

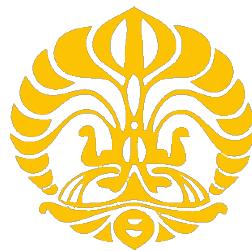
UNIVERSITAS INDONESIA

**SIMULASI WAKTU TUNDA IGNISI
BAHAN BAKAR GASOLIN MULTIKOMPONEN**

SKRIPSI

**JACQUIN SURYADI
0806456625**

**FAKULTAS TEKNIK
PROGRAM STUDI TEKNIK KIMIA
DEPOK
JANUARI 2012**



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SKRIPSI

Diajukan sebagai salah satu syarat untuk memperoleh gelar Sarjana Teknik

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0806456625**

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PROGRAM STUDI TEKNIK KIMIA
DEPOK
JANUARI 2012**

HALAMAN PERNYATAAN ORISINALITAS

Skripsi ini adalah hasil karya saya sendiri, dan semua sumber baik yang dikutip maupun dirujuk telah saya nyatakan dengan benar.

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Telah berhasil dipertahankan di hadapan Dewan Pengaji dan diterima sebagai bagian persyaratan yang diperlukan untuk memperoleh gelar Sarjana Teknik pada Program Studi Teknik Kimia, Fakultas Teknik, Universitas Indonesia

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Tanggal : 17 Januari 2012

KATA PENGANTAR

Puji dan syukur saya panjatkan kepada Tuhan Yang Maha Esa karena atas berkat dan rahmat-Nya, saya dapat menyelesaikan skripsi ini. Penulisan skripsi ini dilakukan sebagai salah satu syarat untuk mencapai gelar Sarjana Teknik Jurusan Teknik Kimia pada Fakultas Teknik Universitas Indonesia. Saya menyadari bahwa, tanpa bantuan dan bimbingan dari berbagai pihak, dari masa perkuliahan sampai pada penyusunan skripsi ini, sangatlah sulit bagi saya untuk menyelesaikan skripsi ini. Oleh karena itu, saya mengucapkan terima kasih kepada:

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Depok, 17 Januari 2012

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(Jacquin Suryadi)

ABSTRAK

Nama : Jacquin Suryadi

Program Studi : Teknik Kimia

Judul : Simulasi Waktu Tunda Ignisi Bahan Bakar Gasolin Multikomponen

Pemodelan kinetika oksidasi dan pembakaran bahan bakar gasolin bertujuan untuk menghasilkan mekanisme reaksi pembakaran yang valid sehingga dapat digunakan untuk memprediksi *ignition delay time*, serta pengaruh temperatur, tekanan dan rasio ekuivalensi pada reaksi oksidasi dan pembakaran bahan bakar tersebut. Penyusunan mekanisme reaksi dilakukan dengan penelusuran literatur. Model yang telah disusun akan divalidasi menggunakan data eksperimen yang diperoleh dengan menggunakan alat *shock tube*, pada rentang temperatur 900-1.150 K, tekanan 25-55 bar, serta rasio ekuivalensi 1. Mekanisme reaksi yang telah divalidasi, kemudian disimulasikan dengan variasi temperatur awal, variasi tekanan awal dan rasio ekuivalensi. Perangkat lunak yang digunakan adalah Chemkin 3.7.1. Mekanisme reaksi yang disusun berhasil memprediksikan data eksperimen dengan kesesuaian yang baik. Dari perbandingan hasil simulasi waktu tunda ignisi dengan data eksperimen, diperoleh nilai deviasi maksimum sebesar 32,36% dan nilai deviasi minimum sebesar 0%.

Kata kunci : waktu tunda ignisi, *shock tube*, gasolin, model kinetika

ABSTRACT

Name : Jacquin Suryadi
Major of Study : Chemical Engineering
Title : Simulation of Ignition Delay Times of Multi-component Gasoline Fuel

The main goals of research on the modeling of kinetic and oxidation of gasoline fuel are to create a valid reaction mechanism that can be used to predict the profile of ignition delay time, and behaviors of its oxidation reaction. Model is arranged by literature study and has to be validated with an experiment data. Experiment data was obtained from shock tube with initial temperature range 900-1.150 K, initial pressure range 25-55 bar, and equivalence ratio 1,0. The valid mechanism will be used for initial temperature, initial pressure and equivalent ratio variation simulation. The software that used in this research is Chemkin 3.7.1. The new reaction mechanism can predict the experiment data successfully. From the comparison of the simulation results of ignition delay time with experimental data, the maximum deviation value is 32,36% and minimum deviation value is 0%.

Keywords: ignition delay time, shock tube, gasoline, kinetic model

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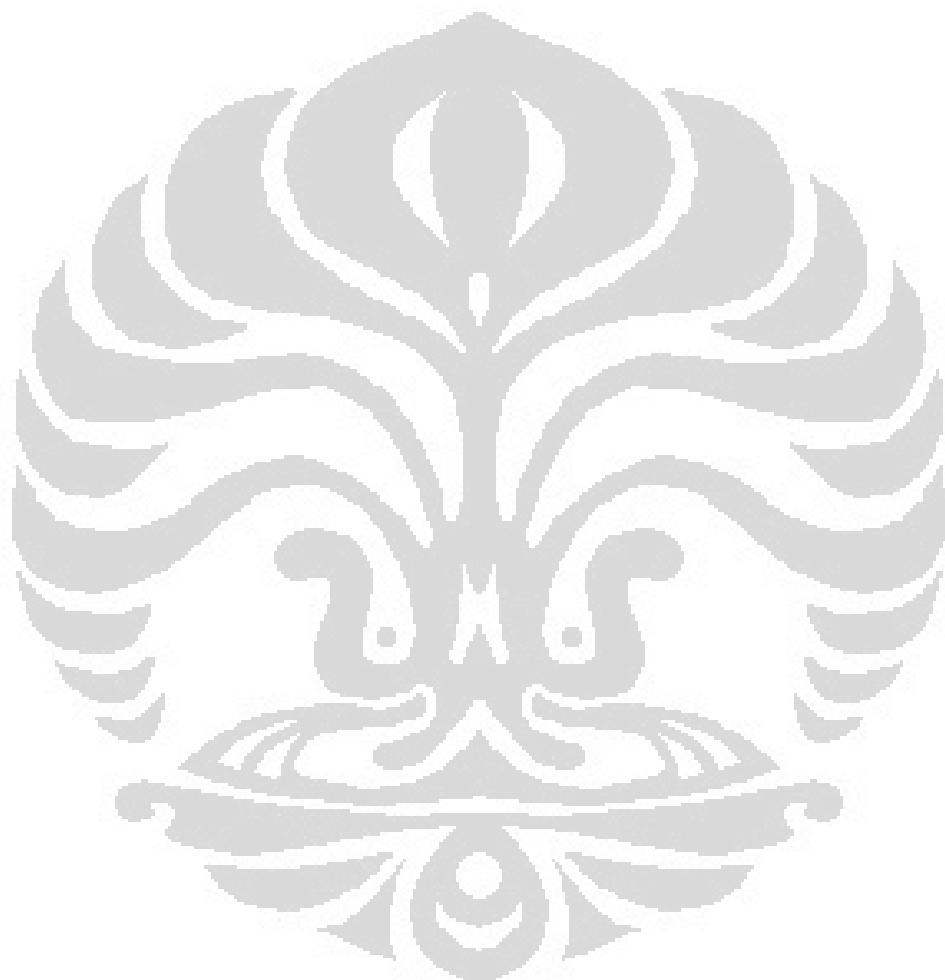
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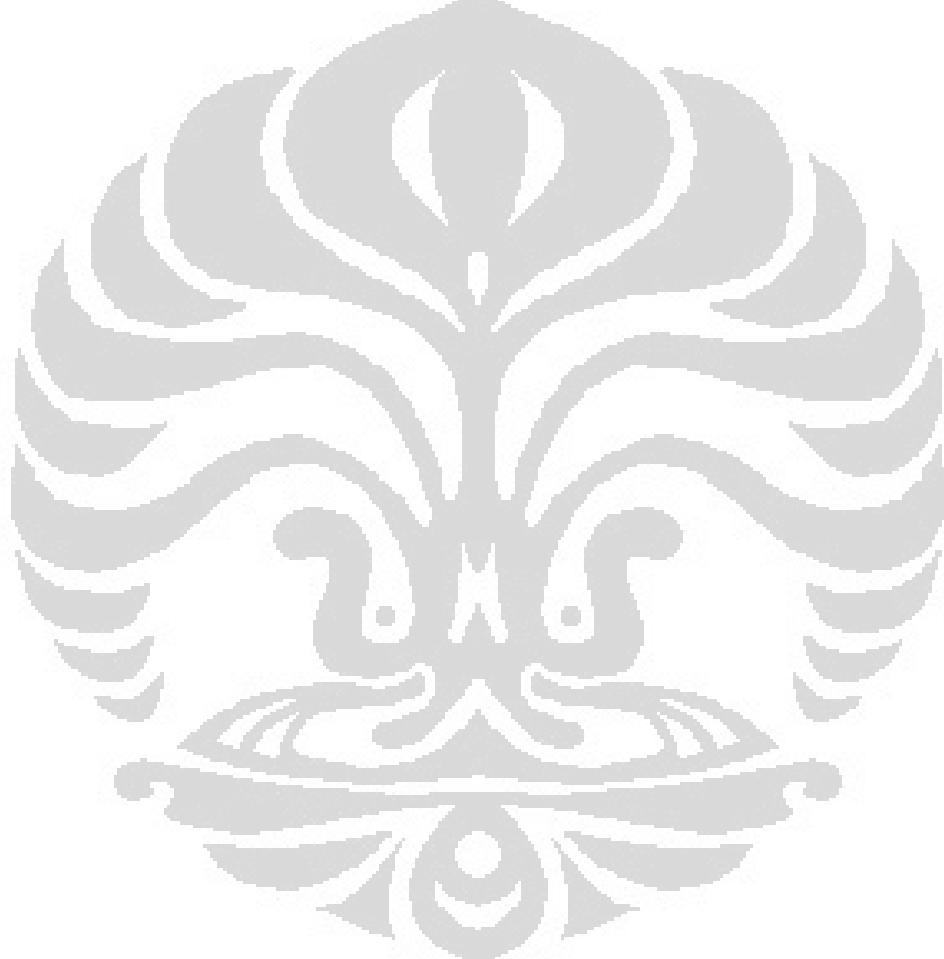


DAFTAR NOTASI

Notasi	Keterangan	Satuan
T	Temperatur	Kelvin
P	Tekanan	Atm
Φ	Rasio ekuivalensi	
k	Koefisien laju reaksi	$\text{cm}^3/\text{mol s}$
E_a	Energi aktivasi	Cal/mol
R	Konstanta gas ideal	Cal/ mol K
A	Faktor pre-eksponensial	cm mol s
b	Eksponen temperatur	
K_p	kesetimbangan tekanan	
p°	Tekanan standar	Atm
K_c	Kesetimbangan konsentrasi	
ΔG°	Energi reaksi standar Gibbs	J/mol
ΔH°	Entalpi standar	J/mol
ΔS°	Entropi reaksi	J/mol K
ΔH_T°	Entalpi standar pada temperatur T	J/mol
ΔS_T°	Entropi reaksi standar pada temperatur T	J/mol K
Cp	Kapasitas panas spesifik	J/mol K
t	Waktu	detik
$v_{rs}^{(c)}$	Koefisien stoikiometri reaktan	
$v_{rs}^{(p)}$	Koefisien stoikiometri produk	
c_i	Konsentrasi dari spesi i	cm^3/mol
k_r	Parameter sistem	$\text{cm}^3/\text{mol s}$
c_i^0	Konsentrasi awal dari spesi i	cm^3/mol
$E_{i,r}$	Sensitivitas absolut	
$E_{i,r}^{rel}$	Sensitivitas relatif	
τ	Waktu tunda ignisi	detik

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BAB 1

PENDAHULUAN

1.1. LATAR BELAKANG MASALAH

Seiring perkembangan zaman, segala sesuatu dituntut untuk lebih cepat dan praktis. Hal ini menjadi salah satu penyebab utama yang mendorong jumlah penjualan kendaraan bermotor kian meningkat dari tahun ke tahun. Jumlah keseluruhan penjualan mobil nasional pada tahun 2010 secara *wholesale* meningkat sebesar 57,13% menjadi 763.751 unit dari penjualan tahun 2009 yang sebesar 486.061 unit [2]. Sedangkan total penjualan sepeda motor mencapai 7,39 juta unit di tahun 2010, meningkat dari penjualan tahun 2009 sebesar 5,88 juta unit [3]. Kuantitas kendaraan bermotor yang bertambah tentu akan menimbulkan berbagai permasalahan transportasi, salah satunya terkait dengan kualitas bahan bakar sebagai sumber energi penggerak transportasi tersebut. Kualitas bahan bakar yang tidak sesuai dengan spesifikasi mesin kendaraan, seperti rasio kompresi, dapat mengakibatkan mesin torak (piston) kendaraan cepat rusak karena terjadi ketukan (*knocking*). Oleh karena itu, bahan bakar kendaraan bermotor menjadi komoditas penting untuk diteliti lebih jauh penggunaannya. Salah satu topik yang menarik perhatian peneliti adalah perilaku dari pembakaran bahan bakar jenis gasolin yang umum digunakan oleh masyarakat luas. Terdapat berbagai cara untuk mempelajari karakteristik pembakaran bahan bakar gasolin, diantaranya melalui pengembangan model kinetika reaksi oksidasi dan pembakaran bahan bakar tersebut.

Untuk mencapainya tujuan yang diinginkan, diperlukan pengetahuan mengenai kimia pembakaran yang ada di dalam proses pembakaran. Kimia pembakaran adalah reaksi kimia yang terjadi di dalam proses pembakaran yang dilengkapi dengan data kinetika yang meliputi faktor pra-eksponensial, faktor eksponensial suhu, serta energi aktivasinya. Setelah mengetahui kimia pembakaran, selanjutnya dapat dibuat suatu model mekanisme pembakaran. Mekanisme pembakaran merupakan sekumpulan reaksi elementer yang terlibat di dalam proses pembakaran. Reaksi pembakaran dapat melibatkan ribuan reaksi elementer. Persamaan-persamaan reaksi elementer itu kemudian diselesaikan

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dengan menggunakan perangkat lunak Chemkin 3.7.1. Perangkat lunak tersebut bekerja dengan mengubah persamaan reaksi elementer yang telah disusun menjadi persamaan diferensial dan diselesaikan secara numeris oleh komputer. Metode ini memiliki beberapa keunggulan yaitu kevalidan atas data eksperimen, murah, dan cepat.

Penelitian Muhamam [4] mengenai model kinetika reaksi oksidasi dari beberapa hidrokarbon rantai panjang menggunakan program MOLEC telah menghasilkan data kinetika dan reaksi elementer dari pembakaran hidrokarbon. Studi Tri [5] tentang model kinetika reaksi oksidasi dan pembakaran bahan bakar gasolin yang mengandung MTBE telah menghasilkan kondisi campuran yang optimum dan model kinetika reaksi yang valid. Pemodelan yang dilakukan Theo [6] untuk mengetahui pengaruh etanol pada kinerja bahan bakar gasolin telah menghasilkan data kinetika laju oksidasi dari etanol dan gasolin, serta model kinetika reaksi yang valid. Pemodelan kinetika campuran iso-oktana dan n-heptana sebagai komponen bahan bakar PRF (*primary reference fuel*) untuk mengetahui waktu tunda ignisi telah berhasil dilakukan oleh Niko [7] dan menghasilkan kesesuaian yang tinggi dengan data eksperimen. Pengembangan model kinetika reaksi oksidasi dan pembakaran bahan bakar gasolin untuk menghasilkan waktu tunda ignisi telah berhasil dibuat Yendha [8]. Namun, model tersebut belum divalidasi dengan menggunakan data eksperimen. Studi oksidasi dan pembakaran dari suatu campuran bahan bakar telah dilakukan oleh Gauthier dkk. [1] pada *shock tube* di tahun 2004. Campuran bahan bakar yang digunakan adalah toluena, n-heptana dan iso-oktana dengan fraksi volume masing-masing sebesar 14%, 17% dan 69%. Percobaan tersebut menghasilkan profil waktu tunda ignisi pada rentang temperatur 900 K - 1.150K, tekanan 25-55 bar dan rasio ekuivalensi 1.

Dengan demikian, penelitian ini dilakukan untuk memvalidasi model kinetika reaksi oksidasi dan pembakaran bahan bakar gasolin dengan menggunakan data eksperimen Gauthier dkk. [1]. Diharapkan setelah divalidasi dengan menggunakan data eksperimen, model kinetika reaksi yang dibuat akan

representatif terhadap kondisi pembakaran dan oksidasi bahan bakar gasolin multikomponen yang sebenarnya.

1.2. RUMUSAN MASALAH

Berdasarkan latar belakang yang telah dikemukakan, maka rumusan masalah yang diajukan dalam penelitian ini adalah sebagai berikut:

- ✚ Bagaimana memperoleh model kinetika reaksi oksidasi dan pembakaran bahan bakar gasolin multikomponen yang valid.
- ✚ Bagaimana menentukan karakteristik pembakaran bahan bakar gasolin multikomponen melalui profil waktu tunda ignisi (*ignition delay time*).

1.3. TUJUAN PENELITIAN

Tujuan dilakukannya penelitian ini adalah

- ✚ Dihasilkan model kinetika reaksi oksidasi dan pembakaran bahan bakar gasolin multikomponen yang valid.
- ✚ Didapatkan profil waktu tunda ignisi dari reaksi oksidasi dan pembakaran bahan bakar gasolin multikomponen pada berbagai variasi tekanan awal dan rasio ekuivalensi.

1.4. BATASAN MASALAH

Batasan dari penelitian yang akan dilakukan adalah sebagai berikut:

- ✚ Bahan bakar gasolin multikomponen direpresentasikan oleh dari 3 komponen yaitu toluena, iso-oktana, dan n-heptana;
- ✚ Reaksi berlangsung dalam fasa gas;
- ✚ Data eksperimen waktu tunda ignisi menggunakan data percobaan yang dilakukan oleh Gauthier dkk. [1] yang diperoleh dari *shock tube*;
- ✚ Model kinetika reaksi oksidasi dan pembakaran yang akan divalidasi menggunakan model yang dikembangkan oleh Yendha [8];

- ✚ Ditambahkan model kinetika reaksi detail n-heptana yang dikembangkan oleh Muharam [4] ke dalam model Yendha [8];
- ✚ Perangkat lunak yang digunakan adalah fasilitas AURORA pada program Chemkin 3.7.1. yang dipakai untuk menunjukkan waktu tunda ignisi;
- ✚ Simulasi dilakukan dengan memvariasikan tekanan awal dan rasio ekuivalensi.

1.5. SISTEMATIKA PENULISAN

Sistematika penulisan dalam makalah ini adalah sebagai berikut :

BAB 1 PENDAHULUAN

Menjelaskan mengenai latar belakang, perumusan masalah, tujuan penelitian, batasan masalah, dan sistematika penulisan.

BAB 2 TINJAUAN PUSTAKA

Menjelaskan studi literatur secara umum dan khusus mengenai topik yang berkaitan dengan penelitian, seperti fenomena pembakaran, bahan bakar gasolin, angka oktan, mesin pembakaran dalam, kinetika kimia, waktu tunda ignisi (*ignition delay time*), peralatan model pembakaran, dan program Chemkin 3.7.1.

BAB 3 METODOLOGI PENELITIAN

Menjelaskan diagram alir penelitian, alat dan bahan penelitian, serta rincian kegiatan penelitian yang akan dilakukan, mencakup tahap pengembangan model kinetika reaksi, validasi dengan data eksperimen, analisis hasil yang diperoleh melalui analisis sensitivitas, serta simulasi model kinetika reaksi yang telah dianalisis dan divalidasi dengan data eksperimen.

BAB 4 VALIDASI

Berisi perbandingan antara data eksperimen terhadap simulasi numeris yang dilakukan dengan program Chemkin 3.7.1. Data eksperimen yang digunakan adalah data eksperimen Gauthier dkk. [1] yang diujikan pada alat *shock tube* di rentang temperatur 900 K - 1.150 K, rentang tekanan 25-55 bar, dan rasio

ekuivalensi 1. Validasi yang dilakukan adalah validasi terhadap waktu tunda ignisi (*ignition delay time*).

BAB 5 ANALISIS SENSITIVITAS

Berisi tentang bagaimana pengaruh dari reaksi elementer yang terlibat di dalam reaksi pembakaran. Semakin besar nilainya, maka semakin besar pengaruh reaksi elementer tersebut terhadap reaksi pembakaran secara keseluruhan. Analisis sensitivitas dilakukan pada temperatur awal rendah (700 K), temperatur awal intermediet (850 K), dan temperatur awal tinggi (1.000 K).

BAB 6 SIMULASI WAKTU TUNDA IGNISI

Menjelaskan mengenai simulasi model kinetika reaksi oksidasi dan pembakaran bahan bakar gasolin berdasarkan profil waktu tunda ignisi yang dihasilkan dari variasi tekanan awal dan rasio ekuivalensi.

BAB 7 KESIMPULAN

Menjelaskan mengenai kesimpulan yang diperoleh dari penelitian ini.

BAB 2

TINJAUAN PUSTAKA

Dalam mencapai tujuan penelitian, perlu dipahami terlebih dahulu konsep fenomena pembakaran secara umum. Studi umum mengenai bahan bakar gasolin multikomponen dan pengaruh angka oktan terhadap kualitasnya juga akan dipelajari. Selain itu, bagaimana cara kerja *internal combustion engine* perlu dijelaskan untuk memberikan gambaran umum mengenai pengaruh waktu tunda ignisi terhadap kondisi ruang pembakaran. Kinetika kimia, mencakup hukum laju reaksi global, reaksi elementer, data termodinamika dan kinetika, mekanisme reaksi oksidasi dan pembakaran, serta ketergantungan koefisien laju reaksi terhadap temperatur dan tekanan juga akan dibahas satu per satu. Waktu tunda ignisi sebagai salah satu topik penting akan dijelaskan definisinya secara singkat. Perangkat peralatan *shock tube* yang dipakai untuk mendapatkan data eksperimen, serta alat yang digunakan dalam penelitian ini, yaitu *software* program Chemkin 3.7.1., akan diangkat untuk memperjelas bagaimana cara perangkat tersebut dapat digunakan untuk menentukan waktu tunda ignisi.

2.1. FENOMENA PEMBAKARAN

Chenn [10] mengatakan bahwa pembakaran dapat didefinisikan sebagai pembakaran bahan bakar dan oksidan untuk menghasilkan panas dan/atau kerja. Pembakaran merupakan reaksi yang bersifat eksotermis dan terjadi melalui sejumlah peristiwa kimia dan fisika, di mana produk reaksi pembakaran yang paling stabil akan membentuk air dan karbon dioksida. Klasifikasi pembakaran dapat dibagi menjadi 4 yakni:

1. Pembakaran Konvensional

Proses pembakaran di mana oksidasi bahan bakar terjadi dengan disertai nyala (*flame*) atau berlangsung pada suhu tinggi.

2. Pembakaran non-Konvensional

Proses pembakaran di mana oksidasi bahan bakar tidak terjadi dengan disertai nyala (*flame*) atau tidak berlangsung pada suhu tinggi.

3. Pembakaran Subsonik (deflagrasi)

Proses pembakaran yang umum terjadi dalam proses pembakaran bahan bakar normal, di mana kecepatan rambat gelombang reaksi pembakaran lebih rendah dari kecepatan suara.

4. Pembakaran Supersonik (detonasi)

Proses pembakaran yang umumnya ingin dihindari terjadi pada pembakaran bahan bakar di mesin torak (piston) kendaraan, di mana kecepatan rambat gelombang reaksi pembakaran lebih tinggi dari kecepatan suara.

Proses pembakaran merupakan interaksi kompleks antara proses fisika (seperti dinamika fluida, perpindahan panas dan massa) dengan proses kimia (seperti termodinamika dan kinetika kimia). Aplikasi praktis dari proses pembakaran melibatkan berbagai bidang ilmu lain, salah satunya yakni teknologi bahan bakar.

2.2. BAHAN BAKAR GASOLIN

Gasolin atau bensin adalah suatu campuran kompleks yang terdiri lebih dari 500 macam hidrokarbon [11]. Gasolin sebagai campuran sejumlah hidrokarbon, kadangkala mengandung etanol yang cukup besar atau sejumlah kecil aditif seperti metil tersier butil eter (MTBE), sebagai zat anti ketukan untuk menambah angka oktan. Rantai hidrokarbon yang biasa digunakan untuk bahan bakar gasolin adalah rantai hidrokarbon C₄ sampai C₁₂ dengan komposisi campurannya terdiri dari alkana 4-8%, alkena 2-5%, isoalkana 25-40%, sikloalkana 3-7%, sikloalkena 1-4%, dan aromatik 20-50% [11].

2.2.1. Produksi dan Analisis Kimia

Gasolin dihasilkan dari kilang minyak. Bahan yang dipisahkan dari minyak mentah melalui proses distilasi disebut sebagai *virgin* atau *straight run gasoline* yang tidak begitu sesuai dengan spesifikasi mesin kendaraan bermotor modern. Aliran-aliran dari pengilangan yang dicampur untuk membuat gasolin memiliki karakteristik-karakteristik tersendiri. Beberapa aliran tersebut antara lain:

 *Reformat*

Dihasilkan dalam reformer berkatalis (*catalytic reformer*) dengan angka oktan dan kandungan aromatik yang tinggi, serta olefin yang sangat rendah.

 *Catalytic Cracked Gasoline*

Dihasilkan dari proses *catalytic cracker*, dengan angka oktan yang tidak terlalu tinggi, kandungan olefin yang tinggi, dan juga kandungan aromatik yang menengah.

 *Hydrocrackate*

Dihasilkan dari sebuah *hydrocracker*, dengan angka oktan menengah sampai rendah dan kandungan aromatik yang menengah.

 *Alkylate*

Dihasilkan dari unit alkilasi dengan angka oktan yang tinggi, di mana biasanya parafin murni yang merupakan rantai bercabang.

 *Isomerate*

Biasanya diperoleh melalui proses isomerasi pentana dan heksana di dalam fraksi naphta ringan yang murni untuk menghasilkan isomer yang berangka oktan lebih tinggi.

Secara keseluruhan, gasolin didominasi oleh campuran parafin (alkana), naphtalen (sikloalkana), dan olefin (alkena). Rasio perbandingan campuran tersebut bergantung pada beberapa hal, antara lain:

-  Unit pengilangan minyak yang menghasilkan gasolin karena tidak semua kilang memiliki pengaturan sama dalam unit prosesnya
-  Minyak mentah yang digunakan sebagai umpan kilang
-  Tingkatan dari gasolin itu sendiri

Kadangkala gasolin mengandung komponen organik, seperti organik eter, ditambah sejumlah kecil pengotor seperti sulfur. Beberapa pengotor seperti thiol dan dihidrogen sulfida harus dibuang karena dapat menyebabkan korosi di dalam mesin kendaraan.

2.2.2. Volatilitas

Gasolin memiliki volatilitas yang lebih tinggi dibandingkan solar maupun kerosin [12]. Tidak hanya disebabkan bahan dasarnya, tetapi juga oleh karena aditif-aditif yang ditambahkan ke dalam gasolin tersebut. Pengendalian akhir dari volatilitas seringkali dilakukan dengan menambahkan butana. Volatilitas gasolin yang diinginkan tergantung pada suhu *ambient*. Pada daerah panas, gasolin akan memiliki berat molekul yang lebih berat. Sebaliknya, di daerah dingin, terlalu sedikit gasolin yang menguap dapat menyebabkan mesin sulit dihidupkan.

2.2.3. Kandungan Energi

Gasolin mengandung kira-kira energi sebesar 34.6 megajoule per liter (MJ/liter) [12]. Besaran ini merupakan rata-rata kandungan energi di dalam gasolin. Disebabkan bervariasinya komposisi campuran dalam gasolin maka energi yang dihasilkan juga akan berbeda-beda. Perbandingan densitas energi volumetrik gasolin dibandingkan beberapa jenis bahan bakar lainnya tercantum pada Tabel 2.1.

Tabel 2.1. Kandungan energi dari beberapa jenis bahan bakar [12]

Jenis Bahan Bakar	MJ/liter	MJ/kg	Research Octane Number (RON)
Regular Gasoline	34.8	44.4	Minimum 91
Autogas (LPG) (60% propane + 40% butane)	26.8	46	108
Ethanol	23.5	31.1	129
Methanol	17.9	19.9	123
Buthanol	29.2	-	91-99
Gasohol (10% ethanol + 90% gasoline)	33.7	-	93/94
Diesel (solar)	38.6	45.4	25 (cetane number)
Jet fuel (kerosene based)	35.1	43.8	-
Hidrogen	25.7	121	130
Aviation Gasoline	33.5	46.8	-

2.3. ANGKA OKTAN

Angka oktan adalah pengukuran ketahanan otoignisi (*autoignition*) dari gasolin atau bahan bakar jenis lainnya yang dipakai untuk mesin pembakaran dalam [13]. Semakin tinggi angka oktan maka akan semakin tinggi energi aktivasi yang dibutuhkan untuk memulai reaksi kimia pembakaran bahan bakar. Dengan demikian, bahan bakar gasolin dengan angka oktan yang lebih tinggi akan lebih sulit terbakar. Semakin besarnya angka oktan juga akan meningkatkan jumlah ikatan karbon-karbon (C-C), yang mengandung energi lebih tinggi dibandingkan ikatan karbon-hidrogen (C-H). Akibatnya, bahan bakar gasolin dengan jumlah ikatan karbon-karbon yang lebih banyak dapat menghasilkan energi yang lebih besar bagi mesin kendaraan.

Di dalam mesin kendaraan, campuran udara dan gasolin (dalam bentuk gas) ditekan oleh mesin torak (piston) sampai dengan volume yang sangat kecil dan kemudian dibakar oleh percikan api yang dihasilkan busi. Karena besarnya tekanan ini, campuran udara dan gasolin juga bisa terbakar secara spontan sebelum percikan api dari busi keluar. Jika campuran gas terbakar karena tekanan yang tinggi (dan bukan karena percikan api dari busi), maka akan terjadi *knocking* atau ketukan di dalam mesin. *Knocking* dapat menyebabkan mesin cepat rusak, sehingga sebisa mungkin harus kita hindari agar mesin awet. Pembakaran secara spontan ini bisa dihindari melalui penyesuaian rasio kompresi mesin dengan jenis bahan bakar gasolin yang digunakan. Faktor yang dijadikan acuan dalam memilih jenis gasolin yang tepat adalah angka oktan, karena ketahanan bahan bakar terhadap ketukan dapat dilihat dari angka oktannya. Dengan demikian kualitas bahan bakar gasolin yang digunakan ditentukan oleh angka oktan yang terkandung di dalamnya.

Umumnya, jenis mesin kendaraan bermotor keluaran tahun 2005 ke atas disertai dengan spesifikasi rasio kompresi mesin yang lebih tinggi. Salah satu tujuan dari meningkatnya rasio kompresi ini adalah untuk meningkatkan tenaga mesin melalui penggunaan bahan bakar gasolin yang berangka oktan lebih tinggi. Besarnya rasio kompresi mesin akan membuat campuran udara dan gasolin lebih mudah terbakar oleh tekanan yang tinggi secara spontan. Hal tersebut dapat

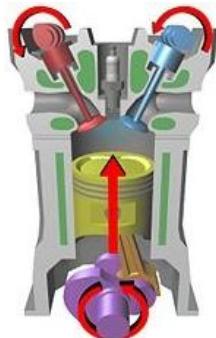
diimbangi dengan bahan bakar gasolin yang berangka oktan tinggi, di mana bahan bakar ini menjadi lebih sulit terbakar secara spontan.

Angka oktan diperkirakan dengan membandingkan karakteristik dari gasolin terhadap iso-oktana (2,2,4-trimetil-pentana) dan n-heptana. Iso-oktana memiliki angka oktan sebesar 100. Hal ini disebabkan karena iso-oktana merupakan komponen dengan rantai bercabang yang terbakar dengan baik. Berbeda dengan n-heptana yang memiliki angka oktan 0, karena merupakan komponen dengan rantai lurus yang sulit terbakar dengan baik. Komponen n-heptana menjadi penyebab ketukan dalam mesin kendaraaan. Bahan bakar gasolin yang keluar dari kilang minyak tanpa pengolahan lebih lanjut memiliki angka oktan sekitar 0. Dengan kata lain, gasolin tersebut memiliki campuran 70% iso-oktana dan 30% n-heptana. Proses *cracking*, isomerisasi, dan proses-proses lainnya dapat dipakai untuk meningkatkan angka oktan dari gasolin.

Ada dua kategori angka oktan, yaitu RON (*Research Octane Number*) dan MON (*Motor Octane Number*). RON diperoleh dari simulasi kinerja bahan bakar saat mesin dioperasikan dalam kondisi standar, sementara MON menunjukkan kinerja bahan bakar saat mesin dioperasikan dalam kondisi lebih berat. Angka oktan MON bisa 10 poin lebih rendah dibandingkan angka oktan RON. Angka oktan yang kita lihat di belakang nama produk gasolin di SPBU-SPBU nasional adalah RON.

2.4. MESIN PEMBAKARAN DALAM

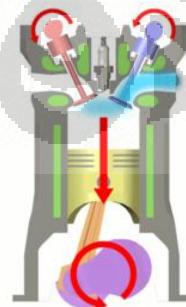
Mesin pembakaran [14] dalam adalah mesin di mana pembakaran bahan bakar dan *oxidizer* (biasanya udara) terjadi dalam ruang tertentu yang disebut ruang bakar (*combustion chamber*). Reaksi yang berlangsung secara eksotermis ini menghasilkan gas dengan tekanan dan temperatur tinggi. Keunggulan dari mesin pembakaran dalam ini adalah kinerja yang dilakukan dengan mengekspansi gas panas secara langsung untuk menggerakkan bagian-bagian padat dari mesin seperti piston atau rotor.



Gambar 2.1. Ilustrasi komponen mesin pembakaran dalam dengan siklus 4 langkah [14]

Mesin pembakaran dalam yang pertama kali diciptakan tidak menggunakan kompresi, melainkan dengan campuran udara dengan bahan bakar yang dihisap atau ditiupkan pada langkah hisap. Perbedaan yang cukup besar antara mesin pembakaran dalam modern dengan mesin pembakaran dalam awal adalah penggunaan kompresi di dalam setiap silindernya. Mesin pembakaran dalam merupakan mesin yang paling sering digunakan sebagai sistem pendorong mobil, motor, lokomotif, dan sebagainya. Mesin ini juga memiliki keunggulan, yaitu karena mesin ini dapat menghasilkan rasio tenaga dan berat yang besar dengan densitas bahan bakar yang tepat. Hampir semua mobil yang digunakan saat ini menggunakan siklus pembakaran 4 langkah untuk mengubah bahan bakar menjadi energi gerak. Siklus 4 langkah juga dikenal sebagai siklus Otto (sebagai penghargaan pada Nikolaus Otto yang menenukannya pada tahun 1867). Siklus 4 langkah dapat divisualisasikan seperti pada Gambar 2.2 sampai Gambar 2.5.

1. Langkah hisap (*Intake*)



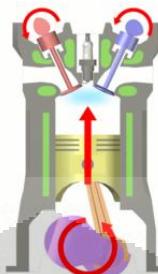
Gambar 2.2. Langkah hisap dalam siklus 4 langkah [15]

Pada siklus ini, bahan bakar yang telah dikabutkan dan bercampur dengan udara akan dihisap masuk ke ruang bakar oleh piston melalui katup masuk (*Inlet*

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Valve). Gerakan piston kearah bawah akan menghasilkan efek vakum yang menyebabkan campuran tersebut terhisap masuk.

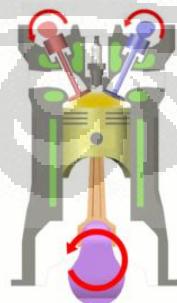
2. Langkah kompresi (*Compression*)



Gambar 2.3. Langkah kompresi dalam siklus 4 langkah [15]

Pada langkah ini, katup masuk dan katup buang akan tertutup. Piston akan bergerak ke atas dan menekan campuran bahan bakar dan udara. Karena ditekan, maka tekanan dan suhu campuran tersebut akan naik secara drastis sebelum dipercik api oleh busi. Di dalam langkah ini, ada peristiwa yang tidak kalah pentingnya selain penekanan campuran udara dan bahan bakar. Peristiwa itu adalah peristiwa otoignisi (*autoignition*). Peristiwa otoignisi terjadi karena bahan bakar yang ditekan piston, terbakar terlebih dahulu sebelum dipercik oleh busi. Pencegahannya adalah dengan menggunakan bahan bakar yang memiliki angka oktan tertentu yang akan dibahas pada sesi angka oktan.

3. Langkah pembakaran (*Combustion*)

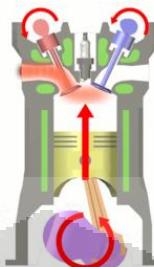


Gambar 2.4. Langkah pembakaran dalam siklus 4 langkah [15]

Saat piston mencapai puncak dari pergerakannya, maka campuran bahan bakar dan udara akan dipercik api oleh busi. Bahan bakar yang terbakar tersebut akan terekspansi dengan suhu dan tekanan tinggi. Gas dengan suhu dan tekanan

yang tinggi tersebut akan mendorong piston turun sekaligus menghasilkan tenaga gerak. Siklus akan memasuki langkah terakhir.

4. Langkah buang (*Exhaust*)



Gambar 2.5. Langkah buang dalam siklus 4 langkah [15]

Pada langkah ini, setelah bahan bakar yang terbakar mendorong piston sampai posisi terendah, maka piston akan naik mendorong gas-gas hasil pembakaran keluar dari ruang bakar melalui katup buang (*exhaust valve*) dan siklus 4 langkah pun selesai.

2.5. KINETIKA KIMIA

Reaksi kimia terjadi ketika molekul dari suatu senyawa bertumbukan dengan senyawa lain yang akan menghasilkan molekul baru. Dalam reaksi kimia atom-atom dari molekul yang bereaksi terdistribusi kembali dalam molekul yang baru. Untuk tercapainya hal ini, molekul yang bereaksi harus memiliki energi kinetik yang cukup sehingga ikatan kimianya dapat terputus dan ikatan baru yang lain terbentuk. Energi ikatan ini tergantung pada sifat alami atom dan faktor geometri, kandungan energi produk tumbuhan mungkin akan berbeda dari kandungan energi molekul yang bertumbukan. Hal ini merupakan dasar dari panas yang dilepaskan atau yang diserap dalam reaksi kimia [16].

2.5.1. Hukum Laju Reaksi Global

Semua reaksi kimia terjadi pada laju tertentu yang bergantung pada kondisi sistem. Kondisi sistem ini seperti konsentrasi reaktan, suhu, dan keberadaan suatu katalis atau inhibitor. Laju reaksi dapat dinyatakan sebagai laju

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berkurangnya konsentrasi reaktan atau laju bertambahnya produk hasil reaksi. Suatu reaksi global, seperti dibawah ini [16]:



dengan A, B, C menunjukkan senyawa yang terlibat dalam reaksi. Laju reaksi yang dilihat dari konsumsi senyawa A dapat dituliskan sebagai berikut:

$$\frac{d[A]}{dt} = -k[A]^a[B]^b[C]^c \quad (2.2)$$

[A], [B], [C], adalah konsentrasi senyawa A, B, C, dengan a, b dan c merupakan orde reaksi serta k merupakan koefisien laju reaksi yang spesifik untuk reaksi global dan bukan fungsi dari konsentrasi reaktan.

Dalam suatu sistem reaksi yang tidak terjadi perubahan konsentrasi suatu senyawa sepanjang reaksi, misalnya konsentrasi B dan C tidak berubah maka akan dihasilkan konstanta laju efektif yang dapat dilihat pada persamaan berikut:

$$k_{\text{eff}} = k[B]^b[C]^c \dots \quad (2.3)$$

sehingga laju reaksinya menjadi:

$$\frac{d[A]}{dt} = -k_{\text{eff}}[A]^a \quad (2.4)$$

Perubahan konsentrasi senyawa A dapat dihitung dengan mengintegralkan persamaan diferensial di atas. Untuk reaksi orde pertama ($a = 1$), maka hasil integrasinya adalah

$$\ln \frac{[A]_t}{[A]_0} = -k_{\text{eff}}(t - t_0) \quad (2.5)$$

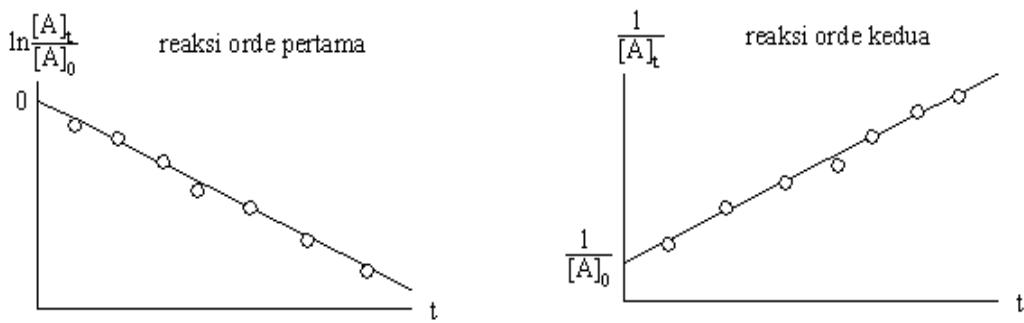
Kemudian, untuk reaksi orde kedua ($a = 2$), hasil integrasinya adalah:

$$\frac{1}{[A]_t} - \frac{1}{[A]_0} = k_{\text{eff}}(t - t_0) \quad (2.6)$$

dan untuk reaksi orde ketiga ($a = 3$), hasil integrasinya adalah:

$$\frac{1}{[A]_t^2} - \frac{1}{[A]_0^2} = 2k_{\text{eff}}(t - t_0) \quad (2.7)$$

dengan $[A]_0$ dan $[A]_t$ menyatakan konsentrasi senyawa A pada waktu t_0 and t . Grafik konsentrasi terhadap waktu pada reaksi orde pertama dan orde kedua ditunjukkan oleh Gambar 2.6.



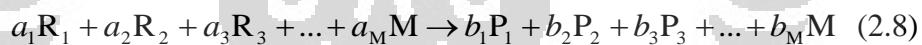
Gambar 2.6. Perubahan konsentrasi terhadap waktu pada reaksi orde 1 dan 2 [16]

2.5.2. Reaksi Elementer

Reaksi elementer terjadi pada tingkat molekular seperti yang dijelaskan pada persamaan reaksi kimia.

2.5.2.1. Hukum Aksi Massa

Hukum aksi massa menyatakan bahwa menghilangnya suatu senyawa kimia sebanding dengan perkalian konsentrasi senyawa kimia yang bereaksi, di mana setiap konsentrasi yang dipangkatkan dengan koefisien stoikiometri. Hal ini hanya berlaku untuk reaksi elementer. Suatu reaksi elementer umum dapat dituliskan berikut ini [16]:



dengan R adalah reaktan, P adalah produk dan M adalah suatu senyawa yang muncul di kedua sisi. Laju konsumsi reaktan dan pembentukan produk dapat dituliskan pada persamaan berikut:

$$\begin{aligned} \frac{d[R_1]}{dt} &= -a_1 r, & \frac{d[R_2]}{dt} &= -a_2 r, & \frac{d[R_3]}{dt} &= -a_3 r, \dots \\ \frac{d[P_1]}{dt} &= b_1 r, & \frac{d[P_2]}{dt} &= b_2 r, & \frac{d[P_3]}{dt} &= b_3 r, \dots \\ \frac{d[M]}{dt} &= b_M r - a_M r \end{aligned} \quad (2.9)$$

dengan r merupakan laju reaksi:

$$r = k[R_1]^{a_1}[R_2]^{a_2}[R_3]^{a_3} \quad (2.10)$$

Persamaan (2.8) menunjukkan reaksi stoikiometri: setiap a_1 mol R_1 bereaksi dengan a_2 mol R_2 , a_3 mol R_3 dan seterusnya, untuk menghasilkan b_1 mol P_1 , b_2 mol P_2 , b_3 mol P_3 dan seterusnya. Jadi banyaknya R_1 yang bereaksi berhubungan dengan banyaknya R_2 , R_3 , dan seterusnya yang telah bereaksi. Jika $b_M = a_M$, M disebut sebagai *third body*. Senyawa ini mungkin tidak berubah tetapi kehadirannya cukup penting untuk keberhasilan suatu reaksi, yaitu untuk menyediakan energi atau mengambil energi dari tumbukan antara reaktan.

2.5.2.2. Tipe Reaksi Elementer

Reaksi elementer dapat diklasifikasikan berdasarkan banyaknya molekul reaktan yang terlibat. Orde keseluruhan ataupun jumlah molekul yang terlibat dalam reaksi disebut juga molekularitas. Berdasarkan molekularitas tipe reaksi elementer adalah sebagai berikut [16]:

2.5.2.2.1. Reaksi unimolekular

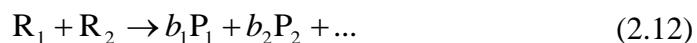
Reaksi di bawah merupakan gambaran ideal, karena molekul tidak mengalami disintegrasi secara spontan.



Maka agar dapat terjadi reaksi, diperlukan adanya tumbukan dengan molekul lain (dengan membuat reaksi secara efektif menjadi orde 2). Laju reaksi orde 1, $r = -k [R_1]$ dan k merupakan koefisien laju reaksi dengan satuan (1/s).

2.5.2.2.2. Reaksi bimolekular

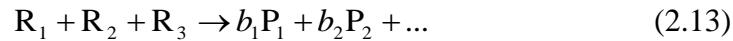
Reaksi di bawah adalah reaksi yang paling umum yang terjadi dalam pembakaran karena sangat besar kemungkinan terjadinya tumbukan antara dua molekul yang ada.



Laju reaksi orde kedua, $r = -k [R_1] [R_2]$, dan k merupakan koefisien laju reaksi dengan satuan $(\text{mol}/\text{cm}^3)^{-1}\text{s}^{-1}$.

2.5.2.2.3. Reaksi trimolekular

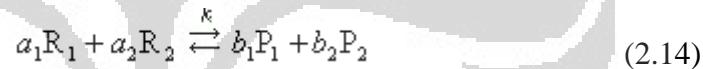
Kemungkinan terjadinya tumbukan tiga molekul secara simultan cukup kecil.



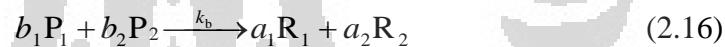
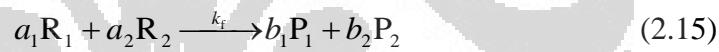
Akan tetapi reaksi orde ketiga merupakan reaksi yang sangat penting. Sebagai contoh, reaksi rekombinasi radikal antara radikal OH dan H untuk membentuk air akan terjadi jika terdapat suatu *third body*, M, yang terlibat dalam tumbukan, dan dengan demikian reaksi ini merupakan reaksi orde ketiga. *Third body* dibutuhkan karena reaksi rekombinasi ini bersifat eksotermik dan *third body* harus menyerap sebagian energinya. Laju reaksi orde ketiga, $r = -k [R_1] [R_2] [R_3]$, dan k merupakan koefisien laju reaksi dengan satuan $(\text{mol/cm}^3)^{-2}\text{s}^{-1}$.

2.5.2.3. Reaksi ke Kanan dan ke Kiri

Reaksi elementer dapat berlangsung dalam dua arah yaitu ke kanan dan ke kiri. Dengan demikian, produk dapat menjadi reaktan dan sebaliknya. Umumnya, laju reaksi spesifiknya sangat berbeda. Sebagai contoh, suatu reaksi:



hal ini berarti bahwa reaksi di atas ekivalen dengan mekanisme berikut:



sehingga laju reaksinya adalah:

$$\frac{d[R_1]}{dt} = -a_1 k_f [R_1]^{a_1} [R_2]^{a_2} + a_1 k_b [P_1]^{b_1} [P_2]^{b_2} \quad (2.17)$$

2.5.3. Ketergantungan Koefisien Laju Reaksi Terhadap Temperatur

Berdasarkan hukum Arrhenius, untuk mendapatkan koefisien laju reaksi dapat digunakan persamaan sebagai berikut [16]:

$$k = A \exp' \left[-\frac{E_a}{RT} \right] \quad (2.18)$$

dengan E_a adalah energi aktivasi. Nilai E_a berasal dari hasil eksperimen atau dari perhitungan mekanika statistik. Tidak semua tumbukan molekular akan menghasilkan suatu reaksi, tetapi hanya yang memiliki energi kinetik yang lebih

tinggi daripada energi yang dibutuhkan untuk memutuskan ikatan dari molekul reaktan. Energi penghalang ini disebut energi aktivasi. Nilai maksimumnya menunjukkan energi ikatan dalam suatu molekul. Pada reaksi disosiasi, energi aktivasi hampir mendekati energi ikatan yang akan diputuskan. Nilai energi aktivasi mungkin dapat lebih kecil atau bahkan nol. Karena reaksi biner elementer menunjukkan kesesuaian dengan hukum Arrhenius pada rentang temperatur sedang, ketergantungan temperatur biasanya digabungkan dengan eksponen tersendiri. Akan tetapi untuk rentang temperatur yang luas yang ditemukan dalam pembakaran, perilaku “non-Arrhenius” pada koefisien laju cenderung terjadi, terutama untuk proses yang memiliki energi *barrier* yang kecil. Oleh karena itu, penggunaan persamaan Arrhenius yang dimodifikasi yang menunjukkan pengaruh temperatur terhadap koefisien laju sangat penting [17].

$$k = AT^n \exp\left[-\frac{E_a}{RT}\right] \quad (2.19)$$

2.5.4 Ketergantungan Koefisien Laju Reaksi Terhadap Tekanan

Ketergantungan koefisien laju reaksi disosiasi (unimolekular) dan rekombinasi (bimolekular) pada tekanan merupakan suatu indikasi bahwa reaksi-reaksi ini tidak elementer. Reaksi-reaksi tersebut merupakan suatu rangkaian dari reaksi-reaksi. Pada kasus yang paling sederhana, ketergantungan pada tekanan dapat dimengerti menggunakan model Lindemann. Mengacu pada model ini, suatu reaksi dekomposisi unimolekular hanya mungkin terjadi jika energi pada molekul cukup untuk memutuskan ikatan. Oleh karenanya, agar reaksi dekomposisi dapat terjadi, energi harus ditambahkan kepada molekul melalui tumbukan dengan molekul lainnya, M (untuk eksitasi dari vibrasi molekular). Molekul tereksitasi kemudian terdekomposisi menjadi produk bergantung pada kekuatan eksitasi, atau terdeaktivasi melalui tumbukan kedua [16].



di mana A^* adalah molekul tereksitasi, k_a , k_{-a} dan k_u adalah koefisien laju aktivasi, deaktivasi dan reaksi unimolekular. Laju rangkaian-rangkaian dari reaksi ini adalah:

$$\frac{d[P]}{dt} = k_u [A^*] \quad (2.23)$$

dan

$$\frac{d[A^*]}{dt} = k_a [A][M] - k_{-a} [A^*][M] - k_u [A^*] \quad (2.24)$$

Dengan mengasumsikan bahwa konsentrasi dari intermediet reaktif A^* berada pada *quasi-steady state*.

$$\frac{d[A^*]}{dt} \approx 0 \quad (2.25)$$

dapat diperoleh [16]

$$[A^*] = \frac{k_a [A][M]}{k_{-a} [M] + k_u} \quad (2.26)$$

dan [16]

$$\frac{d[P]}{dt} = \frac{k_u k_a [A][M]}{k_{-a} [M] + k_u} \quad (2.27)$$

Dua kondisi ekstrim dari reaksi, pada tekanan sangat rendah dan sangat tinggi, dapat dibedakan dari Persamaan (2.27). Pada rentang tekanan yang rendah, konsentrasi rekan tumbukan M sangat kecil dan $k_{-a} [M] \ll k_u$. Oleh karenanya, laju orde kedua dapat diperoleh:

$$\frac{d[P]}{dt} = k_a [A][M] \quad (2.28)$$

Laju reaksi sekarang sebanding dengan konsentrasi senyawa A dan rekan tumbukan M , karena aktivasinya lambat (pembatas laju) pada tekanan rendah.

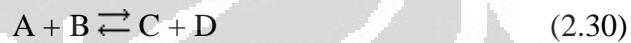
Pada rentang tekanan yang tinggi, konsentrasi rekan tumbukan M besar dan $k_{-a} [M] >> k_u$. Hal ini memberikan laju orde pertama:

$$\frac{d[P]}{dt} = \frac{k_u k_a}{k_{-a}} [A] = k_\infty [A] \quad (2.29)$$

Di sini laju reaksi tidak bergantung pada konsentrasi rekan tumbukan, karena pada tekanan tinggi tumbukan sering terjadi dan dekomposisi molekul teraktivasi A* merupakan pembatas laju, bukan aktivasi. Mekanisme Lindemann mengilustrasikan fakta bahwa orde reaksi dari reaksi kompleks (bukan elementer) bergantung pada kondisi yang dipilih. Meskipun demikian, mekanisme Lindemann sendiri merupakan model yang disederhanakan.

2.5.5. Termodinamika dan Kinetika

Pada reaksi yang memiliki arah ke kanan dan ke kiri, kesetimbangannya bersifat dinamis. Laju kedua arah adalah sama sehingga kesetimbangan konsentrasi dipertahankan. Untuk reaksi berikut [16]:



hubungan ini muncul pada kesetimbangan:

$$\frac{r_f}{r_b} = \frac{k_f [A]_{eq} [B]_{eq}}{k_b [C]_{eq} [D]_{eq}} = 1 \quad (2.31)$$

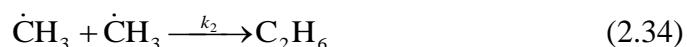
di mana r_f dan r_b adalah laju reaksi ke kanan dan ke kiri dan subskrip eq mengacu ke kesetimbangan. Oleh karenanya:

$$\frac{k_f}{k_b} = \frac{[C]_{eq} [D]_{eq}}{[A]_{eq} [B]_{eq}} \quad (2.32)$$

$$\frac{k_f}{k_b} = K_{11} \quad (2.33)$$

di mana K_{11} adalah konstanta kesetimbangan.

Suatu laju reaksi terkadang lebih mudah diukur pada satu arah daripada arah lainnya. Contoh, rekombinasi radikal metil untuk membentuk etana:



Reaksi dekomposisi ke kiri penting pada proses suhu tinggi, seperti pembakaran, dan kita harus menaruh perhatian terhadap nilai k_{-2} . Laju dekomposisi telah dihitung, namun sulit membuat pengukuran untuk rentang suhu yang luas. Koefisien laju adalah konstan (pada P dan T tertentu) dan tidak berubah selama kesetimbangan dicapai. Oleh karenanya, sangat mungkin untuk

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menggunakan nilai terukur k_2 dan konstanta kesetimbangan K_2 untuk menghitung nilai koefisien laju disosiasi k_{-2} .

$$k_{-2} = \frac{k_2}{K_2} \quad (2.35)$$

Pada umumnya, koefisien laju memiliki unit konsentrasi sehingga K_2 di Persamaan (2.14) adalah K_c . Konstanta K_c ini dapat dikonversi ke K_p (konstanta kesetimbangan yang dinyatakan dalam bentuk kesetimbangan tekanan) melalui:

$$K_c = \frac{K_p}{p^0 RT} \quad (2.36)$$

di mana p^0 adalah tekanan standar, dan Persamaan (2.14) menjadi:

$$k_{-2} = \frac{k_2}{\left(\frac{K_p}{p^0 RT} \right)} \quad (2.37)$$

Dengan menggunakan hubungan antara K_p / p^0 dan perubahan pada energi reaksi standar Gibbs, ΔG^0 :

$$\Delta G^0 = -RT \ln \frac{K_p}{p^0} \quad (2.38)$$

dan hubungan antara ΔG^0 dan perubahan pada entalpi standar dan entropi reaksi, ΔH^0 dan ΔS^0 :

$$\Delta G^0 = \Delta H^0 - T\Delta S^0 \quad (2.39)$$

persamaan berikut dapat diperoleh:

$$k_{-2} = k_2 RT \exp\left(\frac{\Delta H_T^0}{RT}\right) \exp\left(-\frac{\Delta S_T^0}{R}\right) \quad (2.40)$$

di mana ΔH_T^0 & ΔS_T^0 adalah entalpi standar dan entropi standar reaksi pada suhu T:

$$\Delta H_T^0 = \Delta H_{fT}^0(C_2H_6) - 2\Delta H_{fT}^0(CH_3) \quad (2.41)$$

$$\Delta S_T^0 = S_T^0(C_2H_6) - 2S_T^0(CH_3) \quad (2.42)$$

di mana ΔH_{fT}^0 dan S_T^0 adalah entalpi molar standar pembentukan dan hukum ketiga entropi molar untuk spesi tertentu pada suhu T.

2.5.6. Mekanisme Reaksi

Jika banyak terdapat reaksi elementer, jumlah bersih dari reaktan yang dikonsumsi atau produk yang dihasilkan akan muncul dari penambahan kontribusi dari tiap reaksi elementer. Pada umumnya, spesi akan mengambil bagian pada beberapa reaksi sebagai reaktan dan di lainnya sebagai produk. Laju produksi dan konsumsi merupakan hasil bersih dari seluruh reaksi elementer. Untuk suatu mekanisme yang terdiri dari R reaksi elementer, yang tersusun dari S spesi, yang diberikan oleh [16]:



di mana $r = 1, 2, \dots, R$, $v_{rs}^{(e)}$ dan $v_{rs}^{(p)}$ menunjukkan koefisien stoikiometri reaktan dan produk, laju pembentukan suatu spesi i diperoleh dari penambahan seluruh persamaan laju di mana spesi i terlibat,

$$\left(\frac{\partial C_i}{\partial t} \right)_{\text{chem}} = \sum_{r=1}^R k_r (v_{ri}^{(p)} - v_{ri}^{(e)}) \prod_{s=1}^S C_s^{v_{rs}^{(e)}} \quad (2.44)$$

di mana $i = 1, 2, \dots, S$. Notasi C_s menunjukkan konsentrasi dari berbagai spesies s sejumlah S yang terlibat dalam keseluruhan reaksi elementer.

2.5.6.1. Reaksi Rantai

Pembakaran hidrokarbon muncul melalui reaksi rantai, yaitu proses yang menghasilkan produk yang menginisiasi proses selanjutnya dengan jenis yang sama, yang disebut rangkaian yang mampu bertahan sendiri. Reaksi-reaksi di bawah adalah contoh reaksi-reaksi rantai [16]:



Reaksi (2.45) adalah reaksi inisiasi rantai, di mana suatu intermediet reaktif dibentuk dengan bantuan suatu agen seperti panas atau oksigen molekular. Reaksi (2.46) adalah suatu reaksi pencabangan rantai yang menghasilkan lebih banyak radikal. Reaksi (2.47) adalah reaksi perambatan rantai, di mana radikal dapat berubah identitas, namun jumlahnya tidak berubah. Reaksi (2.48) adalah reaksi terminasi rantai, di mana radikal dikonsumsi dan rantai terputus. Reaksi rantai adalah hal yang sangat penting untuk pembakaran. Nyala tidak akan dapat bertahan sendiri jika kimianya tidak memiliki sifat ini. Dengan reaksi rantai, laju reaksi dapat bertambah secara eksponensial dan menyebabkan ledakan. Pada nyala normal, hal ini tidak terjadi karena panas dipindahkan dari daerah reaksi oleh difusi atau konveksi, dan karena konsumsi bahan bakar.

2.5.6.2. Analisis Mekanisme Reaksi

Mekanisme reaksi detail untuk pembakaran hidrokarbon dapat terdiri dari beberapa ribu reaksi elementer. Namun, banyak dari reaksi-reaksi ini tidak penting dan dapat diabaikan. Oleh karenanya, dibutuhkan metode analisis untuk menghilangkan reaksi-reaksi yang dapat diabaikan. Beberapa metode dapat digunakan. Analisis sensitivitas mengidentifikasi langkah reaksi pembatas laju (*rate-limiting reaction step*). Analisis aliran reaksi menentukan karakteristik jalur reaksi. Informasi yang diperoleh dari metode-metode ini dapat digunakan untuk menghilangkan reaksi-reaksi yang tidak penting dan menghasilkan mekanisme reaksi yang tersederhanakan atau tereduksi [16].

2.5.6.2.1. Analisis sensitivitas

Hukum laju dari suatu mekanisme reaksi yang terdiri dari R reaksi diantara S spesi dapat ditulis sebagai suatu sistem persamaan diferensial biasa orde pertama [16]:

$$\frac{dc_i}{dt} = F_i(c_1, \dots, c_S; k_1, \dots, k_R), \quad i=1,2, \dots, S \quad (2.49)$$

$$c_i = c_i^0 \text{ pada } t = t_0$$

Waktu t adalah variabel independen, konsentrasi c_i dari spesi i adalah variabel dependen, dan k_r , parameter sistem; c_i^0 menyatakan kondisi awal.

Hanya koefisien laju dari reaksi kimia yang dipertimbangkan sebagai parameter sistem. Konsentrasi awal, tekanan, dsb dapat menjadi parameter sistem jika diinginkan. Solusi dari sistem persamaan diferensial (2.49) bergantung pada kondisi awal dan juga parameter. Untuk sebagian besar reaksi elementer, perubahan parameter sistem (koefisien laju) hampir tidak memiliki pengaruh pada solusi yang bergantung pada waktu. Bahkan jika reaksinya termasuk secara eksplisit pada mekanisme, itu tidak memerlukan koefisien laju yang sangat akurat. Di sisi lain, untuk sebagian kecil dari reaksi elementer, perubahan koefisien laju memiliki pengaruh yang besar pada keluaran sistem. Akibatnya, koefisien laju yang akurat diperlukan. Beberapa langkah reaksi penting ini adalah penentu laju (*rate-determining steps*) atau pembatas laju (*rate-limiting steps*). Ketergantungan solusi c_i pada parameter k_r disebut dengan sensitivitas. Sensitivitas absolut ($E_{i,r}$) dan sensitivitas relatif ($E_{i,r}^{\text{rel}}$) dapat didefinisikan sebagai:

$$E_{i,r} = \frac{\partial c_i}{\partial k_r} \text{ dan} \quad (2.50)$$

$$E_{i,r}^{\text{rel}} = \frac{k_r}{c_i} \frac{\partial c_i}{\partial k_r} = \frac{\partial \ln c_i}{\partial \ln k_r} \quad (2.51)$$

2.5.6.2.2. Analisis aliran reaksi

Analisis aliran reaksi menghitung persentase kontribusi dari reaksi-reaksi yang berbeda terhadap pembentukan atau konsumsi spesi kimia. Contoh analisis aliran reaksi diberikan di Tabel 2.2.

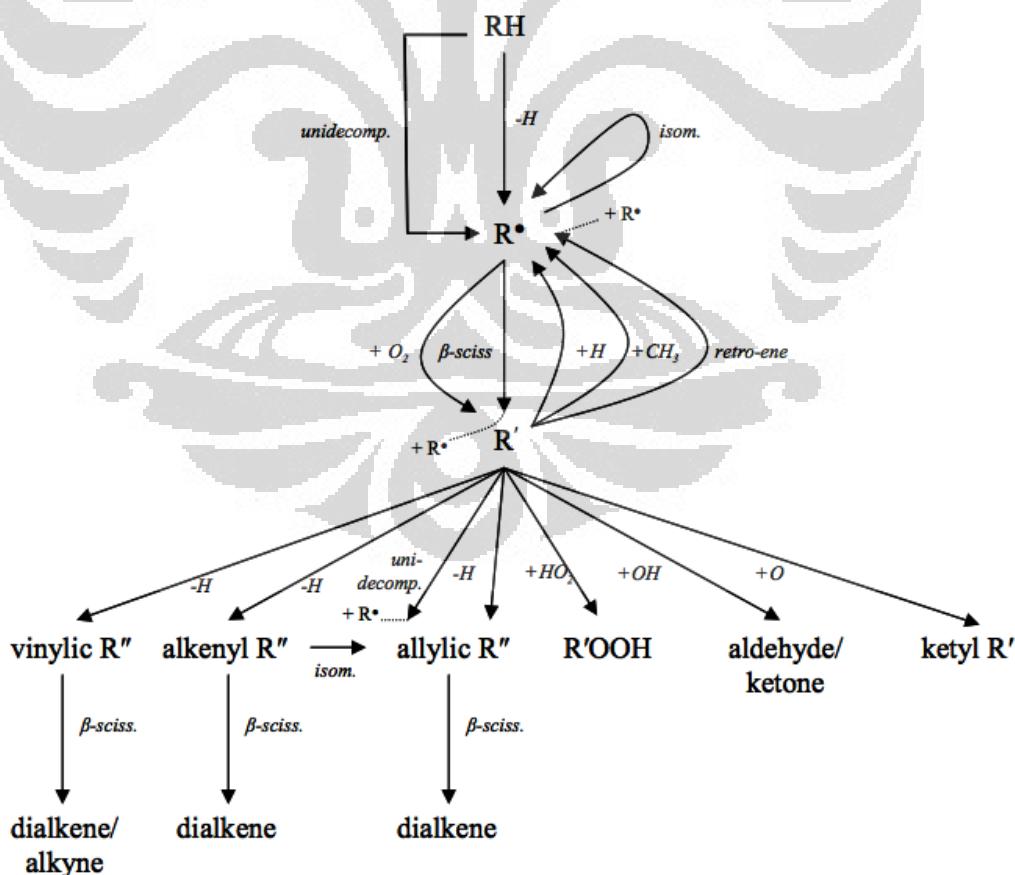
Tabel 2.2. Bagan Ilustrasi Output Dari Suatu Analisis Aliran Reaksi [16]

Reaksi	Spesi					
	1	2	3	...	S - 1	S
1	20%	3%	0	...	0	0
2	0	0	0	...	0	0
3	2%	5%	0	...	100%	90%
.
R - 1	78%	90%	100%	...	0	5%
R	0	2%	0	...	0	0

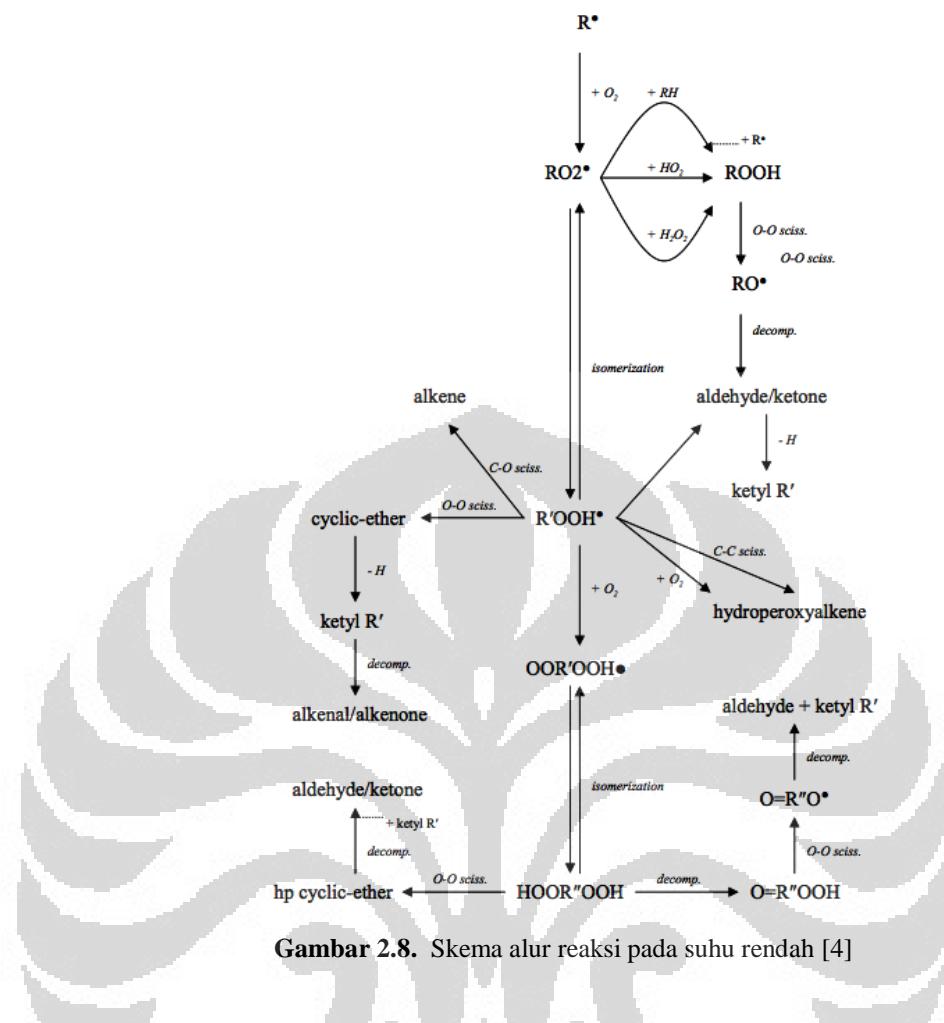
Pada Tabel 2.2., 20% pembentukan spesi 1 berasal dari Reaksi 1, 2% dari Reaksi 3 dan 78% dari Reaksi R-1. Persentase total dari seluruh kontribusi harus 100%. Contoh seperti di atas memperbolehkan konstruksi diagram aliran reaksi yang instruktif.

2.5.6.3. Mekanisme Reaksi Oksidasi dan Pembakaran

Walaupun mekanisme kimia yang detail dari suatu reaksi pembakaran mungkin menyangkut ratusan spesies yang melalui ribuan reaksi elementer, tapi hanya yang memiliki perbedaan tipe reaksi yang ditampilkan. Berdasarkan pengamatan, adalah mungkin untuk merumuskan semua kemungkinan reaksi yang berlangsung dalam oksidasi dan pembakaran hidrokarbon rantai panjang selama koefisien laju reaksi yang digunakan berasal dari aturan yang sederhana. Masing-Masing aturan memberikan tipe reaksi tertentu. Apabila tidak tersedia data pada suatu tipe reaksi tertentu, maka dapat digunakan koefisien laju reaksi yang sama untuk reaksi yang mirip dalam molekul yang berbeda.



Gambar 2.7. Skema alir reaksi pada suhu tinggi [4]



Gambar 2.8. Skema alur reaksi pada suhu rendah [4]

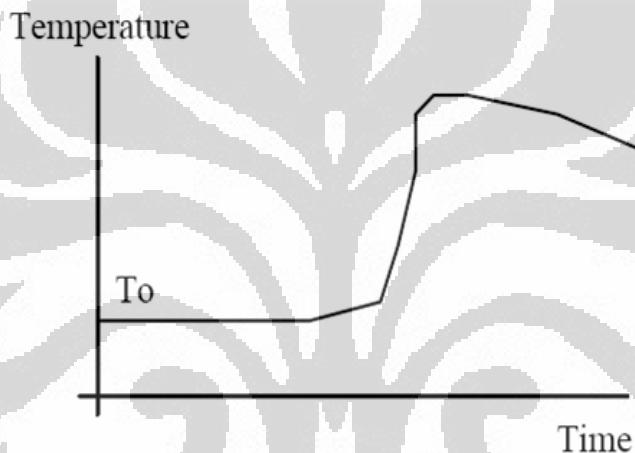
Gambar 2.7. menunjukkan bahwa rangkaian reaksi pada suhu tinggi yang berjumlah ratusan dapat disederhanakan dan dikelompok menjadi tahap-tahap yang sederhana. Sedangkan Gambar 2.8. menunjukkan mekanisme reaksi suhu rendah di mana seperti pada suhu tinggi, mekanisme reaksi oksidasi dan pembakaran dapat disederhanakan dan dikelompokan sehingga mekanisme dari reaksi ini dapat diterapkan dalam program.

2.6. WAKTU TUNDA IGNISI (IGNITION DELAY TIME)

Ignition delay merupakan karakteristik eksplosi rantai-radikal (reaksi kimia yang ditentukan oleh mekanisme percabangan rantai). Selama periode *ignition delay*, populasi kolam radikal meningkat secara eksponensial. Meskipun demikian, jumlah bahan bakar yang terkonsumsi dan bahkan jumlah energi yang dibebaskan masih sangat kecil untuk dideteksi. Oleh karena itu, reaksi kimia

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penting (percabangan rantai, pembentukan radikal) terjadi selama waktu induksi di mana suhu mendekati nilai konstan. Akhirnya, populasi kolam radikal menjadi cukup banyak untuk mengkonsumsi fraksi bahan bakar dengan jumlah yang cukup signifikan dan ignisi cepat dapat terjadi. Definisi yang tepat untuk waktu induksi tergantung pada kriteria yang digunakan, yaitu konsumsi bahan bakar, pembentukan CO, pembentukan OH, peningkatan tekanan dalam suatu bejana bervolume konstan, dan peningkatan suhu dalam suatu bejana adiabatik. Karena reaksi elementer dipengaruhi oleh suhu, maka *ignition delay time* sangat bergantung pada suhu. Sketsa hubungan antara *ignition delay time* dengan suhu dapat dilihat pada Gambar 2.9.



Gambar 2.9. Hubungan waktu tunda ignisi dengan suhu [16]

Warnatz *et al.* [16] menyusun korelasi yang menyatakan bahwa *ignition delay time* tergantung pada suhu secara eksponensial.

$$\tau = A \exp(B/T) \quad (2.52)$$

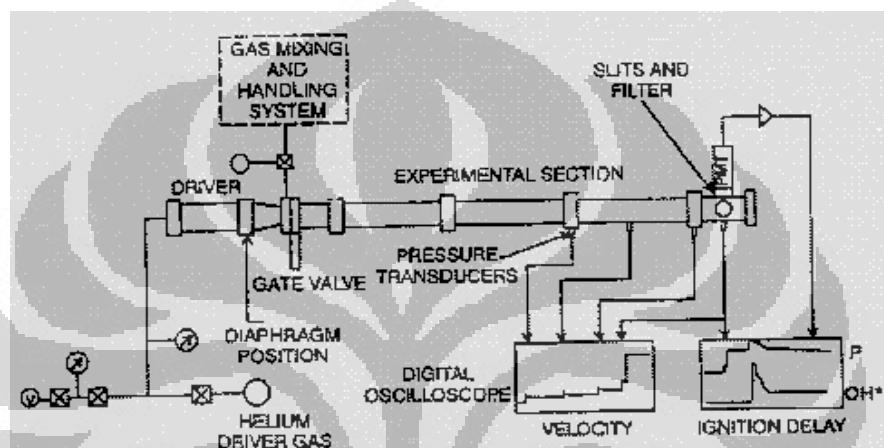
di mana suhu berpengaruh secara langsung pada reaksi elementer selama periode induksi.

2.7. PERALATAN MODEL PEMBAKARAN

Untuk mendapatkan data eksperimen berupa waktu tunda ignisi (*ignition delay time*), digunakan peralatan model pembakaran yang dapat mengkondisikan reaksi oksidasi dan pembakaran bahan bakar pada fasa gas. Peralatan tersebut tersebut adalah *shock tube*.

2.7.1. Shock Tube

Shock tube adalah sebuah alat yang digunakan untuk mempelajari reaksi pembakaran pada fasa gas. *Shock tube* juga dapat digunakan untuk mempelajari aliran aerodinamis pada rentang temperatur dan tekanan yang lebar. *Shock tube* sederhana merupakan sebuah tabung logam yang memisahkan gas pada tekanan rendah dan tinggi dengan sebuah diafragma. Skema sederhana peralatan *shock tube* diperlihatkan pada Gambar 2.10.



Gambar 2.10. Peralatan *shock tube* [18]

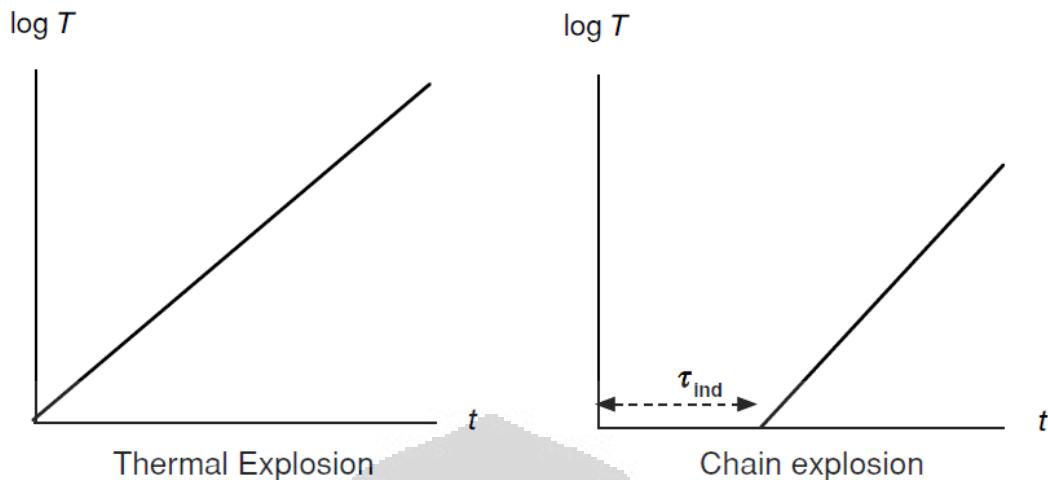
Gas bertekanan rendah pada bagian yang digerakkan menjadi gelombang kejut (*shock wave*). Bagian penggerak mengandung gas bertekanan tinggi (gas penggerak biasanya berupa helium atau hidrogen). Gas-gas ini (yang tidak perlu memiliki komposisi kimia yang sama) dipompa menuju bagian-bagian tabung atau dengan menggunakan pipa gas bertekanan (jika tekanan yang diinginkan kurang dari 1 atmosfer). Gas dipompa keluar dari bagian tabung hingga tekanan yang diinginkan tercapai. Diafragma yang berada di antara bagian tabung harus cukup kuat untuk menahan perbedaan tekanan mula-mula. Diafragma juga harus membuka dengan baik untuk memberikan hasil pengujian yang baik. Permulaan pembakaran menghasilkan peningkatan tekanan secara tiba-tiba sehingga memecahkan diafragma. Metode ini merupakan salah satu metode pemecahan diafragma yang digunakan pada campuran gas yang dapat terbakar dalam *driver*. Setelah diafragma pecah, suatu gelombang bertekanan melewati tabung menuju gas yang akan digerakkan, kemudian secara cepat membentuk suatu *shock front*, yang dikenal sebagai *incident shock wave*. Gelombang kejut ini meningkatkan

temperatur dan tekanan gas yang akan digerakkan dan menginduksi suatu aliran yang bersamaan dengan gelombang kejut (tetapi pada kecepatan yang lebih rendah dari gelombang kejut itu sendiri). Setiap kejutan yang melintas melalui tiap bagian volume akan meningkatkan temperatur. Temperatur akhir sistem biasanya sekitar 10^3 - 10^4 K. Proses pemanasan terjadi dalam waktu yang sangat cepat, yaitu selama $1 \mu\text{s}$ [4].

Ketika *incident shock wave* mencapai ujung *shock tube*, gelombang ini dipantulkan kembali ke dalam gas yang sudah dipanaskan, dan menghasilkan peningkatan yang lebih pada temperatur, tekanan, dan densitas gas. Gelombang ini secara efektif menghasilkan daerah reaksi temperatur dan tekanan tinggi [19]. Baik *incident wave* maupun gelombang terpantulkan dapat digunakan untuk menciptakan kondisi pengujian yang sesuai untuk penelitian otoignisi. Teknik kejutan tepantulkan memiliki tiga keuntungan dibandingkan dengan *incident shock*, yaitu:

1. Dapat menghasilkan temperatur yang lebih tinggi
2. Dapat menghilangkan ignisi sementara yang disebabkan oleh pecahnya diafragma
3. Dapat menciptakan gas yang cukup tenang setelah pantulan gelombang

Teknik *incident shock* memiliki keterbatasan secara fisik. Kejutan yang cukup kuat untuk mengignisi campuran bahan bakar dapat dipercepat dengan gradien densitas yang besar dibelakang gelombang. Peristiwa ini meningkatkan kekuatan kejutan di sepanjang tabung dan dapat mendorong terjadinya detonasi [18]. Pada proses ignisi termal, peningkatan temperatur terjadi sekali. Pada campuran hidrogen atau hidrokarbon-udara, dapat diketahui bahwa peningkatan temperatur dan eksplosi terjadi setelah periode waktu tertentu (*ignition delay time*), yang dapat dilihat pada Gambar 2.11.



Gambar 2.11. Perilaku waktu eksplosi termal (kiri) dan eksplosi percabangan rantai (kanan) dalam suatu sistem adiabatik [16]

Selama periode penundaan ignisi, populasi kumpulan radikal meningkat pada laju eksponensial [20]. Namun banyaknya bahan bakar yang dikonsumsi dan jumlah energi yang dibebaskan sangat kecil untuk dideteksi. Dengan demikian, reaksi kimia penting (percabangan rantai, pembentukan radikal) terjadi selama waktu induksi, yaitu saat temperatur mendekati konstan. Akhirnya, kumpulan radikal menjadi cukup besar untuk mengkonsumsi fraksi bahan bakar secara signifikan dan ignisi cepat akan terjadi [21]. Keakuratan data *shock tube* tergantung pada pengukuran kecepatan kejutan yang tepat. Hal ini biasanya ditentukan dengan mengukur waktu yang diperlukan gelombang kejut untuk melewati empat titik atau lebih, yang dipisahkan dengan jarak tertentu sepanjang tabung, dan merata-ratakan nilainya. *Shock front* yang datang dideteksi oleh *pressure transducers* dan interval waktu direkam oleh suatu pengukur waktu elektrik [21].

2.8. CHEMKIN 3.7.1.

Memahami dan memprediksi *chemistry effects* sangat penting dalam merancang suatu teknologi yang ramah lingkungan, terutama pada sektor transportasi. Dengan semakin kompleksnya desain mesin kendaraan, serta banyaknya jenis bahan bakar komersial yang beredar di masyarakat Indonesia, diperlukan perangkat lunak yang dapat mensimulasikan data-data mengenai

proses pembakaran dan oksidasi bahan bakar sehingga peforma sistem pembakaran bahan bakar tersebut dapat diketahui dan direncanakan penggunaannya secara tepat. Perangkat lunak Chemkin hadir sebagai program yang mampu untuk mensimulasikan reaksi kimia yang kompleks. Dengan kapasibilitas yang tersedia, desain eksperimen dapat diperkirakan kinerjanya melalui parameter yang terukur sebelum konsep *hardware*-nya dibangun.

Dalam sejarahnya, Chemkin telah berevolusi dari bentuk asalnya sebagai kode pembakaran (Chemkin II) yang dibuat oleh Sandia National Laboratory pada awal tahun 1980, menjadi program simulasi komersial terkini yang modern, dengan kontrol bersahabat, kecepatan yang handal, serta memiliki keakuratan yang baik. Sejak 1997, Reaction Design, selaku distributor program Chemkin telah merilis 7 versi dari Chemkin. Versi yang digunakan dalam penelitian ini adalah versi ke-7, yakni Chemkin 3.7.1. Chemkin merupakan sistem yang terdiri dari kumpulan program handal yang dapat menyelesaikan berbagai permasalahan kompleks mengenai kinetika kimia. Masing-masing dari pilihan program aplikasi ini, memiliki karakteristik spesifik terhadap kondisi aliran reaksi tertentu. Salah satu dari kondisi spesifik tersebut mencakup kondisi pembakaran (*combustion*) dalam ruang mesin, yang dapat diselesaikan menggunakan aplikasi Aurora.

2.8.1. Aurora

Aplikasi Aurora bertujuan memprediksi karakteristik tunak dari reaktor yang tercampur dengan baik atau jaringan reaktor. Aurora dapat diaplikasikan pada sistem terbuka maupun tertutup. Model silinder mesin pembakaran dalam (*internal combustion engine*) untuk kinetika reaksi kompresi pembakaran, ikut tercakup dalam aplikasi Aurora. Perhitungan sensitivitas konsentrasi spesi dan temperatur dapat dilakukan Aurora secara dinamik ataupun *steady-state*, pada fasa gas dan laju reaksi permukaan. Untuk permasalahan *steady-state*, aplikasi ini akan menyelesaiannya dengan menggunakan metode hibrid Newton/time-integration yang ditambahkan ke dalam program Chemkin. Untuk permasalahan transien, diselesaikan dengan solver DASPK (*large scale differential algebraic equation solver*) dari U.C. Santa Barbara [22]. Pada penelitian ini, Aurora akan menghasilkan waktu tunda ignisi untuk penentuan karakteristik bahan bakar

gasolin. Aplikasi tersebut akan memerlukan *input* berupa kondisi tekanan awal, suhu awal, dan rasio ekuivalensi (Φ) dari komposisi bahan bakar komersial sampel. Berikut contoh penulisan masukan kondisi di aplikasi Aurora, yaitu:

```

TRAN
ENRG
QLOS 0.0
PRES 54.28
TEMP 1000
REAC NC7H16      0.0030246
REAC I-C8H18     0.0109653
REAC TOLUENE    0.0034541
REAC O2          0.2014239
REAC N2          0.7811319
TIME 0.001
DELT 1.E-4
DTSV 1.E-4
END

```

Keterangan:

- TRAN = kondisi proses adalah transien
- ENRG = permintaan penyelesaian persamaan energi
- QLOS = panas yang hilang diasumsikan nol (sistem adiabatik)
- PRES = tekanan awal bahan bakar sebelum memasuki mesin torak (piston)
- TEMP = suhu awal bahan bakar sebelum memasuki mesin torak (piston)
- REAC = fraksi mol bahan bakar
- TIME = waktu simulasi, satuan detik
- DELT = interval/rentang waktu pencetakan diagnosis file *output*
- DTSV = interval/rentang waktu penulisan data ke dalam *XML Solution File* (XMLdata.zip)
- END = kata kunci akhir untuk file *input*

BAB III

METODOLOGI PENELITIAN

Penelitian mengenai simulasi waktu tunda ignisi bahan bakar gasolin multikomponen ini akan dibagi menjadi lima tahap, yaitu:

1. Menambahkan model kinetika reaksi n-heptana

Tahap ini dilakukan dengan mengumpulkan literatur tentang reaksi-reaksi elementer yang terjadi pada oksidasi dan pembakaran bensin, serta menemukan keterkaitan reaksi elementer n-heptana di antara reaksi-reaksi tersebut. Selanjutnya, data kinetika reaksi yang telah dikumpulkan kemudian ditambahkan ke dalam model kinetika yang sudah ada disertai dengan data termodinamika spesi-spesi baru yang terlibat.

2. Mengembangkan model kinetika reaksi

Pada tahapan ini, disusun model kinetika reaksi oksidasi bahan bakar gasolin multikomponen yang telah ditambahkan model kinetika reaksi detail n-heptana sesuai dengan format Chemkin 3.7.1.

3. Validasi

Setelah penyesuaian selesai, maka model kinetika reaksi tersebut divalidasikan terhadap data eksperimen.

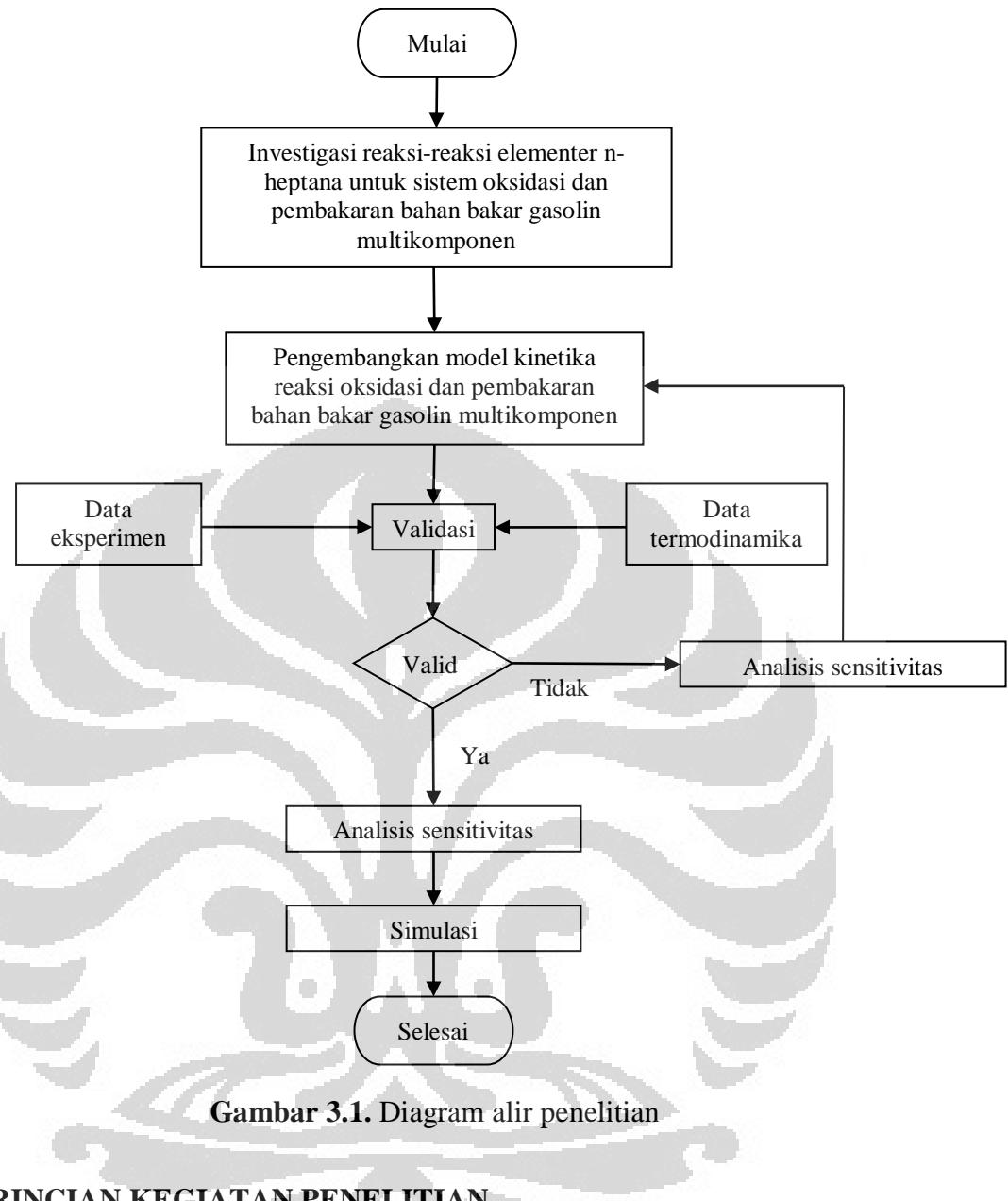
4. Analisis sensitivitas

Untuk menganalisis mekanisme dari pemodelan yang telah dilakukan, maka digunakan analisis sensitivitas.

5. Simulasi

Mensimulasikan model kinetika reaksi yang telah valid tersebut dengan memvariasikan kondisi operasi, seperti temperatur awal, tekanan awal dan rasio ekuivalensi (Φ).

Untuk lebih jelasnya, kelima tahapan di atas beserta alurnya dapat dilihat pada Gambar 3.1.



3.1. RINCIAN KEGIATAN PENELITIAN

3.1.1. Penambahan Model Kinetika Reaksi n-Heptana (C_7H_{16})

Pada tahap ini dilakukan studi pustaka mengenai reaksi-reaksi elementer n-heptana yang terjadi pada reaksi oksidasi dan pembakaran bahan bakar gasolin multikomponen, untuk kemudian menemukan keterkaitan di antara reaksi-reaksi tersebut, serta mengumpulkan data kinetika masing-masing reaksi yang bersangkutan. Data kinetika merupakan koefisien laju reaksi (k) dari persamaan Arrhenius yang terdiri dari faktor pre-exponensial (A), eksponen temperatur (b) dan energi aktivasi (E_a). Kemudian data elemen, spesi, dan mekanisme reaksi

digunakan sebagai masukan *Gas-Phase Kinetics* untuk salah satu utilitas *Chem* dalam *software Chemkin 3.7.1*. Adapun contoh format penulisan mekanisme reaksi pembakaran dan oksidasi gasolin dapat dilihat sebagai berikut [23]:

```

ELEMENTS H O C N AR END
SPECIES H H2 H2O OH O O2 AR N2 HO2 H2O2 CO CO2 OXI CH3CHO CH3 CHO
.....
END

REACTION
!MECHANISM I-C8H18-O2 System at High Temperature
!---H2-O2 reactions
O2 +H =OH +O 9.700E+09 0.0 62.100
H2 +O =OH +H 5.060E+04 2.670 26.300
H2 +OH =H2O +H 1.000E+08 1.600 13.800
OH +OH =H2O +O 1.500E+09 1.140 0.420
H +H =M =H2 +M 1.800E+18 -1.000 0.000
O +O =M =O2 +M 5.400E+13 0.000 -7.4
H +OH =M =H2O +M 5.530E+22 -2.000 0.000
H +O2 =M =HO2 +M 2.100E+18 -0.800 0.0
HO2 +H =OH +OH 1.500E+14 0.0 3.800
HO2 +H =H2 +O2 3.000E+13 0.0 4.000
HO2 +H =H2O +O 3.000E+13 0.0 7.200
HO2 +O =OH +O2 2.000E+13 0.0 0.0
HO2 +OH =H2O +O2 6.000E+13 0.0 0.0
HO2 +HO2 =H2O2 +O2 4.220E+14 0.0 50.140
DUPLICATE
HO2 +HO2 =H2O2 +O2 1.320E+11 0.0 -6.820
DUPLICATE
OH +OH (+M) =H2O2 (+M) 7.230E+13 -0.370 0.0
    / 5.530E+19 -0.760 0.0 /
LOW TROE / 0.500 0.0 0.0 0.0 /
H2O2 +H =H2 +HO2 1.700E+12 0.0 15.700
H2O2 +H =H2O +OH 1.000E+13 0.0 15.000
H2O2 +O =OH +HO2 9.630E+06 2.0 16.630
H2O2 +OH =H2O +HO2 5.400E+12 0.0 4.200
CO +OH =CO2 +H 4.760E+07 1.230 0.290
CO +HO2 =CO2 +OH 1.500E+14 0.0 98.700
CO +O =M =CO2 +M 1.540E+15 0.0 12.560
CO +O2 =CO2 +O 2.500E+12 0.0 200.000
CH +O =CO +H 4.000E+13 0.0 0.0
CH +O2 =CHO +O 3.000E+13 0.0 0.0
.....
END

```

Dalam setiap baris penulisan data reaksi di atas, terdiri dari 2 hal utama yaitu pertama berupa deskripsi simbolik reaksi (bagian kiri) dan kedua berupa koefisien laju Arrhenius (bagian kanan). Pada deskripsi simbolik reaksi, tanda sama dengan (=) menunjukkan bahwa reaksi reversibel dan tanda (\Rightarrow) menunjukkan bahwa reaksi irreversibel , huruf M menunjukkan suatu reaktan atau produk yang berperan sebagai *third body*. Pada bagian kedua yang menunjukkan koefisien laju Arrhenius, urutannya adalah sebagai berikut (dimulai dari kiri) faktor pre-exponensial, eksponen temperatur dan energi aktivasi. Efisiensi *third body* untuk beberapa spesi ditetapkan pada baris berikutnya setelah penulisan reaksi yang mengandung *third body*, M. Reaksi yang tergantung pada tekanan, yang ditandai dengan keterlibatan *third body* dan spesi yang ditulis dalam tanda

kurung seperti (+M) atau (+AR), maka terdapat kata kunci tambahan yaitu LOW dan TROE. Bilangan-bilangan setelah kata LOW merupakan koefisien Arrhenius untuk batas temperatur rendah. Sedangkan bilangan setelah kata TROE adalah parameter *Troe*. Kemudian kata kunci DUPLICATE digunakan untuk reaksi elementer yang sama, namun memiliki koefisien laju yang berbeda. Kata kunci akhir dalam penulisan input mekanisme reaksi yaitu END. Selanjutnya, contoh format penulisan masukan data termodinamika untuk beberapa spesi yaitu [23]:

```

THERMO
 300.000 1000.000 5000.000
H     8/12/99 thermH 10 0 0 0g 300.000 5000.000 1000.000 01
 2.50104422e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00 2
 2.54747466e+04-4.65341317e-01 2.50104422e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00 3
 0.00000000e+00 0.00000000e+00 2.54747466e+04-4.65341317e-01 0.02542060e+02-0.02755062e-03-0.03102803e-07 0.04551067e-10-0.04368052e-14 4
 0.02923080e+06 0.04920308e+02 0.02946429e+02-0.01638166e-01 0.02421032e-04 1
 -0.01602843e-07 0.03890696e-11 0.02914764e+06 0.02963995e+02 0.02991423e+02 0.07000644e-02-0.05633829e-06-0.09231578e-10 0.01582752e-13 2
 -0.08350340e+04-0.01355110e+02 0.03298124e+02 0.08249442e-02-0.08143015e-05 3
 -0.09475434e-09 0.04134872e-11-0.01012521e+05-0.03294094e+02 0.03697578e+02 0.06135197e-02-0.01258842e-05 0.01775281e-09-0.01136435e-13 4
 0.01233930e+05 0.03189166e+02 0.03212936e+02 0.01127486e-01-0.05756150e-05 3
 0.01313877e-07-0.08768554e-11-0.01005249e+05 0.06034738e+02 0.02599754e+00 1.31992406e-03-3.59724670e-07 4.25630800e-11-1.82048016e-15 2
 4.12085374e+03 7.10667307e+00 3.43586219e+00 2.02235804e-04-1.13546412e-07 3
 2.42445149e-10-7.43651031e-14 3.74321252e+03 2.45014127e+00 0.02672146e+02 0.03056293e-01-0.08730260e-05 0.01200996e-08-0.06391618e-13 2
 -0.02989921e+06 0.06862817e+02 0.03386842e+02 0.03474982e-01-0.06354696e-04 3
 0.06968581e-07-0.02506588e-10-0.03020811e+06 0.02590233e+02 0.025852919e-10 1.51139912e-13 8.09181013e+02 1.24191723e-10-7.16400108e-15 2
 3.98127689e+02 3.12515836e+00 3.18310656e+00 3.66767950e-03-9.32385122e-07 3
 -3.25852919e-10 8/12/99 thermH 10 2 0 0g 300.000 5000.000 1390.000 01
 4.10547423e+00 2.38452835e-03-8.06347989e-07 1.24191723e-10-7.16400108e-15 2
 3.98127689e+02 3.12515836e+00 3.18310656e+00 3.66767950e-03-9.32385122e-07 3
 H2O     20387H 20 1 0 0g 300.000 5000.000 1000.00 1
 0.02672146e+02 0.03056293e-01-0.08730260e-05 0.01200996e-08-0.06391618e-13 2
 -0.02989921e+06 0.06862817e+02 0.03386842e+02 0.03474982e-01-0.06354696e-04 3
 0.06968581e-07-0.02506588e-10-0.03020811e+06 0.02590233e+02 0.04573167e+02 0.04336136e-01-0.01474689e-04 0.02348904e-08-0.01431654e-12 2
 -0.01800696e+06 0.05011370e+01 0.03386842e+02 0.06569226e-01-0.01485013e-05 3
 0.04625806e-07 0.02471515e-10-0.01766315e+06 0.06785363e+02 0.02471515e-10-0.01766315e+06 0.04453623e+02 0.03140169e-01-0.01278411e-04 0.02393997e-08-0.01669033e-12 2
 -0.04896696e+06-0.09553959e+01 0.02275725e+02 0.09922072e-01-0.01040911e-03 3
 0.06866687e-07-0.02117280e-10-0.04837314e+06 0.01018849e+03 0.01089825e-06-0.04574885e-10 0.04159922e+05 0.08983614e+02 0.02995606e+02 0.06681321e-01-0.02628955e-04 0.04737153e-08-0.03212517e-12 2
 -0.01532037e+06 0.06912572e+02 0.01652731e+02 0.01263144e+00-0.01888168e-03 3
 CH2O     121286C 1H 20 1 0 0g 300.000 5000.000 1000.00 1
 0.02050031e-06-0.08413237e-10-0.01486540e+06 0.01378482e+03
END

```

Baris pertama pada data termodinamika di atas terdiri dari nama spesi seperti H, O, H₂, dan lain-lain. Simbol G menunjukkan bahwa spesi berada dalam fasa gas. Angka 300, 5.000 dan 1.000 menunjukkan rentang temperatur. Pada baris ke-2 sampai ke-4 merupakan data termodinamika yang terdiri dari bentuk

polinomial untuk menghitung panas spesifik, entalpi standar dan entropi standar. Formatnya dapat menggunakan *Thermodynamic Database* pada *NASA Chemical Equilibrium Code* yang terdiri terdiri dari 14 koefisien, dimana 7 koefisien pertama untuk temperatur rendah dan 7 koefisien kedua untuk temperatur tinggi. Lima koefisien pertama dari masing-masing daerah temperatur, digunakan untuk menghitung kapasitas panas (C_p^0), dan dua koefisien berikutnya digunakan untuk menghitung harga entalpi standar (H^0) dan entropi standar (S^0). Rumus perhitungannya adalah sebagai berikut [23]:

$$\frac{C_p^0}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \quad (3.1)$$

$$\frac{H^0}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T} \quad (3.2)$$

$$\frac{S^0}{R} = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7 \quad (3.3)$$

Persamaan 3.1 – 3.3 digunakan untuk menghitung K_p dengan rumus [24]:

$$K_p = \exp\left(\frac{\Delta S^0}{R} - \frac{\Delta H^0}{RT}\right) \quad (3.4)$$

Nilai ΔH^0 dan ΔS^0 dapat dicari dengan menggunakan persamaan [23]:

$$\frac{\Delta H_i^0}{RT} = \sum_{k=1}^K v_{ki} \frac{H_k^0}{RT} = \sum_{k=1}^K v_{ki} \left(a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T} \right) \quad (3.5)$$

$$\frac{\Delta S_k^0}{R} = \sum_{k=1}^K v_{ki} \frac{S_k^0}{R} = \sum_{k=1}^K v_{ki} \left(a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7 \right) \quad (3.6)$$

dengan v_{ki} merupakan koefisien stoikiometri, k menunjukkan suatu spesi.

3.1.2. Pengembangan Model Kinetika Reaksi

Tahap pengembangan model kinetika dilakukan dengan menggunakan aplikasi yang tersedia di *software Chemkin 3.7.1* yaitu aplikasi AURORA untuk mendapatkan profil *ignition delay* di *shock tube*. Aplikasi AURORA membutuhkan beberapa masukan, yaitu mekanisme reaksi dan data termodinamika dengan format penulisan seperti yang telah dijelaskan pada bagian 3.1.1. di atas. Sedangkan masukan khususnya berdasarkan pada kondisi operasi penelitian. Secara garis besar masukan khusus ini berupa kondisi tekanan awal,

temperatur awal, dan fraksi mol reaktan. Salah satu contoh penulisan masukan kondisi di aplikasi AURORA yaitu [23]:

```

TRAN
ENRG
QLOS 0.0
PRES 54.28
TEMP 1000
REAC NC7H16      0.0030246
REAC I-C8H18      0.0109653
REAC TOLUENE     0.0034541
REAC O2           0.2014239
REAC N2           0.7811319
TIME 0.001
DELT 1.E-4
DTSV 1.E-4
END

```

Keterangan kata-kata kunci pada masukan kondisi di atas telah dijelaskan sebelumnya pada sub-bab 2.8.1.

3.1.3. Validasi

Tahap ini dilakukan dengan membandingkan hasil simulasi dengan data percobaan. Data percobaan yang digunakan untuk memvalidasi mekanisme yang disimulasikan adalah data waktu tunda ignisi (*ignition delay time*) untuk bahan bakar 3 komponen, yaitu toluena, n-heptana dan iso-oktana. Data ini diperoleh Gauthier dkk. [1] dengan menggunakan alat *shock tube* di rentang temperatur 900 K – 1.150 K, rentang temperatur 25-55 bar dan rasio ekuivalensi (Φ) sebesar 1.

3.1.4. Analisis Sensitivitas

Analisis ini digunakan untuk mengidentifikasi laju pembatas dari tahapan-tahapan reaksi. Analisis ini akan ditunjukkan secara detail pada tiap reaksi dalam mekanismenya. Contoh perhitungan numerik untuk analisis sensitivitas dapat dilakukan dengan mengubah koefisien laju reaksi khusus dan perhitungan konsentrasi OH. Perbedaan antara konsentrasi OH sebelum dan sesudah

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perubahan koefisien laju kemudian dihitung. Hasilnya lalu dibandingkan dengan perbedaan terbesar yang dicapai oleh sistem. Hal ini disebut sebagai koefisien sensitivitas. Koefisien sensitivitas dapat bernilai negatif atau positif. Koefisien sensitivitas yang bernilai positif menunjukkan konsentrasi OH yang lebih tinggi dan meningkatkan laju reaksi keseluruhan sedangkan koefisien sensitivitas negative menunjukkan bahwa konsentrasi OH yang rendah dan menurunkan laju reaksi keseluruhan sistem. Koefisien sensitivitas dalam suatu sistem dapat digambarkan dalam diagram batang. Hanya jalur oksidasi utama yang berpengaruh untuk oksidasi bahan bakar.

3.1.5. Simulasi

Tahap simulasi reaksi oksidasi dan pembakaran bahan bakar gasoline multikomponen dijalankan dengan memvariasikan 2 kondisi operasi, yaitu tekanan awal dan rasio ekuivalensi (Φ). Simulasi dilakukan dengan menggunakan program Chemkin 3.7.1. Untuk setiap variasi, hasil simulasi yang diambil adalah waktu tunda ignisi (*ignition delay time*, idt). Profil temperatur dan profil energi hasil pembakaran diperoleh dengan memanfaatkan fitur *Post Process* pada program Chemkin 3.7.1. Profil temperatur yang diambil mewakili suhu adiabatik dari proses pembakaran, di mana suhu adiabatik akan memberikan gambaran mengenai jumlah energi yang dihasilkan oleh proses pembakaran bahan bakar tersebut. Berikut ini merupakan penjelasan proses variasi kondisi operasi dalam simulasi yang dilakukan:

✚ Tekanan Awal

Pada penelitian ini dilakukan variasi tekanan awal 5 bar, 25 bar dan 55 bar, pada rasio ekuivalensi konstan ($\Phi = 1$), dengan rentang suhu antara 700 K - 1.000 K. Variasi tersebut dilakukan dengan cara mengubah nilai tekanan awal pada masukkan Aurora, yaitu sebagai berikut:

TRAN

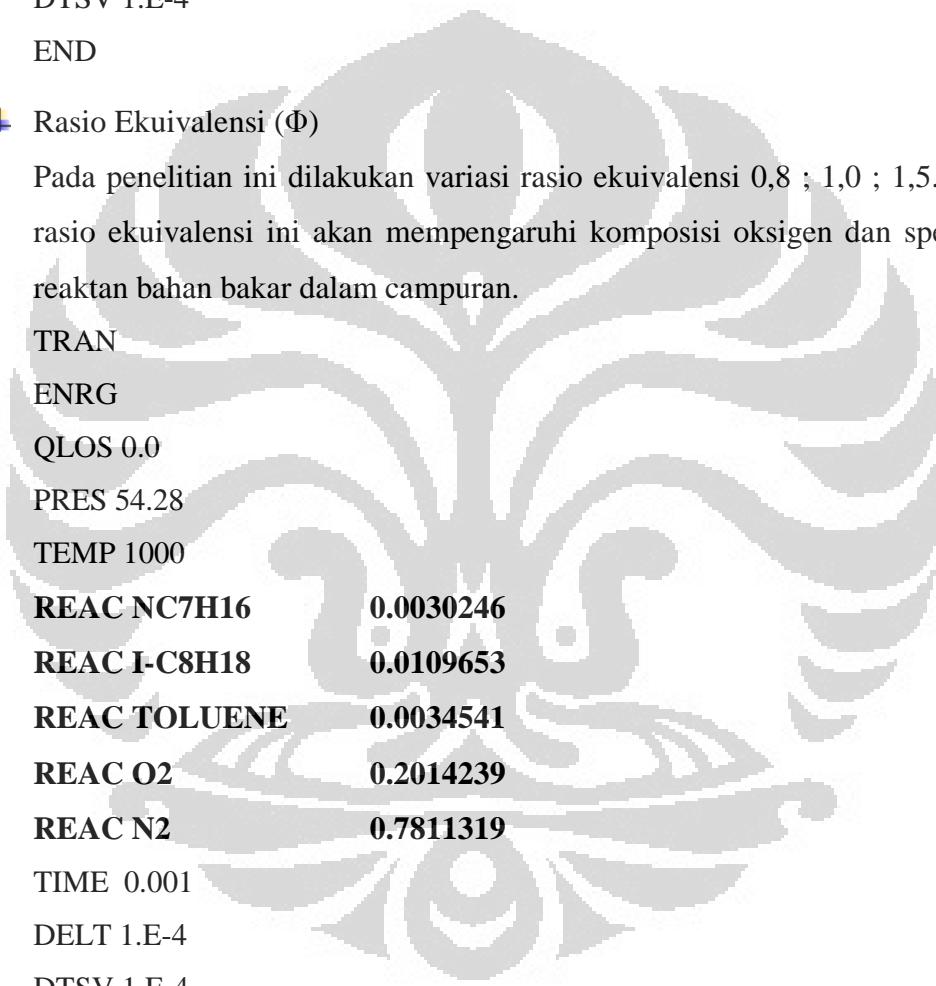
ENRG

QLOS 0.0

PRES 54.28

TEMP 1000

```

REAC NC7H16      0.0030246
REAC I-C8H18     0.0109653
REAC TOLUENE     0.0034541
REAC O2           0.2014239
REAC N2           0.7811319
TIME 0.001
DELT 1.E-4
DTSV 1.E-4
END


```

 Rasio Ekuivalensi (Φ)

Pada penelitian ini dilakukan variasi rasio ekuivalensi 0,8 ; 1,0 ; 1,5. Variasi rasio ekuivalensi ini akan mempengaruhi komposisi oksigen dan spesi-spesi reaktan bahan bakar dalam campuran.

```

TRAN
ENRG
QLOS 0.0
PRES 54.28
TEMP 1000
REAC NC7H16      0.0030246
REAC I-C8H18     0.0109653
REAC TOLUENE     0.0034541
REAC O2           0.2014239
REAC N2           0.7811319
TIME 0.001
DELT 1.E-4
DTSV 1.E-4
END

```

3.2. ALAT DAN BAHAN PENELITIAN

Alat yang digunakan dalam penelitian ini adalah program Chemkin 3.7.1. Bahan penelitian yang digunakan, diambil dari model kinetika reaksi oksidasi dan pembakaran bahan bakar gasolin milik Yendha [8] yang belum divalidasi.

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BAB 4

VALIDASI

Eksperimen untuk mendapatkan waktu tunda ignisi dari campuran 3 komponen bahan bakar telah dilakukan oleh Gauthier dkk. [1] pada tahun 2004. Penelitian tersebut dilakukan pada alat *shock tube* dengan rentang temperatur dari 900 K sampai 1.150 K, di tekanan 25-55 bar, dan rasio ekuivalensi 1. Komponen yang digunakan dalam percobaan adalah toluena, n-heptana dan iso-oktana, dengan perbandingan fraksi volume masing-masing sebesar 14% 17%, dan 69%. Pada percobaan ini, waktu terjadinya ignisi ditandai oleh saat munculnya emisi cahaya pertama yang terlihat. Waktu ignisi untuk eksperimen didefinisikan sebagai waktu yang dibutuhkan untuk mencapai emisi radiasi minimum 366 nm, yang ditandai dengan timbulnya nyala dan hadirnya spesi produk karbondioksida. Sedangkan pada perhitungan secara numeris yang diproses pada CHEMKIN, penentuan waktu ignisi ditentukan berdasarkan beberapa metode, antara lain: pada saat temperatur naik secara drastis, pada saat konversi bahan bakar tinggi, pada saat konsentrasi CO₂ naik drastis, dan pada saat konsentrasi radikal aktif (misal radikal OH) naik secara drastis. Perhitungan numeris waktu tunda ignisi (*ignition delay time*) pada percobaan ini dilakukan dengan menggunakan Aurora yang mengasumsikan bahwa sistem pada keadaan adiabatic ($Q_{lost} = 0$) dan volume tetap.

Untuk melakukan validasi, model kinetika reaksi yang telah disusun sebelumnya akan disimulasikan pada rentang suhu dan temperatur yang sama dengan kondisi operasi eksperimen. Rentang temperatur yang disimulasikan adalah antara 973 K – 1.137 K pada tekanan 25 bar, dan antara 908 K – 1.104 K pada tekanan 55 bar. Model kinetika reaksi oksidasi dan pembakaran bahan bakar gasolin multikomponen terdiri dari 3.895 reaksi elementer dan melibatkan 1.593 spesi. Jumlah fraksi masing-masing komponen yang menjadi masukan Aurora, didasarkan pada perbandingan fraksi mol. Tabel 4.1. menyajikan nilai komposisi campuran bahan bakar gasolin untuk simulasi dengan rasio ekuivalensi sebesar 1.

Tabel 4.1. Komposisi campuran bahan bakar simulasi

Komponen	Bahan Bakar Gasolin
	Fraksi Mol
Toluena	0,0034541
n-Heptana	0,0030246
iso-Oktana	0,0109653

Untuk mendapatkan kesesuaian yang lebih baik dari perbandingan yang dilakukan terhadap data eksperimen dengan data simulasi, maka dilakukan modifikasi pada data model kinetika reaksi. Modifikasi tersebut dilakukan dengan merubah nilai konstanta Arrhenius dari beberapa reaksi yang sensitif. Reaksi tersebut dapat diketahui nilai koefisien sensitivitasnya melalui analisis sensitivitas. Pada penelitian ini, dilakukan analisis sensitivitas terlebih dahulu sebelum dilakukan modifikasi nilai konstanta Arrhenius yaitu pada tekanan 55 bar dan temperatur 1.000 K. Inputan Aurora untuk analisis sensitivitas tersebut, yaitu:

```

TRAN
ENRG
QLOS 0.0
SEN OH
PRES 54.28
TEMP 1000
REAC NC7H16      0.0030246
REAC I-C8H18     0.0109653
REAC TOLUENE    0.0034541
REAC O2          0.2014239
REAC N2          0.7811319
TIME 1.E-3
DELT 1.E-4
DTSV 1.E-4
END

```

Digunakan kata perintah SEN OH untuk menganalisis sensitivitas radikal OH di masing-masing reaksi dalam model kinetika reaksi yang telah disusun. Radikal OH dipilih karena pengaruhnya yang besar dalam menentukan waktu

tunda ignisi pada rentang temperatur tinggi (di atas 900 K). Di mana apabila suatu reaksi elementer memiliki nilai koefisien sensitivitas yang positif, hal ini berarti apabila nilai konstanta Arrheniusnya diperbesar, maka konsentrasi radikal OH akan semakin banyak, yang berakibat laju reaksi keseluruhan sistem akan semakin cepat (nilai waktu tunda ignisi semakin kecil). Demikian juga dengan reaksi elementer yang memiliki nilai koefisien sensitivitas yang negatif, berlaku hal sebaliknya. Modifikasi konstanta Arrhenius yang dilakukan dapat dilihat pada Tabel 4.2.

Tabel 4.2. Modifikasi konstanta Arrhenius

	Reaksi Spesi	Konstanta Arrhenius Awal	Konstanta Arrhenius Modifikasi
Reaksi dengan nilai koefisien sensitivitas positif	$2\text{OH}(+\text{M}) \rightleftharpoons \text{H}_2\text{O}_2(+\text{M})$	5.624E+18	5.624E+18
	$\text{CH}_2\text{O}+\text{HO}_2 \rightleftharpoons \text{HCO}+\text{H}_2\text{O}_2$	6.402E-02	6.402E-02
	$\text{H}+\text{O}_2 \rightleftharpoons \text{O}+\text{OH}$	1.970E+14	1.970E+14
	$\text{I-C}_8\text{H}_{18}+\text{OH} \rightleftharpoons \text{Al-C}_8\text{H}_{17}+\text{H}_2\text{O}$	2.893E+07	2.000E+10
	$\text{I-C}_4\text{H}_8+\text{OH} \rightleftharpoons \text{I-C}_4\text{H}_7+\text{H}_2\text{O}$	5.200E+06	5.200E+06
	$\text{CH}_3\text{O}_2+\text{CH}_3 \rightleftharpoons 2\text{CH}_3\text{O}$	1.650E+13	1.650E+13
	$\text{I-C}_8\text{H}_{18}+\text{HO}_2 \rightleftharpoons \text{Al-C}_8\text{H}_{17}+\text{H}_2\text{O}_2$	2.772E+13	2.772E+13
	$\text{PHCH}_2+\text{HO}_2 \rightleftharpoons \text{PHCH}_2\text{O}+\text{OH}$	3.160E+12	3.160E+12
	$\text{I-C}_8\text{H}_{18}+\text{HO}_2 \rightleftharpoons \text{CI-C}_8\text{H}_{17}+\text{H}_2\text{O}_2$	2.800E+12	2.800E+12
Reaksi dengan nilai koefisien sensitivitas negatif	$\text{TOLUENE}+\text{OH} \rightleftharpoons \text{PHCH}_2+\text{H}_2\text{O}$	1.140E+13	1.140E+13
	$\text{H}_2\text{O}_2+\text{O}_2 \rightleftharpoons 2\text{HO}_2$	5.348E+17	5.348E+17
	$\text{CH}_2\text{O}+\text{OH} \rightleftharpoons \text{HCO}+\text{H}_2\text{O}$	3.087E+10	3.087E+10
	$\text{CH}_3+\text{HO}_2 \rightleftharpoons \text{CH}_4+\text{O}_2$	3.240E+12	3.240E+12
	$\text{C}_3\text{H}_6+\text{OH} \rightleftharpoons \text{A-C}_3\text{H}_5+\text{H}_2\text{O}$	2.814E+06	2.814E+06
	$\text{TOLUENE}+\text{HO}_2 \rightleftharpoons \text{PHCH}_2+\text{H}_2\text{O}_2$	2.70E+14	2.70E+14
	$\text{DI-C}_8\text{H}_{17} \rightleftharpoons \text{C}_3\text{H}_6+\text{NEOC}_5\text{H}_{11}$	2.62E+19	2.62E+19

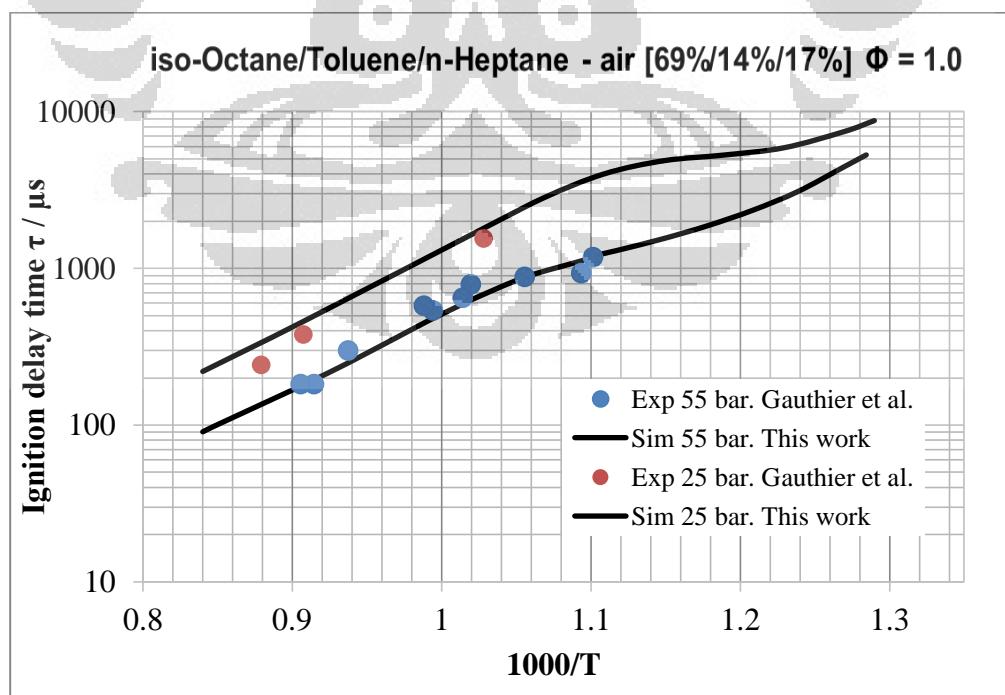
Setelah dilakukan simulasi komputer pada rentang kondisi operasi yang sama dengan data eksperimen, diperoleh data seperti pada Tabel 4.3 untuk tekanan 25 bar dan Tabel 4.4 untuk tekanan 55 bar. Ketika waktu tunda ignisi eksperimen dan simulasi diplotkan secara logaritmik terhadap kebalikan temperatur awal, diperoleh grafik perbandingan seperti yang tercantum pada Gambar 4.1.

Tabel 4.3. Perbandingan waktu tunda ignisi pada tekanan 25 bar

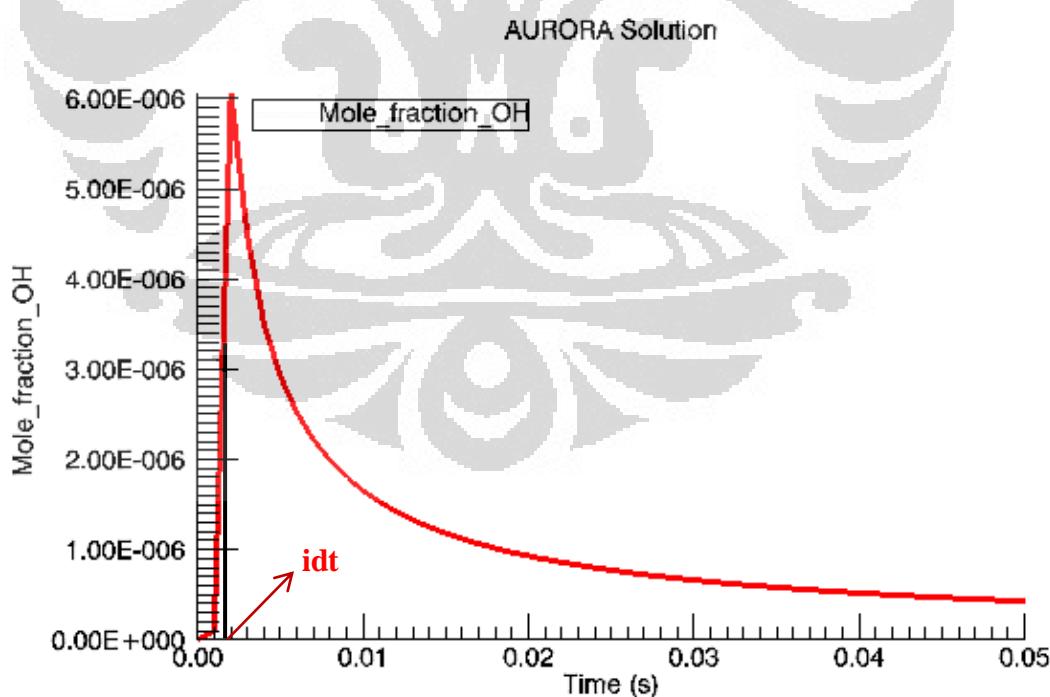
Tekanan 25 bar			
Suhu (K)	1.000/T	Idt Eksperimen (μ sec)	idt Simulasi (μ sec)
973	1,2085	1.545	1.810
1.102	0,908	375	462
1.137	0,8796	241	319

Tabel 4.4. Perbandingan waktu tunda ignisi pada tekanan 55 bar

Tekanan 55 bar			
Suhu (K)	1.000/T	Idt Eksperimen (μ sec)	idt Simulasi (μ sec)
908	1,102	1.168	1.200
915	1,094	928	1.120
947	1,056	880	880
981	1,02	783	631
986	1,0148	645	597
1.006	0,9945	535	481
1.012	0,9885	575	450
1.067	0,938	298	251
1.093	0,915	182	196
1.104	0,906	182	178

**Gambar 4.1.** Plot logaritmik data simulasi dan data eksperimen

Dari hasil plot di Gambar 4.1., terlihat bahwa model kinetika reaksi bahan bakar gasolin yang telah dikembangkan Yendha [8] dan sudah ditambahkan dengan model kinetika reaksi detail n-heptana, secara umum menunjukkan kesesuaian terhadap data eksperimen. Kesesuaian ini dicapai setelah dilakukan *tuning* (pengubahan) pada konstanta Arrhenius berupa faktor pre-eksponensial (A). Pengubahan hanya dilakukan pada reaksi yang menunjukkan sensitivitas tinggi seperti yang ditunjukkan pada Tabel 4.2. Jika mengambil deviasi maksimal sebesar 24%, hanya ada 1 titik dari 13 titik yang tidak memenuhi kriteria. Selain itu, juga terlihat dari Gambar 4.1. bahwa semakin tinggi temperatur yang digunakan, maka waktu tunda ignisi akan semakin kecil. Pada tekanan yang lebih tinggi dengan rasio ekivalen yang sama, waktu tunda ignisi pun akan semakin kecil. Hal ini menunjukkan bahwa pada temperatur yang semakin tinggi dan tekanan yang lebih tinggi, waktu tunda untuk mencapai ignisi semakin pendek sehingga ignisi bahan bakar semakin cepat tercapai. Gambar 4.2. menunjukkan cara penentuan waktu tunda ignisi melalui profil konsentrasi radikal OH. Waktu tunda ignisi diperoleh dari titik di mana konsentrasi radikal OH naik secara dratis.



Gambar 4.2. Profil temperatur pada tekanan awal 25 bar; temperatur awal 973⁰K; rasio ekivalensi (Φ) = 1,0

BAB 5

ANALISIS SENSITIVITAS

Studi yang dilakukan mengenai model kinetika reaksi oksidasi dan pembakaran lengkap suatu hidrokarbon melibatkan ribuan reaksi elementer yang membentuk mekanisme reaksi kompleks. Masing-masing laju reaksi elementer dalam mekanisme pembakaran tersebut memiliki perbedaan yang besar. Untuk banyak reaksi elementer, perubahan koefisien laju reaksi hampir tidak memiliki pengaruh yang signifikan pada hasil keluaran sistem. Namun sebaliknya, sebagian kecil reaksi elementer dapat mempengaruhi hasil keluaran sistem secara signifikan apabila terdapat perubahan koefisien laju reaksi. Reaksi elementer inilah yang disebut sebagai reaksi laju pembatas. Oleh karena itu, diperlukan suatu analisis mekanisme reaksi yang dapat membedakan suatu reaksi laju pembatas dengan reaksi elementer lainnya. Salah satu jenis analisis mekanisme yang umum dilakukan untuk mencapai tujuan tersebut adalah analisis sensitivitas.

Mekanisme reaksi yang lengkap untuk sistem oksidasi dan pembakaran hidrokarbon terdiri dari ribuan reaksi elementer. Untuk memvalidasi mekanisme reaksi yang dibuat, maka harus dilakukan pengaturan nilai konstanta Arrhenius setiap reaksi. Beberapa dari reaksi elementer itu memiliki kemungkinan termasuk dalam reaksi yang tidak penting sehingga dapat diabaikan dalam pengaturan parameter kinetika tersebut. Analisis sensitivitas akan digunakan untuk mengidentifikasi reaksi-reaksi sensitif (reaksi laju pembatas) yang terlibat dalam mekanisme reaksi pembakaran. Mengidentifikasi reaksi-reaksi yang penting bukan berarti reaksi-reaksi yang tidak penting dapat dieliminasi. Mengeliminasi reaksi-reaksi yang tidak penting dapat berakibat hilangnya jalur reaksi dari seluruh reaksi berantai yang telah disusun. Dengan melakukan analisis sensitivitas diharapkan dapat mempermudah untuk mengatur nilai konstanta Arrhenius masing-masing reaksi agar hasil simulasi yang diperoleh dapat sesuai dengan data eksperimen.

Perhitungan numeris untuk analisis sensitivitas dilakukan dengan mengubah koefisien laju reaksi tertentu dan kemudian menghitung konsentrasi

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OH. Perubahan konsenterasi OH sebelum dan sesudah perubahan koefisien laju reaksi kemudian dihitung. Hasil ini kemudian dibandingkan dengan perbedaan terbesar yang diperoleh dari sistem. Inilah yang disebut dengan koefisien sensitivitas. Koefisien sensitivitas dapat bernilai positif atau negatif. Koefisien sensitivitas yang bernilai positif mengindikasikan ketika nilai konstanta Arrhenius reaksi tersebut dinaikkan, maka laju reaksi keseluruhan akan meningkat (waktu tunda ignisi semakin singkat) karena konsentrasi radikal OH yang juga meningkat. Sebaliknya, untuk koefisien sensitivitas yang bernilai negatif akan berakibat penurunan laju reaksi secara keseluruhan ketika ketika nilai konstanta Arrhenius dinaikkan (waktu tunda ignisi semakin lambat), karena konsentrasi radikal OH menjadi berkurang. Perbandingan nilai koefisien sensitivitas masing-masing reaksi yang sensitif terhadap perubahan konsentrasi radikal OH, dapat digambarkan ke dalam bentuk diagram batang seperti pada Gambar 5.1. sampai dengan Gambar 5.3.

Analisis sensitivitas mekanisme yang sudah divalidasi, dilakukan pada tekanan 55 bar dan rasio ekuivalensi 1. Rentang suhu yang digunakan adalah mulai dari suhu rendah (700 K), sedang (850 K), dan tinggi (1.000 K).

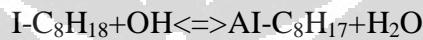
5.1. ANALISIS SENSITIVITAS PADA TEMPERATUR RENDAH

Dapat diambil suatu sudut pandang bahwa pada pembakaran bahan bakar gasolin pada temperatur rendah merupakan awal terjadinya sistem reaksi yang sangat kompleks. Tabel 5.1. memuat reaksi-reaksi yang mempunyai koefisien sensitivitas paling tinggi atau paling sensitif pada reaksi oksidasi dan pembakaran bahan bakar gasolin dengan temperatur awal rendah.

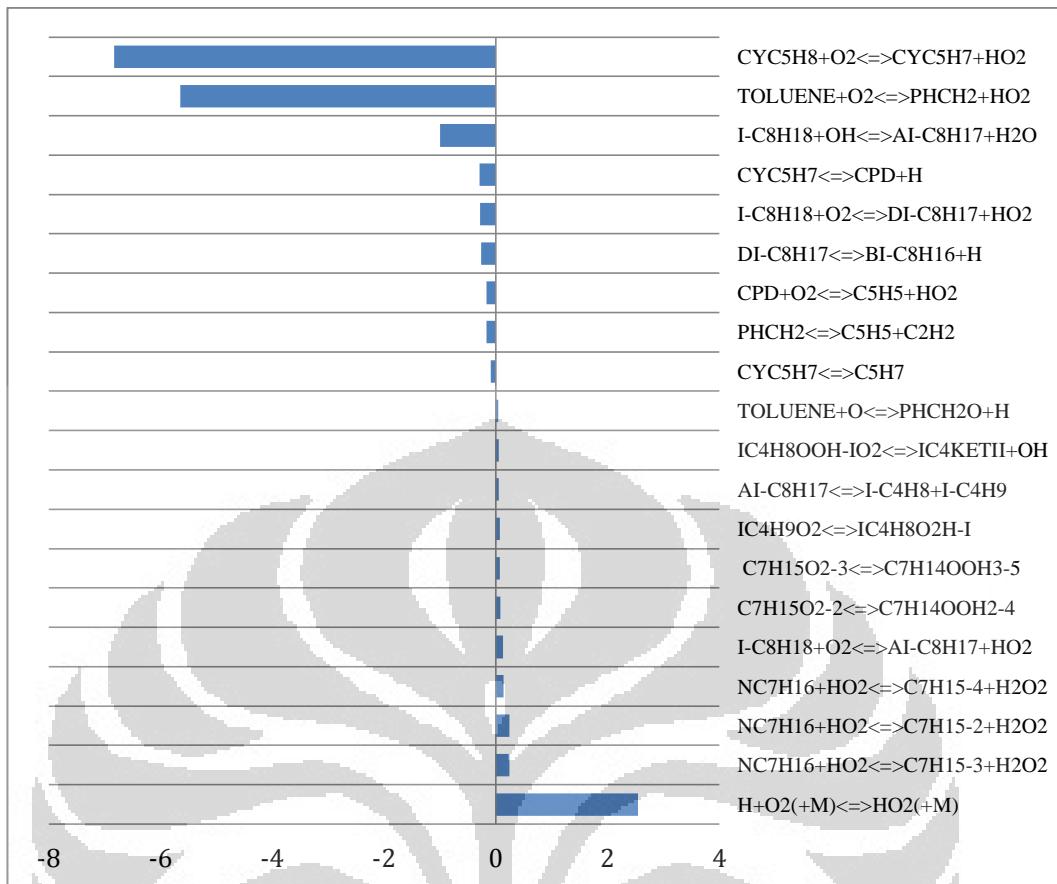
Tabel 5.1. Daftar reaksi yang paling sensitif beserta nilai koefisien sensitivitas pada suhu 700 K

Reaksi	Koefisien Sensitivitas
$H+O_2(+M) \rightleftharpoons HO_2(+M)$	2,546
$CYC_5H_8+O_2 \rightleftharpoons CYC_5H_7+HO_2$	-6,826
$TOLUENE+O_2 \rightleftharpoons PHCH_2+HO_2$	-5,648
$I-C_8H_{18}+OH \rightleftharpoons AI-C_8H_{17}+H_2O$	-0,997

Berdasarkan data pada Tabel 5.1., terlihat bahwa terjadi pembentukan radikal-radikal aktif HO₂ melalui abstraksi atom H pada 3 reaksi sensitif teratas. Radikal HO₂ ini akan memicu terjadinya reaksi konsumsi dan produksi secara berantai dalam proses oksidasi dan pembakaran bahan bakar gasolin. Untuk reaksi yang melibatkan senyawa oksigen, jalannya reaksi akan berlangsung secara lambat karena energi aktivasi oksigen yang tinggi (> 167 kJ/mol), selanjutnya radikal yang dihasilkan reaksi tersebut akan memulai reaksi rantai dan populasi radikal meningkat secara eksponensial dengan cepat akibat adanya pencabangan rantai setelah tahap propagasi (tahap di mana senyawa lain akan mengalami reaksi dengan HO₂ hasil reaksi). Tahapan selanjutnya adalah reaksi propagasi secara cepat yang didominasi oleh reaksi pengikatan radikal OH oleh reaktan iso-oktana.



Isooktana akan bereaksi dengan radikal yang ada sehingga terjadi abstraksi atom H dan terbentuk radikal alkil yang lebih kecil. Lalu radikal alkil yang lebih kecil ini akan terdekomposisi untuk membentuk radikal-radikal alkil yang lebih kecil lagi untuk memicu terjadinya reaksi-reaksi yang lebih kompleks dalam proses oksidasi dan pembakaran bahan bakar gasolin. Jadi pada temperatur rendah ini, kedua tipe reaksi tersebut (tahap inisiasi dan tahap propagasi cepat) merupakan reaksi yang paling sensitif untuk dapat mempercepat atau menaikkan laju reaksi secara keseluruhan apabila dilakukan perubahan terhadap parameter kinetik reaksi tersebut. Hal ini sangat berkaitan dengan proses validasi mekanisme reaksi dengan data eksperimen yang ada di mana prediksi parameter kinetik harus tepat supaya dihasilkan mekanisme reaksi yang benar. Reaksi yang paling sensitif sangat berpengaruh untuk memperlambat atau mempercepat laju reaksi keseluruhan agar diperoleh hasil yang sesuai dengan data eksperimen untuk validasi. Gambar 5.1. memperlihatkan reaksi-reaksi yang memiliki koefisien sensitivitas tertinggi dari semua reaksi yang terlibat pada reaksi pembakaran bahan bakar gasolin di temperatur rendah (700 K).



Gambar 5.1. Diagram batang analisis sensitivitas pada kondisi operasi temperatur awal 700 K, tekanan awal 55 bar dan rasio ekuivalensi 1

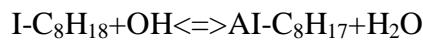
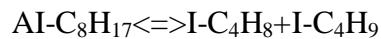
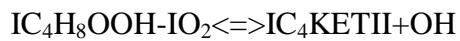
5.2. ANALISIS SENSITIVITAS PADA TEMPERATUR INTERMEDIET

Analisis sensitivitas pada temperatur intermediet dilakukan pada temperatur awal 850 K dengan campuran bahan bakar-udara yang stoikiometri dan tekanan awal 55 bar. Tabel 5.2. memuat reaksi-reaksi yang mempunyai koefisien sensitivitas paling tinggi atau paling sensitif pada reaksi oksidasi dan pembakaran bahan bakar gasolin dengan temperatur awal intermediet.

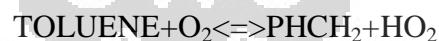
Tabel 5.2. Daftar reaksi yang paling sensitif beserta nilai koefisien sensitivitas pada suhu 850 K

Reaksi	Koefisien Sensitivitas
$\text{IC}_4\text{H}_8\text{OOH}-\text{IO}_2 \rightleftharpoons \text{IC}_4\text{KETII}+\text{OH}$	0,647
$\text{AI-C}_8\text{H}_{17} \rightleftharpoons \text{I-C}_4\text{H}_8+\text{I-C}_4\text{H}_9$	0,601
$\text{I-C}_8\text{H}_{18}+\text{OH} \rightleftharpoons \text{AI-C}_8\text{H}_{17}+\text{H}_2\text{O}$	-0,998
$\text{TOLUENE}+\text{O}_2 \rightleftharpoons \text{PHCH}_2+\text{HO}_2$	-1,096
$\text{CYC}_5\text{H}_8+\text{O}_2 \rightleftharpoons \text{CYC}_5\text{H}_7+\text{HO}_2$	-1,262

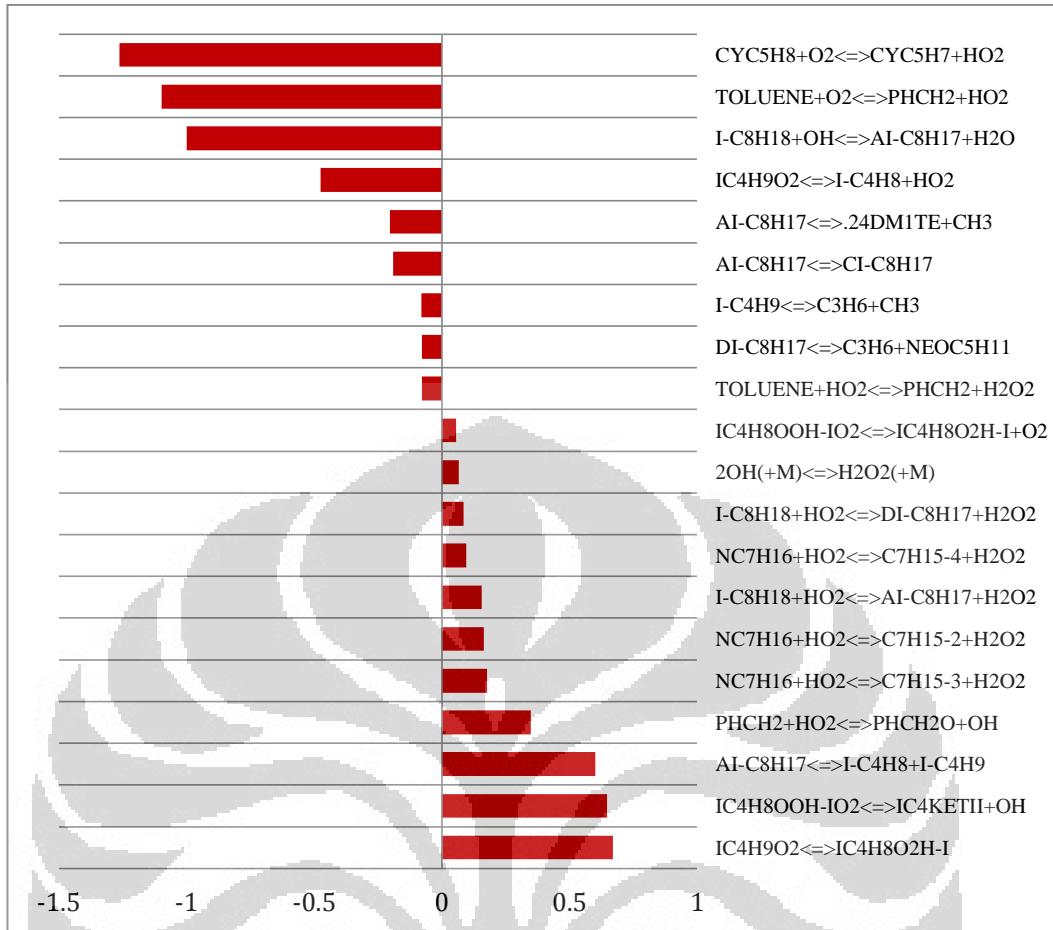
Dari daftar tipe-tipe reaksi yang sensitif pada temperatur intermediet di atas, yang paling menonjol adalah reaksi berikut:



Pada tiga reaksi ini, terjadi keterkaitan antara satu dengan yang lain , yaitu adanya pembentukan radikal OH yang kemudian akan segera dikonsumsi oleh komponen bahan bakar (iso-oktana), di mana hasilnya akan dengan cepat terdekomposisi secara unimolekular. Hal ini menandakan ketiga reaksi di atas mempunyai sensitifitas yang besar, terlihat dari nilai koefisien sensitifitasnya yang cukup signifikan. Jadi pada temperatur intermediet ini, tipe reaksi tersebut merupakan reaksi yang paling sensitif untuk dapat mempercepat atau menaikkan laju reaksi secara keseluruhan apabila dilakukan perubahan terhadap parameter kinetik reaksi tersebut. Dengan memperbesar atau memperkecil parameter kinetik reaksi ini maka akan berpengaruh terhadap laju reaksi secara keseluruhan agar hasil yang diperoleh dapat sesuai dengan data validasi. Sedangkan, reaksi dengan koefisien sensitivitas negatif yang paling besar masih didominasi oleh reaksi pembentukan radikal aktif HO₂, yaitu:



Jenis kedua reaksi ini diketahui sebagai reaksi yang *reversible*, berjalan lambat, serta memiliki energi aktivasi yang besar. Gambar 5.2. memperlihatkan reaksi-reaksi yang memiliki koefisien sensitivitas tertinggi dari semua reaksi yang terlibat pada pembakaran bahan bakar gasolin di temperatur intermediet (850 K).



Gambar 5.2. Diagram batang analisis sensitivitas pada kondisi operasi temperatur awal 850 K, tekanan awal 55 bar dan rasio ekuivalensi 1

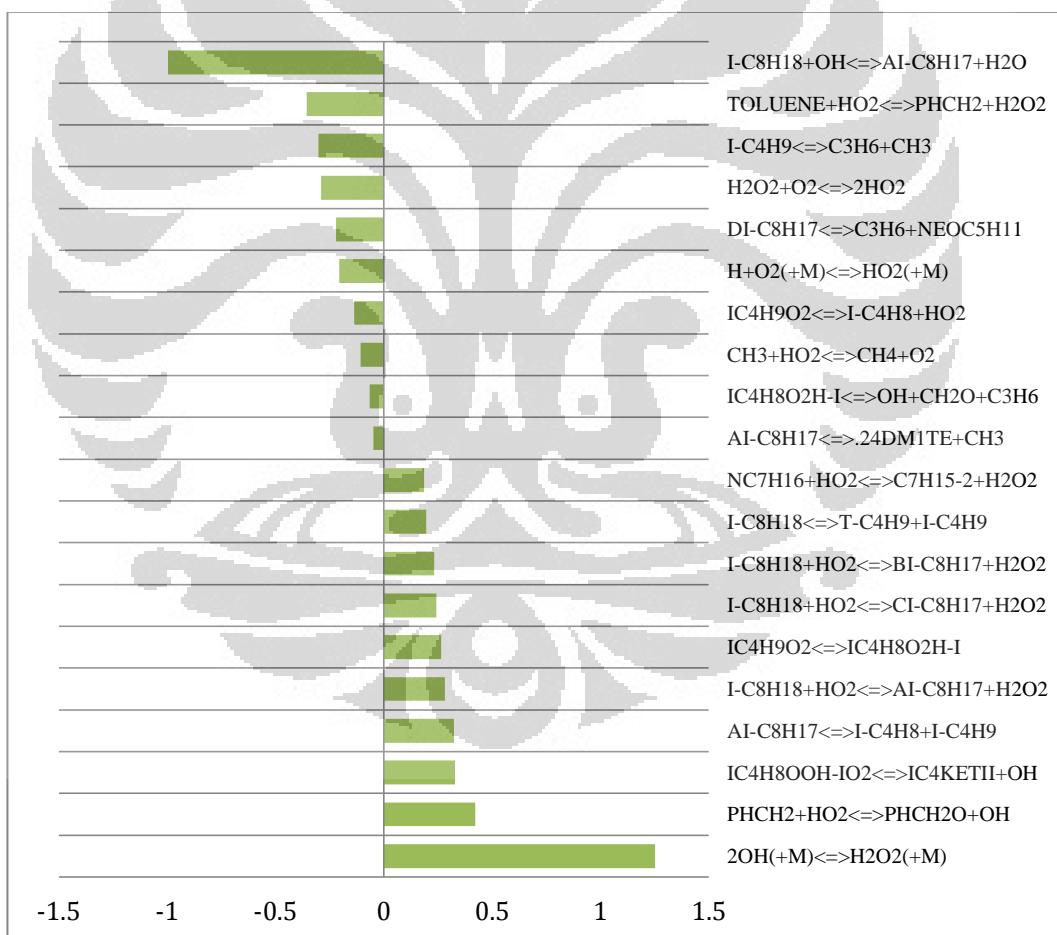
5.3. ANALISIS SENSITIVITAS PADA TEMPERATUR TINGGI

Analisis sensitivitas dilakukan pada temperatur awal 1.000 K pada campuran bahan bakar-udara yang stoikiometri dan tekanan awal 55 bar. Menurut Gambar 5.3 di bawah, jelas terlihat perbedaan yang sangat mencolok bila dibandingkan dengan hasil analisis sensitivitas pada temperatur awal 850 K (Gambar 5.1), yakni reaksi yang melibatkan *third body* menjadi jauh lebih sensitif. Reaksi-reaksi yang dianggap paling sensitif dimuat pada Tabel 5.3.

Tabel 5.3. Daftar reaksi yang paling sensitif beserta nilai koefisien sensitivitas pada suhu 1.000 K

Reaksi	Koefisien Sensitivitas
$2\text{OH}(\text{+M}) \rightleftharpoons \text{H}_2\text{O}_2(\text{+M})$	1,252
$\text{TOLUENE} + \text{HO}_2 \rightleftharpoons \text{PHCH}_2 + \text{H}_2\text{O}_2$	-0,355
$\text{I-C8H18} + \text{OH} \rightleftharpoons \text{AI-C8H17} + \text{H}_2\text{O}$	-0,996

Berdasarkan tipe reaksi pada tabel di atas, terjadi konsumsi radikal OH dan HO₂ oleh komponen bahan bakar yang cukup signifikan, terutama oleh senyawa toluena dan iso-oktana. Radikal aktif ini akan berkurang konsentrasi karena mengabstraksi atom H yang terdapat pada senyawa toluena dan iso-oktana. Dengan demikian ketiga reaksi di atas dapat dijadikan dasar bahwa pada rentang temperatur tinggi, dengan semakin meningkatnya temperatur, maka konsentrasi radikal OH dan HO₂ akan semakin aktif bereaksi dengan bahan bakar karena adanya reaksi pemutusan atom H, akibatnya bahan bakar akan semakin cepat mengalami ignisi. Di samping itu, keterlibatan *third body* juga mempengaruhi reaktivitas reaksi secara keseluruhan, karena perannya sebagai penyedia energi dalam pemutusan ikatan atom H.



Gambar 5.3. Diagram batang analisis sensitivitas pada kondisi operasi temperatur awal 1.000 K, tekanan awal 55 bar dan rasio ekuivalensi 1

BAB 6

SIMULASI WAKTU TUNDA IGNISI

Simulasi dilakukan setelah model kinetika reaksi yang digunakan untuk memvalidasi data eksperimen dinyatakan valid. Simulasi ini dilakukan pada berbagai variasi kondisi operasi yang meliputi variasi tekanan awal dan variasi rasio ekuivalensi. Tujuan dari dilakukannya simulasi ini adalah untuk mengetahui bagaimana perilaku dari reaksi oksidasi dan pembakaran bahan bakar gasolin tanpa harus mengujinya di laboratorium. Perilaku yang akan dipelajari adalah waktu tunda ignisi dari proses pembakaran tersebut. Proses simulasi dijalankan dengan program Chemkin 3.7.1. Pada tahap ini, ada beberapa variabel yang divariasikan di mana hasil simulasi yang diambil adalah waktu tunda ignisi (*ignition delay time*). Variabel yang divariasikan, antara lain :

- ✚ Variasi tekanan awal pada kondisi rasio ekuivalensi konstan
Untuk variasi tekanan awal, tekanan yang diambil adalah 5, 25, dan 55 bar
- ✚ Variasi rasio ekuivalensi pada kondisi tekanan awal konstan
Untuk variasi rasio ekuivalensi, kondisi yang diambil adalah rasio ekuivalensi 0,8 (*lean fuel*), 1 (stoikiometri), dan 1,5 (*rich fuel*)

Simulasi ini menggunakan tiga tipe campuran bahan bakar dengan oksigen, yaitu *lean fuel*, stoikiometri, dan *rich fuel*. Tabel 6.1. sampai Tabel 6.3. memperlihatkan komposisi bahan bakar gasolin (toluena, n-heptana, iso-oktana) untuk setiap campuran yang sudah dinormalisasi dan merupakan komposisi yang digunakan untuk menjalankan simulasi.

Tabel 6.1. Komposisi bahan bakar gasolin dalam campuran *lean fuel*

Komponen	Komposisi
Toluena	0,0027729
n-Heptana	0,0024282
iso-Oktana	0,0088029
O ₂	0,2021292
N ₂	0,7838668

Tabel 6.2. Komposisi bahan bakar gasolin dalam campuran stoikiometri

Komponen	Komposisi
Toluena	0,0034541
n-Heptana	0,0030246
iso-Oktana	0,0109653
O ₂	0,2014239
N ₂	0,7811319

Tabel 6.3. Komposisi bahan bakar gasolin dalam campuran *rich fuel*

Komponen	Komposisi
Toluena	0,0051364
n-Heptana	0,0044977
iso-Oktana	0,0163057
O ₂	0,1996823
N ₂	0,7743779

6.1. VARIASI RASIO EKUIVALENSI (TEKANAN AWAL KONSTAN)

Untuk mengetahui pengaruh bahan bakar gasolin terhadap oksigen (udara), maka dilakukan penelitian waktu tunda ignisi gasolin pada berbagai rasio ekuivalensi yang hasilnya seperti terlihat pada Gambar 6.1. - Gambar 6.3. yang memperlihatkan profil waktu tunda ignisi dengan variasi rasio ekuivalensi pada setiap variasi tekanan awal konstan, serta temperatur awal dari 700 K sampai 1.000 K. Pada penelitian ini digunakan tiga campuran agar ketiga jenis campuran bahan bakar pada saat operasi pembakaran dapat terwakili yaitu campuran dengan kondisi bahan bakar sedikit (*lean fuel*), campuran dengan kandungan bahan bakar yang sebanding dengan banyaknya oksigen (stoikiometri) dan yang terakhir yaitu kandungan bahan bakar yang dalam campurannya melebihi rasio kecukupan secara teoritis untuk jumlah keperluan oksigen (*rich fuel*). Tabel 6.4. sampai Tabel 6.6. memuat data simulasi pada tekanan awal konstan dan variasi rasio ekuivalensi.

Tabel 6.4. Data simulasi pada tekanan awal konstan 5 bar

Temperatur awal, K	Tekanan awal, bar	idt sim, RE=0,8	idt sim, RE=1	idt sim, RE=1,5
700	5	90,4	105	118
850	5	56	71	81,3
1.000	5	9,04	9,15	10,1

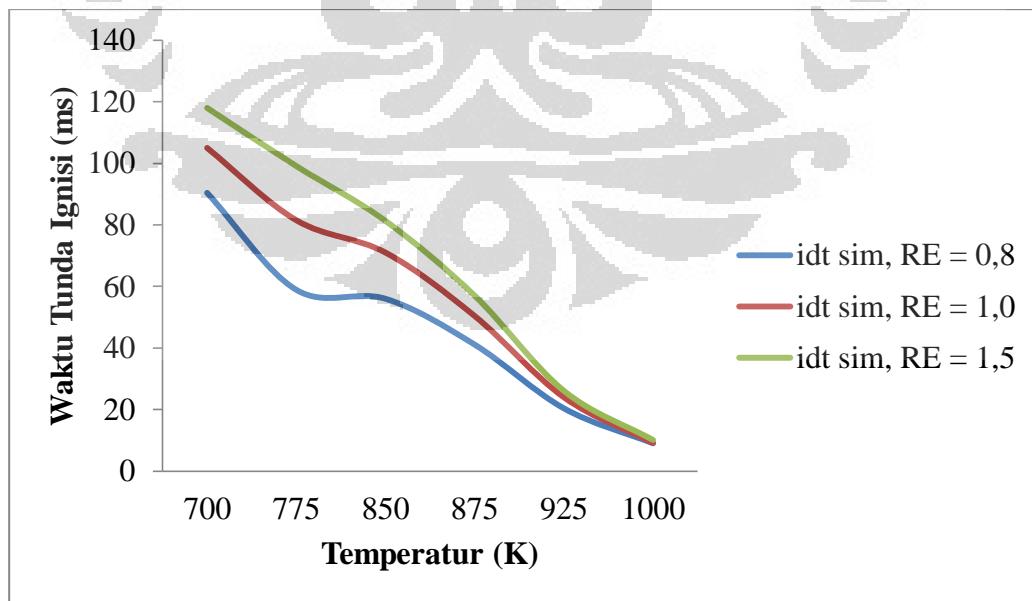
Tabel 6.5. Data simulasi pada tekanan awal konstan 25 bar

Temperatur awal, K	Tekanan awal, bar	idt sim, RE=0,8	idt sim, RE=1	idt sim, RE=1,5
700	25	52,2	56,2	59,5
850	25	4,16	5,18	6
1.000	25	1,13	1,24	1,29

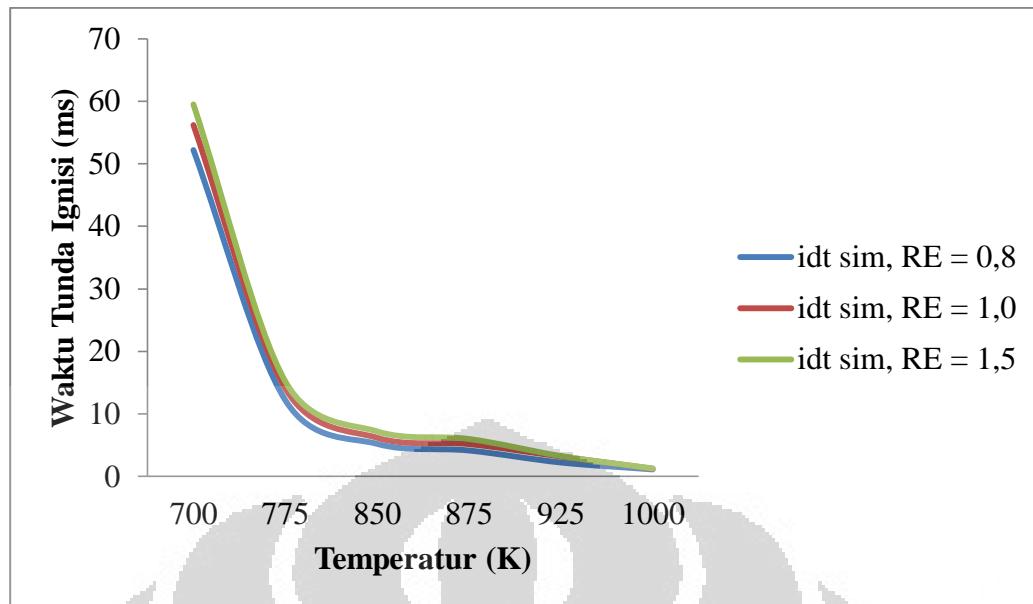
Tabel 6.6. Data simulasi pada tekanan awal konstan 55 bar

Temperatur awal, K	Tekanan awal, bar	idt sim, RE=0,8	idt sim, RE=1	idt sim, RE=1,5
700	55	50	54	56,3
850	55	1,52	1,85	2,08
1.000	55	0,406	0,506	0,584

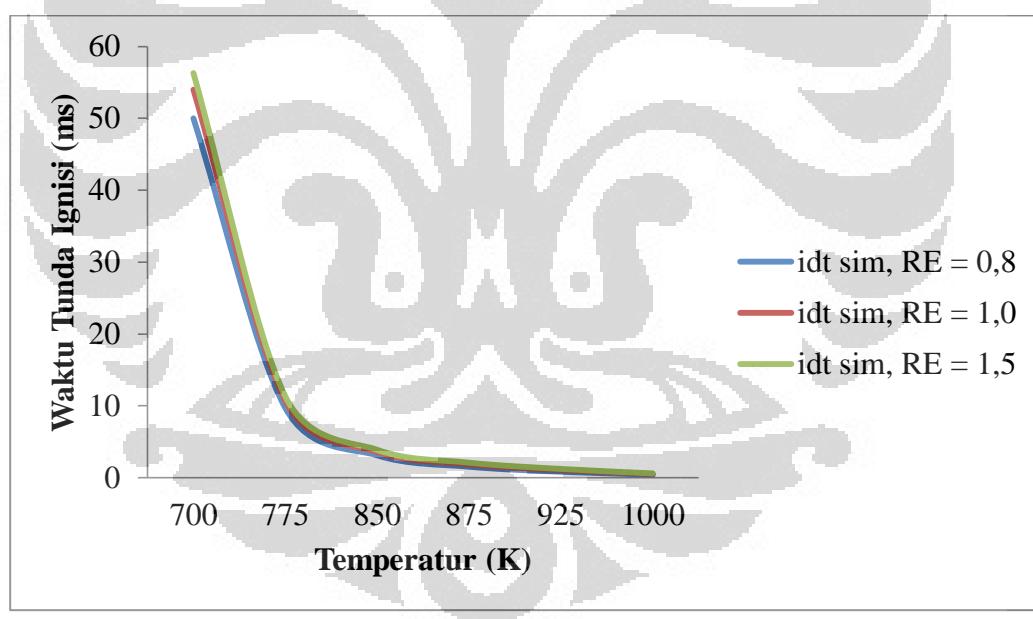
Berikut ini merupakan profil waktu tunda ignisi yang diperoleh dari simulasi pada tekanan konstan dan variasi rasio ekivalensi:



Gambar 6.1. Perbandingan *ignition delay time* pada kondisi tekanan awal = 5 bar untuk variasi rasio ekuivalensi (Φ) = 0,8; 1,0 dan 1,5



Gambar 6.2. Perbandingan *ignition delay time* pada kondisi tekanan awal = 25 bar untuk variasi rasio ekuivalensi (Φ) = 0,8; 1,0 dan 1,5



Gambar 6.3. Perbandingan *ignition delay time* pada kondisi tekanan awal = 55 bar untuk variasi rasio ekuivalensi (Φ) = 0,8; 1,0 dan 1,5

Berdasarkan profil waktu tunda ignisi yang telah dihasilkan di atas, dapat terlihat bahwa pada setiap nilai tekanan awal (5, 25 dan 55 bar) yang konstan dan setiap variasi rasio ekivalensi yang semakin kecil, waktu tunda ignisi terjadi semakin cepat. Secara umum, waktu tunda ignisi akan semakin cepat seiring

dengan naiknya temperatur, yang akan membantu proses inisiasi bahan bakar berjalan lebih cepat di mana populasi radikal OH yang paling sensitif dan radikal lainnya semakin cepat terbentuk dan populasinya yang semakin besar akan menyebabkan sistem semakin reaktif. Radikal-radikal tersebut kemudian akan mengkonsumsi bahan bakar secara berantai.

Selain faktor temperatur, pengaruh rasio ekuivalensi juga besar terhadap waktu tunda ignisi. Rasio ekuivalensi merupakan kondisi perbandingan antara bahan bakar dengan oksidator pada kondisi aktual terhadap bahan bakar dan oksidator pada kondisi stoikiometri. Oksigen merupakan oksidator utama untuk proses pembakaran. Reaksi bahan bakar dengan oksigen, walaupun berjalan lambat, tapi merupakan reaksi yang penting karena akan menghasilkan radikal-radikal bebas pengkonsumsi bahan bakar. Jika diamati dari data hasil simulasi, terlihat bahwa pada kondisi miskin bahan bakar (*lean fuel*), waktu tunda ignisi berjalan paling cepat. Hal ini disebabkan oksigen tersedia secara berlebih. Radikal-radikal pengkonsumsi bahan bakar pun terbentuk lebih cepat dan mengakibatkan reaksi pembakaran berjalan secara cepat (waktu tunda ignisi menjadi singkat). Berbeda ketika reaksi berjalan secara kaya bahan bakar. Pada kondisi ini, oksigen tersedia yang akan bereaksi dengan bahan bakar jauh lebih sedikit jumlahnya dibandingkan dengan yang diperlukan oleh bahan bakar. Akibatnya, radikal-radikal yang berperan untuk mengkonsumsi bahan bakar terbentuk sangat sedikit di awal reaksi pembakaran dan berdampak pada melambatnya laju reaksi pembakaran secara keseluruhan (waktu tunda ignisi menjadi lambat).

6.2. VARIASI TEKANAN AWAL (RASIO EKUIVALENSI KONSTAN)

Pada simulasi ini dilakukan variasi dari tekanan awal untuk mengetahui pengaruh tekanan awal terhadap proses oksidasi dan pembakaran bahan bakar gasolin. Hasil simulasi dapat terlihat pada Gambar 6.4. – Gambar 6.6. yang memperlihatkan profil waktu tunda ignisi dengan variasi tekanan awal pada setiap rasio ekuivalensi yang konstan, serta temperatur awal dari 700 K sampai 1.000 K. Pada penelitian ini digunakan tiga variasi kondisi tekanan awal, yaitu 5 bar (tekanan

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rendah), 25 bar (tekanan sedang) dan 55 bar (tekanan tinggi). Tabel 6.7. sampai Tabel 6.9. memuat data simulasi pada rasio ekuivalensi konstan dan variasi tekanan awal.

Tabel 6.7. Data simulasi pada rasio ekuivalensi = 0,8

Temperatur awal, K	Rasio Ekuivalensi	Tekanan awal 5 bar	Tekanan awal 25 bar	Tekanan awal 55 bar
700	0,8	90,4	52,2	50
850	0,8	56	4,16	1,52
1.000	0,8	9,04	1,13	0,406

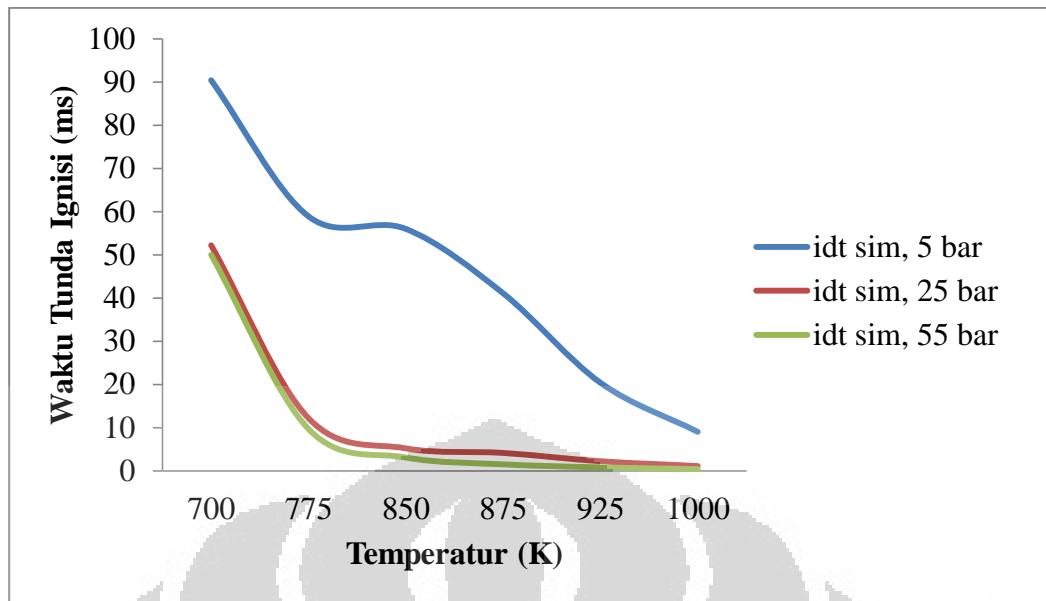
Tabel 6.8. Data simulasi pada rasio ekuivalensi = 1,0

Temperatur awal, K	Rasio Ekuivalensi	Tekanan awal 5 bar	Tekanan awal 25 bar	Tekanan awal 55 bar
700	1,0	105	56,2	54
850	1,0	71	5,18	1,85
1.000	1,0	9,15	1,24	0,506

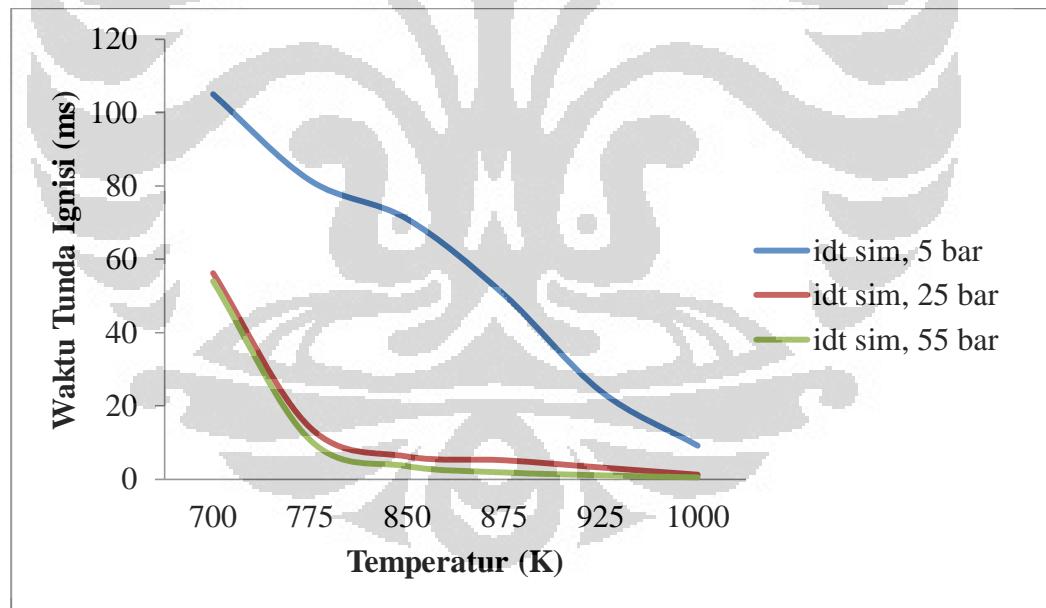
Tabel 6.9. Data simulasi pada rasio ekuivalensi = 1,5

Temperatur awal, K	Rasio Ekuivalensi	Tekanan awal 5 bar	Tekanan awal 25 bar	Tekanan awal 55 bar
700	1,5	118	59,5	56,3
850	1,5	81,3	6	2,08
1.000	1,5	10,1	1,29	0,584

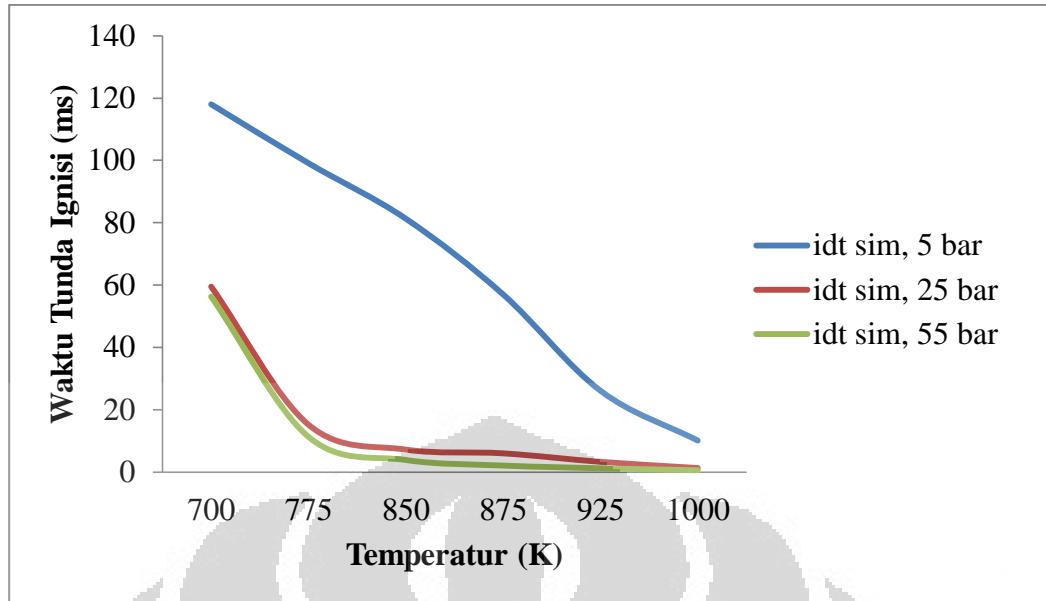
Berikut adalah profil waktu tunda ignisi yang diperoleh dari simulasi pada rasio ekuivalensi konstan dan variasi tekanan awal:



Gambar 6.4. Perbandingan *ignition delay times* pada kondisi rasio ekuivalensi ($\Phi = 0,8$) untuk variasi tekanan awal = 5, 25, dan 55 bar



Gambar 6.5. Perbandingan *ignition delay times* pada kondisi rasio ekuivalensi ($\Phi = 1,0$) untuk variasi tekanan awal = 5, 25, dan 55 bar



Gambar 6.6. Perbandingan *ignition delay times* pada kondisi rasio ekuivalensi ($\Phi = 1,5$) untuk variasi tekanan awal = 5, 25, dan 55 bar

Dari hasil simulasi di atas, untuk variasi rasio ekuivalensi mulai dari 0,8; 1; dan 1,5 terlihat bahwa bahan bakar yang dimasukkan dengan tekanan awal 5 bar akan memiliki waktu tunda ignisi yang lebih lambat. Berbeda ketika tekanan awal dinaikkan menjadi 25 bar, bahan bakar memiliki waktu tunda ignisi yang lebih cepat dibandingkan ketika dimasukkan dengan tekanan awal 5 bar. Fenomena ini terjadi pula di mana ketika tekanan awal dinaikkan lagi menjadi 55 bar, maka bahan bakar akan semakin cepat terignisi. Dengan demikian, semakin besar tekanan awal yang diberikan pada reaktan, maka reaksi yang terjadi akan semakin cepat. Peningkatan kecepatan reaksi dapat terlihat dari semakin pendeknya waktu tunda ignisi ketika tekanan awal dinaikkan. Kejadian ini dipengaruhi oleh dua faktor yaitu kenaikan temperatur dan keterlibatan spesi M atau biasa disebut sebagai *third body*.

Ketika tekanan awal semakin tinggi maka secara bersamaan temperatur akan semakin tinggi pula dan waktu tunda ignisi akan semakin cepat. Hal tersebut dapat dijelaskan melalui persamaan Arrhenius yang dimodifikasi di bawah ini:

$$k = AT^n \exp\left[-\frac{E_a}{RT}\right]$$

Semakin tinggi temperatur (T) akan meningkatkan energi kinetik dari molekul-molekul senyawa yang terlibat dalam reaksi. Kenaikan energi kinetik tersebut akan meningkatkan jumlah tumbukan antar molekul yang terjadi selama reaksi (A), yang akan memperbesar energi melebihi energi aktivasi sehingga reaksi dapat terjadi lebih cepat. Jadi, semakin tinggi temperatur (T) akan meningkatkan jumlah tumbukan antar molekul (A) sehingga reaksi dapat terjadi lebih cepat dimana hal ini diperlihatkan dengan nilai waktu tunda ignisi yang semakin singkat.

Selain itu, reaksi-reaksi yang melibatkan komponen *third body* (M) juga berpengaruh dalam menurunkan waktu tunda ignisi ketika tekanan dinaikkan, terutama pada reaksi yang berlangsung secara unimolekular. *Third body* ini sendiri merupakan spesi selain reaktan, yang membawa energi pada molekul saat terjadi pada proses dekomposisi unimolekular. Pada kondisi awal, ketika sistem diberikan tekanan dengan nilai tertentu, maka besarnya tekanan awal yang diterima oleh *third body* itu sama dengan tekanan awal yang diterima oleh sistem tersebut. Tekanan awal merupakan suatu bentuk energi yang akan dipindahkan pada reaktan. Dengan demikian, saat reaktan bertemu dengan *third body*, maka akan terjadi suatu perpindahan energi dari *third body* ke reaktan. Energi yang diterima akan meningkatkan gerakan molekul. Tumbukan antar molekul pun akan semakin sering seiring dengan meningkatnya tekanan di dalam sistem. Tumbukan ini pula yang menyebabkan reaktan terdekomposisi secara unimolekular ketika energi yang diterima cukup untuk memutuskan ikatan kimia dari molekul itu sendiri. Dekomposisi unimolekular ini biasa terjadi di awal tahapan reaksi berantai. Selain itu, dekomposisi unimolekular pada umumnya menghasilkan radikal-radikal yang aktif mengkonsumsi bahan bakar. Semakin cepat radikal-radikal pengkonsumsi bahan bakar ini terbentuk, maka semakin cepat pula reaksi berlangsung. Dan salah satu cara untuk mempercepat reaksi berantai tersebut adalah dengan menaikkan tekanan awal.

BAB 7

KESIMPULAN

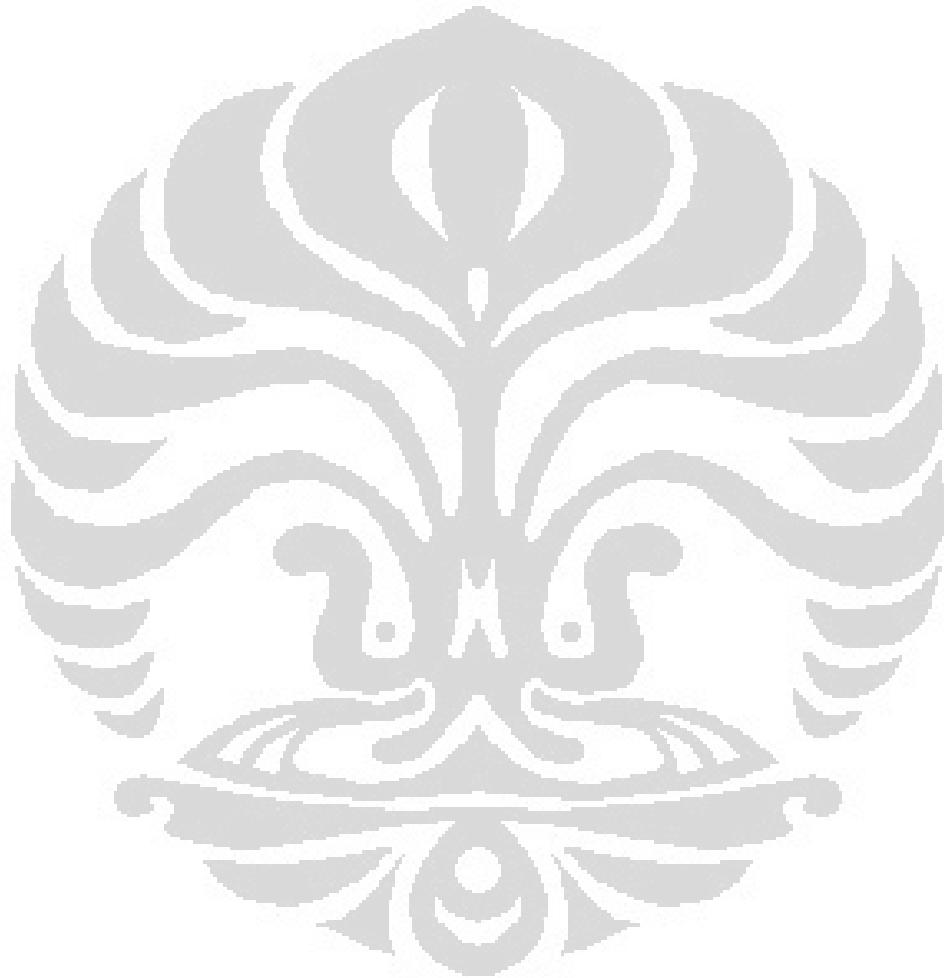
Berdasarkan pembahasan pada bab-bab sebelumnya, maka dapat diambil kesimpulan sebagai berikut:

1. Model kinetika reaksi oksidasi bahan bakar gasolin multikomponen yang sudah ditambahkan model kinetika reaksi detail n-heptana menunjukkan kesesuaian yang baik dengan data eksperimen saat disimulasikan pada rentang kondisi operasi yang sama.
2. Analisis sensitivitas yang dilakukan menunjukkan bahwa reaksi yang paling sensitif dalam reaksi oksidasi dan pembakaran bahan bakar yaitu :
 - a. Pada temperatur rendah (700^0K), reaksi yang memiliki koefisien sensitivitas paling positif adalah reaksi $\text{H} + \text{O}_2 (+\text{M}) \leftrightarrow \text{HO}_2 (+\text{M})$, dan reaksi yang memberikan sensitivitas paling negatif adalah $\text{CYC}_5\text{H}_8 + \text{O}_2 \leftrightarrow \text{CYC}_5\text{H}_7 + \text{HO}_2$.
 - b. Pada temperatur intermediate (850^0K), reaksi yang paling memiliki koefisien sensitivitas paling positif adalah reaksi $\text{IC4H9O2} \leftrightarrow \text{IC4H8O2H-I}$, dan reaksi yang memberikan sensitivitas paling negatif adalah $\text{TOLUENE} + \text{O}_2 \leftrightarrow \text{PHCH}_2 + \text{HO}_2$ dan $\text{CYC}_5\text{H}_8 + \text{O}_2 \leftrightarrow \text{CYC}_5\text{H}_7 + \text{HO}_2$.
 - c. Pada temperatur tinggi (1.000^0K), reaksi yang paling memiliki koefisien sensitivitas paling positif adalah reaksi $2\text{OH} (+\text{M}) \leftrightarrow \text{H}_2\text{O}_2 (+\text{M})$, serta reaksi yang memiliki koefisien sensitivitas paling negatif adalah reaksi $\text{I-C}_8\text{H}_{18} + \text{OH} \leftrightarrow \text{AI-C}_8\text{H}_{17} + \text{H}_2\text{O}$
3. Hasil simulasi waktu tunda ignisi pada variasi rasio ekuivalensi menunjukkan bahwa campuran bahan bakar *lean fuel* ($\Phi = 0,8$) akan memiliki waktu tunda ignisi yang paling cepat apabila dibandingkan dengan campuran bahan bakar stokimetri ($\Phi = 1,0$), dan *rich fuel* ($\Phi = 1,5$).
4. Hasil simulasi waktu tunda ignisi pada bahan bakar gasolin menunjukkan bahwa semakin tinggi tekanan dan temperatur awal proses pembakaran, maka

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waktu tunda ignisi proses oksidasi dan pembakaran bahan bakar gasolin akan semakin cepat pula.

5. Waktu tunda ignisi paling cepat terjadi pada tekanan 55 bar, temperatur 1.000^0K , dan campuran bahan bakar *lean fuel* ($\Phi = 0,8$) yaitu 0,406 milisekon.
6. Waktu tunda ignisi paling lambat terjadi pada tekanan 5 bar, temperatur 700^0K , dan campuran bahan bakar *rich fuel* ($\Phi = 1,5$) yaitu 118 milisekon.



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LAMPIRAN

Lampiran 1: Inputan aurora

a) Inputan Aurora pada Rasio Ekuivalensi *Lean Fuel*

```
TRAN
ENRG
QLOS 0.0
PRES 54.28
TEMP 1000
REAC NC7H16      0.0024282
REAC I-C8H18     0.0088029
REAC TOLUENE    0.0027729
REAC O2          0.2021292
REAC N2          0.7838668
TIME 1
DELT 1.E-3
DTSV 1.E-3
END
```

b) Inputan Aurora pada Rasio Ekuivalensi *Stokimetri*

```
TRAN
ENRG
QLOS 0.0
PRES 54.28
TEMP 1000
REAC NC7H16      0.0030246
REAC I-C8H18     0.0109653
REAC TOLUENE    0.0034541
REAC O2          0.2014239
REAC N2          0.7811319
TIME 1
DELT 1.E-3
DTSV 1.E-3
END
```

Lampiran 1: Inputan aurora (lanjutan)

c) Inputan Aurora pada Rasio Ekuivalensi *Rich Fuel*

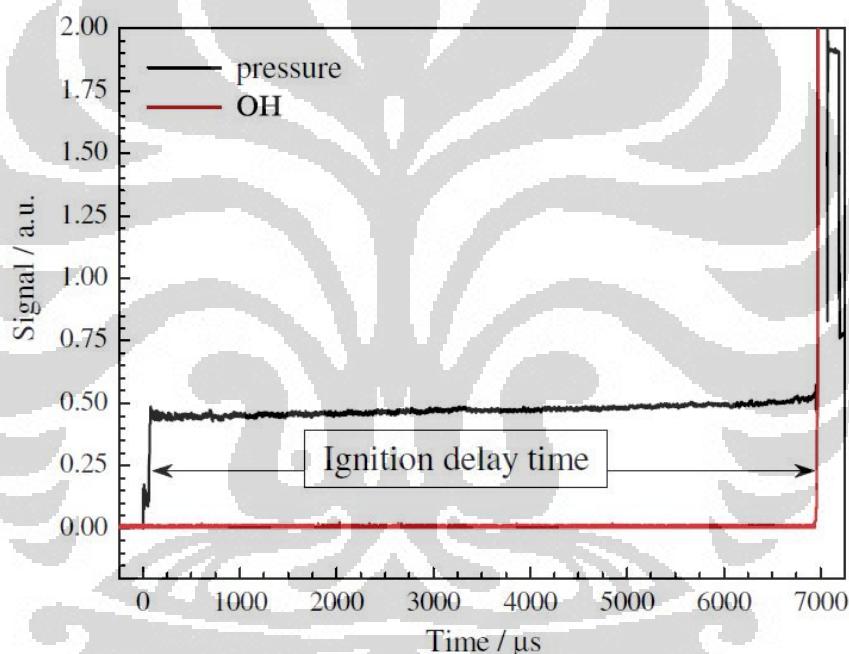
TRAN
ENRG
QLOS 0.0
PRES 54.28
TEMP 1000
REAC NC7H16 0.0044977
REAC I-C8H18 0.0163057
REAC TOLUENE 0.0051364
REAC O2 0.1996823
REAC N2 0.7743779
TIME 10
DELT 1.E-2
DTSV 1.E-2
END

Lampiran 2 : Rangkuman hasil simulasi

Rasio Ekuivalensi	Tekanan Awal (bar)	Temperatur Awal (K)	Waktu Tunda Ignisi (milidetik)	Temperatur Nyala Adiabatik (K)
0,8 <i>(lean fuel)</i>	5	700	90,4	1.100
		850	56	1.250
		1.000	9,04	1.400
	25	700	52,2	1.100
		850	4,16	1.250
		1.000	1,13	1.400
	55	700	50	1.100
		850	1,52	1.250
		1.000	0,406	1.400
1,0 <i>(stokimetri)</i>	5	700	105	1.100
		850	71	1.250
		1.000	9,15	1.400
	25	700	56,2	1.100
		850	5,18	1.250
		1.000	1,24	1.400
	55	700	54	1.100
		850	1,85	1.250
		1.000	0,506	1.400
1,5 <i>(rich fuel)</i>	5	700	118	1.100
		850	81,3	1.250
		1.000	10,1	1.400
	25	700	59,5	1.100
		850	6	1.250
		1.000	1,29	1.400
	55	700	56,3	1.100
		850	2,08	1.250
		1.000	0,584	1.400

Lampiran 3 : Penentuan waktu tunda ignisi eksperimen

Eksperimen dilakukan pada alat *shock tube* bertekanan tinggi, di mana kecepatan *shock* diukur antar dua interval menggunakan tiga *piezo-electric pressure gauges*. Data tekanan kemudian direkam dengan skala waktu $0,1 \mu\text{s}$. Eksperimen dilakukan dengan udara sintesis (kandungan N_2 dan O_2 masing-masing sebesar 79,5% dan 20,5%). Waktu tunda ignisi eksperimen ditentukan dari pengukuran emisi OH pada panjang gelombang 431,5 nm. Ekstrapolasi dilakukan pada titik di mana terjadi kenaikan jejak signal OH paling dratis, seperti yang ditunjukkan oleh Gambar 1.



Gambar 1. Penentuan waktu tunda ignisi berdasarkan jejak signal OH

Lampiran 4 : Reaksi-reaksi pada model kinetika reaksi oksidasi dan pembakaran bahan bakar gasolin multikomponen

REACTIONS CONSIDERED	(k = A T ^b *b exp(-E/RT))	A	b	E	Reverse Arrhenius coefficients:	A	b	E
1. IC4H8OOH-IO2<=>IC4KETII+OH	5.00E+10 0.0 21340.0				73. AI-C8H17+HO2-A-C8H17O+OH	1.86E-10 0.6 26190.0		
Reverse Arrhenius coefficients:	1.99E+03 1.5 44420.0				Reverse Arrhenius coefficients:	7.00E+12 0.0 -1000.0		
2. CYCSH8+O2-CYCSH7+HO2	1.28E+10 0.0 25002.4				Reverse Arrhenius coefficients:	1.39E+16 -0.7 26700.0		
3. OH+OH(+M)-H2O2(+M)	5.62E+18 -0.4 0.0				Reverse Arrhenius coefficients:	7.00E+12 0.0 -1000.0		
Low pressure limit: 0.30410E+31 -0.46300E+01 0.20490E+04					75. I-C8H18=BI-C8H17+H	1.36E+18 -1.3 31470.0		
TROE centering: 0.47000E+00 0.10000E+03 0.20000E+04 0.10000E+16					76. BI-C8H17=24DM2TE+CH3	1.82E+55 -11.6 119800.0		
H2 Enhanced by 2.500E+00					Reverse Arrhenius coefficients:	7.00E+12 0.0 -1000.0		
H2O Enhanced by 1.200E+01					77. BI-C8H17=44DM2TE+CH3	1.15E+17 -1.1 29840.0		
CO Enhanced by 1.900E+00					Reverse Arrhenius coefficients:	8.50E+10 0.0 12950.0		
CO2 Enhanced by 3.800E+00					78. BI-C8H17-AI-C8H16+H	1.14E+15 -0.7 26370.0		
4. C2H5OH(+M)=CH3+CH2OH(+M)	8.94E+28 -1.7 91163.0				Reverse Arrhenius coefficients:	1.10E+11 0.0 8275.0		
Low pressure limit: 0.28800E+86 -0.18900E+02 0.10991E+06					79. I-C8H18=CI-C8H17+H	6.41E+15 -0.8 37060.0		
TROE centering: 0.50000E+00 0.20000E+03 0.89000E+03 0.46000E+04					80. BI-C8H17+02-BI-C8H16+HO2	1.00E+13 0.0 2500.0		
H2O Enhanced by 5.000E+00					Reverse Arrhenius coefficients:	3.56E+54 -11.4 115800.0		
H2 Enhanced by 2.000E+00					Reverse Arrhenius coefficients:	1.50E-19 0.0 4000.0		
CO2 Enhanced by 3.000E+00					Reverse Arrhenius coefficients:	2.00E-19 0.0 17500.0		
CO Enhanced by 2.000E+00					81. BI-C8H17+A-C8O2-B-C8H17O+A-C8H17O	9.00E+12 0.0 -1000.0		
5. C2H5OH(+M)=C2H5+OH(+M)	1.25E+23 -1.5 96005.0				Reverse Arrhenius coefficients:	9.04E+15 -0.8 31350.0		
Low pressure limit: 0.32520E+86 -0.18810E+02 0.11493E+06					82. BI-C8H17-B-C8O2-B-C8H17O+B-C8H17O	7.00E+12 0.0 -1000.0		
TROE centering: 0.50000E+00 0.30000E+03 0.90000E+03 0.50000E+04					Reverse Arrhenius coefficients:	6.96E+15 -0.8 30220.0		
H2 Enhanced by 2.000E+00					83. BI-C8H17-C-C8O2-B-C8H17O+C-C8H17O	7.00E+12 0.0 -1000.0		
CO2 Enhanced by 3.000E+00					Reverse Arrhenius coefficients:	6.07E+15 -0.8 32160.0		
CO Enhanced by 2.000E+00					84. BI-C8H17-D-C8O2-B-C8H17O+D-C8H17O	7.00E+12 0.0 -1000.0		
6. C2H5OH(+M)=C2H4+H2O(+M)	2.79E+13 0.1 66136.0				Reverse Arrhenius coefficients:	4.54E+15 -0.8 31350.0		
Low pressure limit: 0.25700E+84 -0.18850E+02 0.86452E+05					85. BI-C8H17-H2O2-B-C8H17O+OH	7.00E+12 0.0 -1000.0		
TROE centering: 0.70000E+00 0.35000E+03 0.80000E+03 0.38000E+04					Reverse Arrhenius coefficients:	1.94E+18 -1.4 28690.0		
H2O Enhanced by 5.000E+00					86. BI-C8H17+CH3O2-B-C8H17O+CH3O	7.00E+12 0.0 -1000.0		
H2 Enhanced by 2.000E+00					Reverse Arrhenius coefficients:	1.90E+20 -1.9 33450.0		
CO2 Enhanced by 3.000E+00					87. I-C8H18=DI-C8H17+H	3.76E+54 -11.4 121700.0		
CO Enhanced by 2.000E+00					88. DI-C8H17+44DMITE+CH3	8.18E+15 -0.9 28450.0		
7. C2H5OH(+M)=CH3CHO+H2(+M)	7.24E+11 0.1 91007.0				Reverse Arrhenius coefficients:	1.00E+11 0.0 10200.0		
Low pressure limit: 0.44600E+88 -0.19420E+02 0.11559E+06					89. DI-C8H17=CH3H6+NEOC5H11	2.62E+19 -1.8 32110.0		
TROE centering: 0.90000E+00 0.90000E+03 0.11000E+04 0.35000E+04					Reverse Arrhenius coefficients:	5.00E+10 0.0 13100.0		
H2O Enhanced by 5.000E+00					90. DI-C8H17-BI-C8H16+H	5.16E+16 -0.9 34910.0		
8. C2H5OH-CH3+CH2OH	3.10E+15 0.0 80538.8				Reverse Arrhenius coefficients:	1.00E+13 0.0 2500.0		
9. C2H5OH-C2H5+OH	5.00E+16 0.0 91143.6				91. DI-C8H17+02-BI-C8H16+HO2	1.50E-19 0.0 4000.0		
10. C2H5OH-C2H4+H2O	1.00E+14 0.0 76645.6				Reverse Arrhenius coefficients:	2.00E-19 0.0 17500.0		
11. C2H5OH-OH-S-C2H4OH+H2O	5.25E+05 2.0 453.8				92. I-C8H18=A3-C7H15+CH3	7.51E+49 -9.4 96330.0		
12. C2H5OH-OH-S-C2H4OH+H2O	3.64E+10 0.1 0.0				93. DI-C8H17+A-C8O2-D-C8H17O+A-C8H17O	7.00E+12 0.0 -1000.0		
13. C2H5OH-OH-C2H5+H2O	1.15E+06 2.0 907.6				Reverse Arrhenius coefficients:	3.25E+13 -0.2 28560.0		
14. C2H5OH-OH-C2H5+H2O	7.46E+10 0.2 1634.0				94. DI-C8H17+B-C8O2-D-C8H17O+B-C8H17O	7.00E+12 0.0 -1000.0		
15. C2H5OH-OH-P-C2H4OH+H2O	2.13E+05 2.0 597.1				Reverse Arrhenius coefficients:	2.50E+13 -0.1 27430.0		
16. C2H5OH-OH-P-C2H4OH+H2O	1.74E+10 0.3 600.0				95. DL-C8H17+C-C8O2-D-C8H17O+C-C8H17O	7.00E+12 0.0 -1000.0		
17. C2H5OH-O-S-C2H4OH+OH	7.94E+12 0.0 3248.3				Reverse Arrhenius coefficients:	2.18E+13 -0.2 29370.0		
18. C2H5OH-O-S-C2H4OH+OH	1.88E+07 1.9 1824.0				96. DJ-C8H17-D-C8O2-B-C8H17O+D-C8H17O	7.00E+12 0.0 -1000.0		
19. C2H5OH-O-C2H5+OH	4.79E+13 0.0 6854.9				Reverse Arrhenius coefficients:	1.63E+13 -0.2 28560.0		
20. C2H5OH-O-C2H5+OH	1.58E+06 2.0 4448.0				97. DI-C8H17+HO2-D-C8H17O+OH	7.00E+12 0.0 -1000.0		
21. C2H5OH-O-P-C2H4OH+OH	1.00E+14 0.0 7475.9				Reverse Arrhenius coefficients:	6.98E+15 -0.7 25900.0		
22. C2H5OH-O-P-C2H4OH+OH	9.41E+07 1.7 5459.0				98. DL-C8H17+CH3O2-B-C8H17O+CH3O	7.00E+12 0.0 -1000.0		
23. C2H5OH-H-S-C2H4OH+H2	9.40E+10 0.0 4562.0				Reverse Arrhenius coefficients:	6.82E+17 -1.3 30670.0		
24. C2H5OH-H-S-C2H4OH+H2	2.58E+06 1.6 2827.0				99. BI-C8H16+H-A1C8H15+H2	3.70E+13 0.0 3900.0		
25. C2H5OH-H-C2H5+H2O	5.90E+11 0.0 3439.4				Reverse Arrhenius coefficients:	3.48E+14 -0.4 21050.0		
26. C2H5OH-H-P-C2H4OH+H2	1.23E+05 1.8 5098.0				100. I-C8H18-B2-C7H15+CH3	1.18E+50 -9.8 98640.0		
27. C2H5OH-H-C2H5+H2O	1.50E+06 1.6 3038.0				101. BI-C8H16+OH-A1C8H15+H2O	3.70E+13 0.0 3900.0		
28. C2H5OH-H-O2-S-C2H4OH+H2O2	9.30E+11 0.0 19370.4				Reverse Arrhenius coefficients:	1.51E+15 -0.4 36210.0		
29. C2H5OH-H-O2-S-C2H4OH+H2O2	8.20E+05 2.5 10750.0				102. I-C8H18-T-C4H9+L-C4H9	1.94E+57 -11.8 98980.0		
30. C2H5OH-H-O2-P-C2H4OH+H2O2	1.23E+04 2.5 15750.0				103. BI-C8H16+CH3-A4C8H15+CH4	2.00E+12 0.4 7300.0		
31. C2H5OH-H-O2-C2H5+H2O2	2.50E+12 0.0 24000.0				Reverse Arrhenius coefficients:	4.92E+14 -0.4 24930.0		
32. C2H5OH-CHO-C2H5+CH2O	6.50E+09 0.0 13662.0				104. I-C8H18-NEOC5H11+L-C3H7	5.75E+49 -9.7 98040.0		
33. C2H5OH-CH3-S-C2H4OH+CH4	2.04E+11 0.0 8694.0				Reverse Arrhenius coefficients:	1.00E+11 0.0 -4000.0		
34. C2H5OH-CH3-S-C2H4OH+CH4	7.28E+02 3.0 7948.0				105. BI-C8H16+O-C2H20+PC7H15	0.00E+00 0.0 0.0		
35. C2H5OH-CH3-P-C2H4OH+CH4	2.04E+11 0.0 8694.0				Reverse Arrhenius coefficients:	0.00E+00 0.0 -1050.0		
36. C2H5OH-CH3-P-C2H4OH+CH4	2.19E+02 3.2 9622.0				Reverse Arrhenius coefficients:	0.00E+00 0.0 0.0		
37. C2H5OH-CH3-C2H5+CH4	7.49E+10 0.0 9386.6				107. I-C8H18-A1-C8H17+H2	7.34E+05 2.8 8147.0		
38. C2H5OH-CH3-C2H5+CH4	1.45E+02 3.0 7649.0				108. I-C8H18-B1-C8H17+H2	5.74E-05 2.5 4124.0		
39. C2H5OH-CH30-S-C2H4OH+CH3OH	2.00E+11 0.0 6998.4				109. I-C8H18-H-C1-C8H17+H2	5.42E-05 2.4 2583.0		
40. C2H5OH-CH20-C2H5O-C2H4OH	1.53E+12 0.0 79583.4				110. CI-C8H17-C4H9+T-C4H9+T-C4H9	3.41E+22 -2.7 32360.0		
41. C2H5OH-C2H5O-C2H5OH-C2H4OH	2.00E+11 0.0 6998.2				Reverse Arrhenius coefficients:	5.00E+10 0.4 12600.0		
42. I-C5H12+AC5H11O3=>A-C5H11+CSH1103H	1.20E+13 0.0 20000.0				111. CI-C8H17=AI-C8H16+H	1.84E+15 -0.5 40360.0		
43. I-C5H12+AC5H11O3=>C-C5H11+CSH1103H	1.50E+12 0.0 15111.5				Reverse Arrhenius coefficients:	1.00E+13 0.0 2500.0		
44. I-C5H12+AC5H11O3=>C-C5H11+CSH1103H	3.00E+12 0.0 17500.0				112. CI-C8H17-CI-C8H16+H	8.64E+14 -0.4 39900.0		
45. I-C5H12+AC5H11O3=>D-C5H11+CSH1103H	6.00E+12 0.0 20000.0				Reverse Arrhenius coefficients:	1.00E+13 0.0 2500.0		
46. I-C5H12+BC5H11O3=>A-C5H11+CSH1103H	1.20E+13 0.0 20000.0				113. AI-C8H16+B3-C3C8H15+H2	3.70E+13 0.0 3900.0		
47. I-C5H12+BC5H11O3=>B-C5H11+CSH1103H	1.50E+12 0.0 15111.5				Reverse Arrhenius coefficients:	3.48E+14 -0.4 21050.0		
48. I-C5H12+BC5H11O3=>C-C5H11+CSH1103H	3.00E+12 0.0 17500.0				114. AI-C8H16+O-B3-C3C8H15+OH	3.70E+13 0.0 3900.0		
49. I-C5H12+BC5H11O3=>D-C5H11+CSH1103H	6.00E+12 0.0 20000.0				Reverse Arrhenius coefficients:	1.53E+14 -0.4 18960.0		
50. C5H12+AC5H11O3=>1-C5H11+CSH1103H	1.20E+13 0.0 20000.0				115. AI-C8H16+OH-B3-C3C8H15+H2O	3.70E+13 0.0 3900.0		
51. C5H12+AC5H11O3=>2-C5H11+CSH1103H	6.00E+12 0.0 17500.0				Reverse Arrhenius coefficients:	1.51E+15 -0.4 36210.0		
52. C5H12+AC5H11O3=>3-C5H11+CSH1103H	3.00E+12 0.0 17500.0				116. AI-C8H16+CH3-B3-C3C8H15+CH4	2.00E+12 0.4 7300.0		
53. C5H12+BC5H11O3=>1-C5H11+CSH1103H	1.20E+13 0.0 20000.0				Reverse Arrhenius coefficients:	4.92E+14 -0.4 24930.0		
54. C5H12+BC5H11O3=>2-C5H11+CSH1103H	6.00E+12 0.0 17500.0				117. AI-C8H16+OH-C2H20+PC7H15	1.00E+11 0.0 -4000.0		
55. C5H12+BC5H11O3=>3-C5H11+CSH1103H	3.00E+12 0.0 17500.0				Reverse Arrhenius coefficients:	0.00E+00 0.0 0.0		
56. I-C8H18+AC5H11O3=>AI-C8H17+CSH1103H	1.80E+13 0.0 20000.0				118. AI-C8H16+O-C2H20+PC7H14	1.00E+11 0.0 -1050.0		
57. I-C8H18+AC5H11O3=>BI-C8H17+CSH1103H	3.00E+12 0.0 17500.0				Reverse Arrhenius coefficients:	0.00E+00 0.0 0.0		
58. I-C8H18+AC5H11O3=>C-C8H17+CSH1103H	1.50E+12 0.0 15111.5				119. CI-C8H17+O2-AI-C8H16+H2O	3.00E-19 0.0 5000.0		
59. I-C8H18+AC5H11O3=>DI-C8H17+CSH1103H	1.20E+13 0.0 20000.0				Reverse Arrhenius coefficients:	2.00E-19 0.0 17500.0		
60. I-C8H18+BC5H11O3=>AI-C8H17+CSH1103H	1.80E+13 0.0 20000.0				120. I-C8H18+H-DI-C8H17+H2	1.88E-05 2.8 6280.0		
61. I-C8H18+BC5H11O3=>BI-C8H17+CSH1103H	3.00E+12 0.0 17500.0				Reverse Arrhenius coefficients:	7.00E+12 0.0 -1000.0		
62. I-C8H18+BC5H11O3=>C-C8H17+CSH1103H	1.50E+12 0.0 15111.5				Reverse Arrhenius coefficients:	1.46E+17 -1.1 30460.0		
63. I-C8H18+BC5H11O3=>D-C8H17+CSH1103H	1.20E+13 0.0 20000.0				122. CI-C8H17+B-C8O2-C8H17O+B-C8H17O	7.00E+12 0.0 -1000.0		
64. I-C8H18+AI-C8H17+H	1.83E+55 -11.4 12500.0				Reverse Arrhenius coefficients:	1.12E+17 -1.0 29330.0		
65. AI-C8H17-24DMITE+CH3	3.62E+17 -1.3 29700.0				Reverse Arrhenius coefficients:	7.00E+12 0.0 -1000.0		
66. AI-C8H17-I-C4H8+I-C4H9	1.00E+11 0.0 12700.0				123. CI-C8H17+C-C8O2-C8H17O+C-C8H17O</td			

134. I-C8H18+OH=BI-C8H17+H2O	9.90E+05	2.0	-1133.0	244. C5H5+O=C5H4O+H	5.81E+13	0.0	19991.4		
135. I-C8H18+OH=CI-C8H17+H2O	1.70E+06	1.9	-1451.0	245. C5H5+O-N-C4H5+CO	2.00E+14	0.0	0.0		
136. I-C8H18+OH=DI-C8H17+H2O	1.78E+07	1.8	1431.0	246. C5H5+C5H5=NAPHT+H2	1.00E+13	0.0	7000.6		
137. I-C8H18+CH3=AI-C8H17+CH4	4.26E-14	8.1	4154.0	247. CPD+HO2-C5H5+H2O2	2.00E+12	0.0	11660.5		
138. I-C8H18+CH3=BI-C8H17+CH4	2.70E+04	2.3	7287.0	248. CPD+OH=C5H5+H2O	3.43E+09	1.2	-446.6		
139. I-C8H18+CH3=CL-C8H17+CH4	6.01E-10	6.4	893.0	249. CPD+H-C5H5+H2	2.19E+08	1.8	2999.9		
140. I-C8H18+CH3=DI-C8H17+CH4	1.47E-01	3.9	6808.0	250. CPD+H-C3H3+C2H4	2.00E+14	0.0	10000.5		
141. I-C8H18+HO2=AI-C8H17+H2O2	2.77E+13	0.0	20440.0	251. CPD+O-C5H5+OH	1.81E+13	0.0	3081.1		
142. I-C8H18+HO2=BI-C8H17+H2O2	6.16E+12	0.0	17690.0	252. CPD+CH3-C5H5+CH4	3.11E+11	0.0	5500.6		
143. I-C8H18+HO2=CI-C8H17+H2O2	2.80E+12	0.0	16010.0	253. CPD+C2H3-C5H5+C2H6	3.11E+11	0.0	5500.6		
144. I-C8H18+HO2=DI-C8H17+H2O2	1.68E+13	0.0	20440.0	254. CPD+C2H5-C5H5+C2H6	3.11E+11	0.0	5500.6		
145. I-C8H18+CH3O=AI-C8H17+CH3OH	4.74E+11	0.0	7000.0	255. CPD+N-C4H5-C5H5+C4H6	3.11E+11	0.0	5500.6		
146. I-C8H18+CH3O=BI-C8H17+CH3OH	1.10E+11	0.0	5000.0	256. CPD+I-C4H5-C5H5+C4H6	3.11E+11	0.0	5500.6		
147. I-C8H18+CH3O=CI-C8H17+CH3OH	1.90E+10	0.0	2800.0	257. CPD+CH5-C5H5+C6H6	3.11E+11	0.0	5500.6		
148. I-C8H18+CH3O=DI-C8H17+CH3OH	3.20E+11	0.0	7000.0	258. CPD+O2=>C3H4O+CH2CO	3.00E+08	0.0	2999.9		
149. I-C8H18+O2=AI-C8H17+H2O2	6.30E+13	0.0	50760.0	259. C6H5OH+CH5-C6H5O+CH6	3.00E+02	3.0	7650.2		
150. I-C8H18+O2=BI-C8H17+H2O2	1.40E+13	0.0	48210.0	260. C6H5O+CH5+CO	8.00E+13	0.0	55402.7		
151. I-C8H18+O2=CI-C8H17+H2O2	7.00E+12	0.0	46060.0	261. C6H5O+H+(M)=C6H5OH+M	2.50E+14	0.0	0.0		
152. I-C8H18+O2=DI-C8H17+H2O2	4.20E+13	0.0	50760.0	Low pressure limit: 0.10000E+95 -0.21840E+02 0.13879E+05					
153. I-C8H18+O2=CH3=AI-C8H17+CH2H6	1.50E+11	0.0	13400.0	TROE centering: 0.43000E+01 0.30400E+03 0.60000E+05 0.14092E+07					
154. I-C8H18+O2=CH3=BI-C8H17+CH2H6	5.00E+10	0.0	10400.0	262. PHCH2+PHCH2OH+TOLUENE+PHCH2O	1.05E+11	0.0	9500.0		
155. I-C8H18+O2=CH3=CI-C8H17+CH2H6	1.00E+11	0.0	7900.0	263. PHCH2OH+O2=PHCH2+HO2+H	2.00E+14	0.0	41401.6		
156. I-C8H18+O2=CH3=DI-C8H17+CH2H6	1.00E+11	0.0	13400.0	264. PHHO+PHCO+H	3.98E+15	0.0	83705.9		
157. I-C8H18+O2=CH3=AI-C8H17+CH2H4	1.50E+12	0.0	18000.0	265. PHHO+O2=PHCO+HO2	1.02E+13	0.0	39001.2		
158. I-C8H18+O2=CH3=BI-C8H17+CH2H4	4.00E+11	0.0	16800.0	266. PHCO+H+CH5+CO	3.98E+14	0.0	29401.9		
159. I-C8H18+O2=CH3=CI-C8H17+CH2H4	2.00E+11	0.0	14300.0	267. PHCO+HO2=>CH5+CO2+OH	3.00E+10	0.0	2870.9		
160. I-C8H18+O2=CH3=DI-C8H17+CH2H4	1.00E+12	0.0	18000.0	268. PHCO+HO2=>CH5+CO2+OH	2.00E+13	0.0	0.0		
161. TOLUENE=C6H5+CH3	1.40E+16	0.0	99800.0	269. PHHC+HO2=>PHCO+H2O2	2.00E+12	0.0	11665.2		
162. C6H5+H-C6H6	2.20E+14	0.0	0.0	270. PHHC+OH=>PHCO+H2O	1.71E+09	1.2	-446.6		
163. C6H5+O2=CH5O+O	2.09E+12	0.0	7471.1	271. PHHC+OH=C6H5OH+CHO	1.20E+13	0.0	5123.2		
164. C6H5+HO2=C6H5O+OH	5.00E+13	0.0	1000.8	272. PHHC+O+PHCO+OH	9.04E+12	0.0	3081.1		
165. C6H5+OH=C6H5O+H	5.00E+13	0.0	0.0	273. PHHC+H+PHCO+H2	5.00E+13	0.0	4927.4		
166. C6H5+O2=C2H-PHC2H	3.00E+08	0.0	1390.1	274. PHHC+H+C6H6+CHO	1.20E+13	0.0	5147.1		
167. C6H5+C2H4-STYRENE+H	1.43E+08	1.2	3539.7	275. PHHC+CH3+PHCO+CH4	2.77E+03	2.8	5772.9		
168. STYRENE=C6H6+C2H2	1.60E+11	0.0	58440.8	276. PHHO+CH5+PHCO+C6H6	7.01E+11	0.0	4399.5		
169. N-C4H5+C4H4-STYRENE+H	3.16E+11	0.0	3699.7	277. PHCH2OH+O=>PHCO+H2O+H	8.43E+12	0.0	2584.3		
170. C4H4+CH4-STYRENE	1.48E+14	0.0	38005.2	278. PHCH2OH+H-C6H6+CH2O	1.20E+13	0.0	5147.1		
171. C6H5+C2H2-PHC2H+H	1.00E+13	0.0	764.3	279. PHCH2OH+H-PHC2H+H->PHCO+TOLUENE+H	2.11E+11	0.0	9501.3		
172. C6H5+C2H4-PHC2H+C2H	2.00E+13	0.0	0.0	280. PHCH2OH+H-C6H6+>PHCO+C6H6-H	1.40E+12	0.0	4399.5		
173. C6H5+C4H4-PHC2H+C2H3	1.00E+13	0.0	764.3	281. PHHC+PHC2H+PHCO+TOLUENE	2.77E+03	2.8	5773.0		
174. C6H5+C2H5-PHC2H5	1.00E+13	0.0	0.0	282. PHCH2OH+H-TOLUENE+OH	2.21E+13	0.0	7910.0		
175. PHC2H3+PHC2H+CH3	1.00E+15	0.0	70003.3	283. 3-C5O2+CH5H12=>3C5OOH+I-C5H11	6.00E+12	0.0	13996.4		
176. PHC2H5-BPHC2H4+H	2.51E+15	0.0	81264.9	284. 3-C5O2+CH5H12=>3C5OOH+I-C5H11	2.00E+12	0.0	11010.8		
177. PHC2H5+APHC2H4+H	2.51E+15	0.0	83264.1	285. 3-C5O2+CH5H12=>3C5OOH+I-C5H11	4.00E+12	0.0	11010.8		
178. APHC2H4-STYRENE+H	3.16E+13	0.0	50673.6	286. 3-C5O2+I-C5H12=>3C5OOH+D-C5H11	3.00E+12	0.0	13996.4		
179. APHC2H5+CH5-C2H4	1.00E+14	0.0	12584.8	287. 3-C5O2+I-C5H12=>3C5OOH+A-C5H11	6.00E+12	0.0	13996.4		
180. PHC2H5+HO2-BPHC2H4+H2O2	9.80E+10	0.0	12584.8	288. 3-C5O2+I-C5H12=>3C5OOH+C-C5H11	2.00E+12	0.0	11010.8		
181. PHC2H5+O2-STYRENE+H	3.16E+15	0.0	50673.6	289. 3-C5O2+I-C5H12=>3C5OOH+B-C5H11	1.00E+12	0.0	8001.3		
182. PHC2H5+OH-BPHC2H4+H2O2	5.20E+12	0.0	0.0	290. C-5H11=>3-C5O2	2.00E+12	0.0	0.0		
183. PHC2H5+O2-BPHC2H4+H2	8.00E+05	1.2	334.4	291. 3-C5H11=>I-C4H8+CH3	8.00E+12	0.0	33008.5		
184. PHC2H5+CH3-BPHC2H4+CH4	1.00E+12	0.0	10000.5	292. 3-C5H11=>2-C5H10-HO2	1.00E+09	0.0	3898.0		
185. PHC2H5+H-C6H6+C2H5	2.40E+13	0.0	5123.2	293. D-C5H11=>2-C5-C5O2	2.00E+12	0.0	0.0		
186. PHC2H5-C6H6+C2H4	1.15E+09	0.0	51700.6	294. D-C5H11=>I-C3H7+CH4	1.30E+13	0.0	29497.5		
187. C3H3+C3H3-C6H5+H	1.00E+13	0.0	0.0	295. D-C5H11=>A-C5H11	6.00E+11	0.0	21090.1		
188. N-C4H3+C2H2-C6H5+H	2.80E+03	2.9	1399.6	296. D-C5H11=>2-M1BE+HO2	5.00E+08	0.0	3898.0		
189. TOLUENE=PHC2H+H	3.00E+15	0.0	88198.6	297. A-C5H11=>2-A-C5O2	2.00E+12	0.0	0.0		
Declared duplicate reaction...									
190. PHCH2-C4H4+C3H3	2.00E+14	0.0	83603.2	298. A-C5H11=>I-C4H8+CH3	1.00E+13	0.0	26010.3		
191. PHCH2-C5H5+CH2H2	6.03E+13	0.0	70003.3	299. A-C5H11=>C2H5+C3H6	1.30E+13	0.0	29497.5		
192. PHCH2-O2-PHCH2+O	6.31E+12	0.0	43001.8	300. A-C5H11=>D-C5H11	3.00E+11	0.0	21090.1		
193. PHCH2-HO2=PHCH2+O+H	3.16E+12	0.0	0.0	301. A-C5H11=>2-M1BE+HO2	2.50E+08	0.0	2450.6		
194. PHCH2-O+PHCH2+O+H	1.30E+14	0.0	1101.1	302. B-C5H11=>2-C5-C5O2	2.00E+12	0.0	0.0		
195. PHCH2-O+PHCH2+O+H	2.00E+13	0.0	0.0	303. B-C5H11=>I-C4H8+CH3	8.00E+12	0.0	33008.5		
196. PHCH2-O+PHCO+O+H	1.58E+13	0.0	0.0	304. B-C5H11=>2-M2BE+HO2	5.00E+08	0.0	3898.0		
197. PHCH2-O+C6H5+C2H2	1.00E+13	0.0	0.0	305. B-C5H11=>2-M1BE+HO2	1.50E+09	0.0	6195.7		
198. PHCH2-C3H3+TOLUENE+C3H2	1.00E+12	0.0	0.0	306. C-C5H11=>2-E-C5O2	2.00E+12	0.0	0.0		
199. PHCH2-C6H5OH+TOLUENE+C6H5O	1.05E+11	0.0	9501.3	307. C-C5H11=>2-C4H8+CH3	1.00E+13	0.0	26010.3		
200. TOLUENE+O2-PHCH2+H2O2	4.50E+15	0.0	42992.0	308. C-C5H11=>2-M2BE+HO2	2.50E+08	0.0	2450.6		
201. TOLUENE+O+PHCH2+H2O2	2.70E+14	0.0	22012.0	309. C-C5H11=>2-M1BE+HO2	7.50E+08	0.0	6195.7		
202. TOLUENE+OH+PHCH2+H2O2	1.14E+13	0.0	2583.0	310. B-C5O2+I-C5H12=>B-C5OOH+D-C5H11	3.00E+12	0.0	13996.4		
203. TOLUENE+H+PHC2H+H2	1.20E+13	0.0	8235.0	311. B-C5O2+I-C5H12=>B-C5OOH+A-C5H11	6.00E+12	0.0	13996.4		
204. TOLUENE+C6H6+C2H2	1.20E+11	0.0	5148.0	312. B-C5O2+I-C5H12=>E-C5OOH+D-C5H11	2.00E+12	0.0	11010.8		
205. C6H6=C4H4+C2H2	9.00E+15	0.0	10743.5	313. E-C5O2+I-C5H12=>E-C5OOH+C-C5H11	6.00E+12	0.0	13996.4		
206. C6H6+O2=>C6H5+H2O2	6.30E+13	0.0	60002.9	314. E-C5O2+I-C5H12=>E-C5OOH+D-C5H11	3.00E+12	0.0	11010.8		
207. C6H6+H2O2=>C6H5+H2O2	1.52E+11	0.0	17001.0	315. E-C5O2+I-C5H12=>E-C5OOH+C-C5H11	2.00E+12	0.0	11010.8		
208. C6H6+OH=>C6H5+H2O2	2.11E+13	0.0	4569.1	316. C-C5O2+I-C5H12=>E-C5OOH+B-C5H11	1.00E+12	0.0	8001.3		
209. C6H6+O=>C6H5+H2	2.50E+14	0.0	16000.3	317. A-C5O2+I-C5H12=>A-C5OOH+D-C5H11	3.00E+12	0.0	13996.4		
210. C6H6+O=>C6H5O+H	3.56E+01	3.8	941.1	318. A-C5O2+I-C5H12=>A-C5OOH+C-C5H11	6.00E+12	0.0	13996.4		
211. C6H6+CH3=>C6H5+CH4	2.00E+12	0.0	15001.9	319. A-C5O2+I-C5H12=>A-C5OOH+C-C5H11	2.00E+12	0.0	11010.8		
212. C6H6+C2H5=>C6H5+C2H6	2.00E+12	0.0	15001.9	321. A-C5O2+I-C5H12=>A-C5OOH+B-C5H11	1.00E+12	0.0	8001.3		
213. C6H6+C2H3=>C6H5+C2H4	2.00E+12	0.0	15001.9	322. C-C5O2+I-C5H12=>C-C5OOH+C-C5H11	3.00E+12	0.0	13996.4		
214. C6H6+N-C4H5=>C6H5+C4H6	2.00E+12	0.0	15001.9	323. C-C5O2+I-C5H12=>C-C5OOH+A-C5H11	6.00E+12	0.0	11010.8		
215. C6H6+I-C4H5=>C6H5+C4H6	2.00E+12	0.0	15001.9	324. C-C5O2+I-C5H12=>C-C5OOH+B-C5H11	2.00E+12	0.0	11010.8		
216. C3H3+C3H4-C6H6+H	1.40E+12	0.0	12799.8	325. C-C5O2+I-C5H12=>C-C5OOH+B-C5H11	1.00E+12	0.0	8001.3		
217. C3H3+C3H4-C6H6+H	3.00E+11	0.0	0.0	326. C5H12+R-C5O2=>1-C5H11-B-C5OOH	6.00E+12	0.0	13996.4		
218. C4H4+C2H4-C6H6+H	1.90E+12	0.0	3511.0	327. B-C5O2+R=RF-C5O0H	5.96E+12	0.0	27880.5		
219. N-C4H5+C2H3-C6H6+H	2.80E+03	2.9	1399.6	328. B-C5O2+R=CE-C5O0H	1.79E+13	0.0	29679.0		
220. N-C4H3+C2H3-C6H6	2.87E+14	0.0	816.9	329. B-C5O2+R=RG-C5O0H	7.41E+11	0.0	23884.6		
221. TOLUENE+O-PHCH2+O+H	1.63E+13	0.0	3418.0	330. B-C5O2+H02=>B-C5OOH+O2	1.75E+10	0.0	-3272.2		
222. TOLUENE+CH3-C2H3+CH2+CH4	2.84E+11	0.0	9500.0	331. B-C5O2+H02=>B-C5OOH+					

356. C5H12+CH3=>3-C5H11+CH4	4.00E+11	0.0	9506.1	470. C5H7+H=>13-C5H8	1.00E+14	0.0	0.0
357. C5H12+CH3=>2-C5H11+CH4	8.00E+11	0.0	9506.1	471. 13-C5H8+O2>C2H3CHO+CH3CHO	2.00E+08	1.5	30202.1
358. C5H12+HO2=>1-C5H11+H2O2	1.12E+13	0.0	19394.3	472. 13-C5H8+HO2=>C2H3CHO+C2H4+OH	5.00E+11	0.0	19000.2
359. C5H12+HO2=>3-C5H11+H2O2	3.36E+12	0.0	17005.8	473. 13-C5H8+HO2=>C4H6+CH2O+OH	5.00E+11	0.0	19000.2
360. C5H12+HO2=>2-C5H11+H2O2	6.72E+12	0.0	17005.8	474. 13-C5H8+OH=>C3H3CHO+C3H5	6.00E+12	0.0	-394.1
361. C5H12+OH=>1-C5H11+H2O	2.57E+09	1.1	1810.5	475. 13-C5H8+OH=>CH2O+C4H7	6.00E+12	0.0	-394.1
362. C5H12+OH=>3-C5H11+H2O	3.90E+08	1.3	702.2	476. 13-C5H8+O=>C2H3CHO+C2H4	4.50E+08	1.4	-857.5
363. C5H12+OH=>2-C5H11+H2O	7.80E+08	1.3	702.2	477. 13-C5H8+O=>C2H2O+C4H6	4.50E+08	1.4	-857.5
364. C5H12+O2=>1-C5H11+H2O2	2.52E+13	0.0	49011.2	478. 13-C5H8+H=>C5H7+H2	7.00E-06	2.0	0.0
365. C5H12+O2=>3-C5H11+H2O2	2.00E+13	0.0	47602.0	479. 13-C5H8+H=>C3H5+C2H4	3.35E+08	1.5	1999.1
366. C5H12+O2=>2-C5H11+H2O2	4.00E+13	0.0	47602.0	480. 13-C5H8+OH=>C5H7+H2O	7.00E-06	2.0	0.0
367. C5H12+O2=>1-C5H11+OH	1.00E+14	0.0	7858.0	481. 13-C5H8+HO2=>C5H7+H2O2	2.00E+11	0.0	12601.5
368. C5H12+O2=>3-C5H11+OH	2.80E+13	0.0	5206.8	482. 13-C5H8+CH3=>C5H7+CH4	2.00E+14	0.0	22800.2
369. C5H12+O2=>2-C5H11+OH	5.60E+13	0.0	5206.8	483. N-C4H5+CH3=>13-C5H8	2.00E+13	0.0	0.0
370. C5H12+H=>1-C5H11+H2	5.61E+07	2.0	7690.8	484. C3H5+C2H3=>13-C5H8	1.00E+13	0.0	0.0
371. C5H12+H=>3-C5H11+H2	9.00E+07	2.0	4991.9	485. I-C4H5+CH3=>13-C5H8	4.80E+37	-7.6	11359.5
372. C5H12+H=>2-C5H11+H2	1.80E+07	2.0	4991.9	486. C5H7+CPD+H	2.00E+11	0.0	18001.8
373. I-C5H12+CH2H=>D-C5H11+C2H4	5.00E+11	0.0	17987.5	487. CYC5H7+O2>C2H3CHO+CH2CHO	4.00E+10	0.0	5001.4
374. I-C5H12+CH2H=>A-C5H11+C2H4	1.00E+12	0.0	17987.5	488. CYC5H7+O2>CPD+HO2	1.01E+12	0.0	13353.9
375. I-C5H12+CH2H=>C-C5H11+C2H4	4.00E+11	0.0	16788.5	489. CYC5H7+HO2=>CPD+H2O2	2.65E+12	0.0	0.0
376. I-C5H12+CH2H=>B-C5H11+C2H4	2.00E+11	0.0	14290.1	490. CYC5H7+HO=>CPD+H2O	6.02E+12	0.0	0.0
377. I-C5H12+CH2H=>D-C5H11+C2H6	5.00E+10	0.0	13392.1	491. CYC5H7+O=>CPD+OH	1.80E+13	0.0	0.0
378. I-C5H12+CH2H=>A-C5H11+C2H6	1.00E+11	0.0	13392.1	492. CYC5H7+H=>CPD+H2	3.16E+13	0.0	0.0
379. I-C5H12+CH2H=>C-C5H11+C2H6	5.00E+10	0.0	10392.2	493. CYC5H8+HO2=>CYC5H7+H2O2	1.60E+11	0.0	17060.8
380. I-C5H12+CH2H=>B-C5H11+C2H6	1.00E+11	0.0	7893.9	494. CYC5H8+HO=>CYC5H7+H2O	1.28E+09	0.0	300.9
381. I-C5H12+CH3O=>D-C5H11+CH3OH	1.58E+11	0.0	6995.8	495. CYC5H8+O=>CYC5H7+OH	2.78E+11	0.0	2507.9
382. I-C5H12+CH3O=>A-C5H11+CH3OH	3.16E+11	0.0	6995.8	496. C6H9CY2+HO2=>CYC5H8+CHO+OH	4.50E+12	0.0	0.0
383. I-C5H12+CH3O=>C-C5H11+CH3OH	1.10E+11	0.0	4996.7	497. C6H9CY2+O=>CYC5H8+CHO	8.26E+13	0.0	0.0
384. I-C5H12+CH3O=>B-C5H11+CH3OH	1.90E+10	0.0	2799.3	498. 33DM1BE+HO2=>B-C5H11+O2	2.00E+11	0.0	19919.8
385. I-C5H12+CH3O2=>D-C5H11+CH3O2H	1.26E+13	0.0	20469.1	499. 2M2ITE+HO2=>A-C5H11+O2	2.00E+11	0.0	19919.8
386. I-C5H12+CH3O2=>A-C5H11+CH3O2H	2.52E+13	0.0	20469.1	500. 2M1TE+HO2=>A-C5H11+O2	2.00E+11	0.0	19919.8
387. I-C5H12+CH3O2=>C-C5H11+CH3O2H	3.00E+12	0.0	17005.8	501. 4M1TE+HO2=>A-C5H11+O2	2.00E+11	0.0	19919.8
388. I-C5H12+CH3O2=>B-C5H11+CH3O2H	3.00E+12	0.0	14999.5	502. 2M2ITE+HO2=>A1-C5H11+O2	2.00E+11	0.0	19919.8
389. I-C5H12+CH3=>D-C5H11+CH4	6.60E+11	0.0	11607.9	503. 4M2TE+HO2=>A4-C5H11+O2	2.00E+11	0.0	19919.8
390. I-C5H12+CH3=>A-C5H11+CH4	1.32E+12	0.0	11607.9	504. 4M1TE+HO2=>A4-C6H11+O2	2.00E+11	0.0	19919.8
391. I-C5H12+CH3=>C-C5H11+CH4	4.00E+11	0.0	9506.1	505. B3-C6H13+O2=>F-C6O2	2.00E+12	0.0	0.0
392. I-C5H12+CH3=>B-C5H11+CH4	1.00E+11	0.0	7905.8	506. B3-C6H13=>T-C4H9+C2H4	1.30E+13	0.0	29497.5
393. I-C5H12+HO2=>D-C5H11+H2O2	5.61E+12	0.0	19394.3	507. B3-C6H13=>B1-C6H13	9.00E+11	0.0	21090.1
394. I-C5H12+HO2=>A-C5H11+H2O2	1.12E+13	0.0	19394.3	508. B3-C6H13+O2=>33DM1BE+HO2	5.00E+08	0.0	3898.0
395. I-C5H12+HO2=>C-C5H11+H2O2	3.36E+12	0.0	17005.8	509. A2-C6H13+O2=>B-C6O2	2.00E+12	0.0	0.0
396. I-C5H12+HO2=>B-C5H11+H2O2	1.00E+12	0.0	14402.4	510. A2-C6H13=>A4-C4H8+C2H5	2.00E+13	0.0	28566.0
397. I-C5H12+OH=>D-C5H11+H2O	1.29E+09	1.1	18104.5	511. A2-C6H13=>A5-C6H13	3.00E+11	0.0	21090.1
398. I-C5H12+OH=>A-C5H11+H2O	2.57E+09	1.1	18104.5	512. A2-C6H13+O2=>2M2TE+HO2	5.00E-08	0.0	3898.0
399. I-C5H12+OH=>C-C5H11+H2O	3.90E+08	1.3	7022.1	513. A2-C6H13+O2=>2M1TE+HO2	1.50E-09	0.0	6195.7
400. I-C5H12+OH=>B-C5H11+H2O	1.20E+12	0.0	4418.6	514. A5-C6H13+O2=>D-C6O2	2.00E+12	0.0	0.0
401. I-C5H12+O2=>D-C5H11+H2O	1.26E+13	0.0	4901.1	515. A5-C6H13=>C4H9+C2H4	2.00E+13	0.0	28566.0
402. I-C5H12+O2=>A-C5H11+H2O	2.77E+13	0.0	4901.1	516. A5-C6H13=>A2-C6H13	1.00E+11	0.0	16098.2
403. I-C5H12+O2=>C-C5H11+H2O	1.80E+12	0.0	4760.2	517. A5-C6H13=>A1-C6H13	6.00E+11	0.0	14077.6
404. I-C5H12+O2=>B-C5H11+H2O	2.00E+12	0.0	4600.2	518. A5-C6H13+O2=>4M1TE+HO2	5.00E-08	0.0	3898.0
405. I-C5H12+O2=>D-C5H11+OH	5.01E+09	0.0	785.8	519. A1-C6H13=>A-C6O2	2.00E+12	0.0	0.0
406. I-C5H12+O=>A-C5H11+OH	1.00E+14	0.0	785.8	520. A1-C6H13=>1-C5H10+CH3	1.00E+13	0.0	26010.3
407. I-C5H12+O=>C-C5H11+OH	2.80E+13	0.0	5207.	521. A1-C6H13=>N-C5H7+C3H6	1.30E+13	0.0	29497.5
408. I-C5H12+H=>B-C5H11+H2	1.00E+13	0.0	327.2	522. A1-C6H13=>A4-C6H13	2.00E+11	0.0	18071.1
409. I-C5H12+H=>D-C5H11+H2	2.80E+07	2.0	769.1	523. A1-C6H13=>A5-C6H13	3.00E+11	0.0	14077.6
410. I-C5H12+H=>A-C5H11+H2	5.61E+07	2.0	769.1	524. A1-C6H13+O2=>2M1TE+HO2	2.50E-08	0.0	2450.6
411. I-C5H12+H=>C-C5H11+H2	9.00E+06	2.0	499.2	525. A4-C6H13+O2=>C-C6O2	2.00E+12	0.0	0.0
412. I-C5H12+H=>B-C5H11+H2	1.26E+14	0.0	730.9	526. A4-C6H13=>A1-C6H13	6.00E+11	0.0	21090.1
413. C-S8O2+CH2=>N-C3H7+C2H5	8.30E+22	-1.6	88210.6	527. A4-C6H13=>1-C3H7+CH3	1.30E+13	0.0	29497.5
414. C5H12+P=C4H9+CH3	3.50E+19	-0.9	87030.7	528. A4-C6H13+O2=>4M2TE+HO2	5.00E-08	0.0	3898.0
415. I-C5H12=>C-C4H9+CH3	1.75E+19	0.9	87030.7	529. A4-C6H13+O2=>4M1TE+HO2	7.50E-08	0.0	6195.7
416. I-C5H12=>1-C3H7+C2H5	3.09E+21	-1.4	85562.1	530. F-C6O2=>RZ-C6O0H	5.96E+12	0.0	27880.5
417. I-C5H12=>S-C4H9+CH3	1.21E+18	-0.6	84434.4	531. F-C6O2=>RY-C6O0H	1.85E+11	0.0	21085.3
418. C5H12=>3-C5H11+H	2.58E+18	-0.8	99273.9	532. F-C6O2+HO2=>G-C6O0H+O2	1.75E-10	0.0	-3272.2
419. C5H12=>2-C5H11+H	5.16E+18	-0.8	99273.9	533. F-C6O2+H2O2=>G-C6O0H+HO2	2.41E+12	0.0	9933.6
420. C5H12=>1-C5H11+H	1.67E+22	-1.7	10373.8	534. B-C6O2=>RG-C6O0H	5.96E+12	0.0	27880.5
421. C5H12=>D-C5H11+H	8.37E+21	-1.7	10373.8	535. B-C6O2=>RF-C6O0H	1.79E+13	0.0	29679.0
422. C5H12=>C-C5H11+H	2.58E+18	-0.8	99273.9	536. B-C6O2=>RH-C6O0H	4.96E+11	0.0	22136.2
423. C5H12=>B-C5H11+H	1.45E+20	-1.4	97046.6	537. B-C6O2=>R1-C6O0H	6.18E+10	0.0	21085.3
424. I-C5H12=>A-C5H11+H	1.67E+22	-1.7	10373.8	538. D-C6O2=>RS-C6O0H	5.96E+12	0.0	27880.5
425. C-S8O2+CH2=>C-C8O0H+1-C5H11	6.00E+12	0.0	13996.4	539. D-C6O2=>RR-C6O0H	4.96E+11	0.0	22136.2
426. C-S8O2+CH2=>C-S8O0H+3-C5H11	2.00E+12	0.0	11010.8	540. D-C6O2=>RQ-C6O0H	1.80E+10	0.0	16389.6
427. C-S8O2+CH2=>B-C8O0H+2-C5H11	4.00E+12	0.0	13996.4	541. D-C6O2=>RP-C6O0H	1.03E+10	0.0	23884.6
428. C-S8O2+CH2=>C-C8O0H+D-C5H11	3.00E+12	0.0	13996.4	542. A-C6O2=>RC-C6O0H	2.59E+12	0.0	25382.2
429. C-S8O2+CH2=>C-C8O0H+A-C5H11	6.00E+12	0.0	13996.4	543. A-C6O2=>RC-C6O0H	4.96E+11	0.0	22136.2
430. C-S8O2+CH2=>D-C8O0H+C-C5H11	2.00E+12	0.0	11010.8	544. A-C6O2=>RA-C6O0H	7.41E+11	0.0	23884.6
431. C-S8O2+CH2=>C-S8O0H+B-C5H11	1.00E+12	0.0	8001.3	545. A-C6O2=>RD-C6O0H	4.12E+10	0.0	19337.0
432. D-C8O2+CH2=>D-C8O0H+1-C5H11	6.00E+12	0.0	13996.4	546. A-C6O2=>RE-C6O0H	5.16E+09	0.0	23884.6
433. B-C8O2+CH2=>B-C8O0H+1-C5H11	2.00E+12	0.0	11010.8	547. E-C6O2=>RN-C6O0H	5.96E+12	0.0	27880.5
434. B-C8O2+CH2=>C-C8O0H+3-C5H11	4.00E+12	0.0	11010.8	548. C-C6O2=>RO-C6O0H	8.94E+12	0.0	29679.0
435. B-C8O2+CH2=>B-C8O0H+D-C5H11	3.00E+12	0.0	13996.4	549. C-C6O2=>RM-C6O0H	2.16E+11	0.0	19685.7
436. B-C8O2+CH2=>B-C8O0H+A-C5H11	6.00E+12	0.0	13996.4	550. C-C6O2=>RL-C6O0H	1.24E+11	0.0	21085.3
437. B-C8O2+CH2=>C-C8O0H+C-C5H11	2.00E+12	0.0	11010.8	551. BI-C6H13+O2=>E-C6O2	2.00E+12	0.0	0.0
438. B-C8O2+CH2=>B-C8O0H+B-C5H11	1.00E+12	0.0	8001.3	552. BI-C6H13+>2M1BE+C3H3	1.00E-13	0.0	29784.1
439. D-C8O2+CH2=>D-C8O0H+1-C5H11	9.00E+12	0.0	13996.4	553. BI-C6H13+>1-C4H8+C2H5	1.30E+13	0.0	29497.5
440. D-C8O2+CH2=>D-C8O0H+B-C5H11	1.00E+12	0.0	8001.3	554. BI-C6H13+>B3-C6H11	3.00E-11	0.0	21090.1
441. D-C8O2+CH2=>B-C8O0H+1-C5H11	2.00E+12	0.0	11010.8	555. E-C6O2=>RU-C6O0H	4.96E+11	0.0	22136.2
442. D-C8O2+CH2=>D-C8O0H+C1-C5H11							

584. .2M1TE+CH3=>A2-C6H11+CH4	1.50E+12	0.0	7294.4	698. RT-C6OOH=>2M1BE+COOH	2.00E+13	0.0	28661.5
585. 2M1TE+OH=>A3-C6H11+H2O	3.00E+13	0.0	1229.1	699. RU-C6OOH=>2M2BE+COOH	2.00E+13	0.0	28661.5
586. 2M1TE+OH=>A2-C6H11+H2O	4.50E+13	0.0	1229.1	700. RL-C6OOH=>1C3OOH2+C3H6	2.00E+13	0.0	28661.5
587. 2M1TE+O=>A3-C6H11+OH	2.62E+11	0.5	11892.1	701. RM-C6OOH=>I-C4H8+CH3COOH	2.00E+13	0.0	28661.5
588. 2M1TE+O=>A2-C6H11+OH	3.92E+11	0.5	11892.1	702. RE-C6OOH=>RB-C4OOH+C2H4	2.00E+13	0.0	28661.5
589. 2M1TE+H=>A3-C6H11+H2	3.70E+13	0.0	3898.0	703. RD-C6OOH=>2C3OOH3+C3H4	2.00E+13	0.0	28661.5
590. 2M1TE+H=>A2-C6H11+H2	5.55E+13	0.0	3898.0	704. RA-C6OOH=>I-C5H10+COOH	2.00E+13	0.0	28661.5
591. 4M1TE=>I-C3H7+C3H5	1.00E+16	0.0	70961.1	705. RC-C6OOH=>2-C5H10+COOH	2.00E+13	0.0	28661.5
592. 4M1TE+OH=>D-C5H11+CH2O	1.00E+11	0.0	-3997.3	706. RP-C6OOH=>1C3OOH3+C3H6	2.00E+13	0.0	28661.5
593. 4M1TE+OH=>IC5H10O+CH3	1.00E+11	0.0	-3997.3	707. RQ-C6OOH=>I-C4H8+.1C2OOH2	2.00E+13	0.0	28661.5
594. 4M1TE+O=>D-C5H11+CHO	1.00E+11	0.0	-1049.2	708. RR-C6OOH=>.3M1BE+COOH	2.00E+13	0.0	28661.5
595. 4M1TE+O=>A-C5H9O+CH3	1.00E+11	0.0	-1049.2	709. RI-C6OOH=>RE-C4OOH+C2H4	2.00E+13	0.0	28661.5
596. 4M1TE+HO2=>RO-C6OOH	1.00E+11	0.0	10523.5	710. RH-C6OOH=>2C3OOH3+C3H6	2.00E+13	0.0	28661.5
597. 4M1TE+HO2=>RS-C6OOH	1.00E+11	0.0	10523.5	711. RJ-C6OOH=>F-C6O2	1.00E+11	0.0	12491.6
598. 4M1TE+CH3=>D3-C6H11+CH4	1.00E+12	0.0	7294.4	712. RY-C6OOH=>F-C6O2	1.00E+11	0.0	7499.8
599. 4M1TE+OH=>D3-C6H11+H2O	3.00E+13	0.0	1229.1	713. RU-C6OOH=>E-C6O2	1.00E+11	0.0	6592.1
600. 4M1TE+O=>D3-C6H11+OH	2.62E+11	0.5	11892.1	714. RT-C6OOH=>E-C6O2	1.00E+11	0.0	6592.1
601. 4M1TE+H=>D3-C6H11+H2	3.70E+13	0.0	3898.0	715. RV-C6OOH=>E-C6O2	1.00E+11	0.0	6998.2
602. 1-C5H10-HO2=>2-C5H11+O2	2.00E+11	0.0	19919.8	716. RN-C6OOH=>C-C6O2	1.00E+11	0.0	12491.6
603. 1-C5H10-HO2=>1-C5H11+O2	2.00E+11	0.0	19919.8	717. RO-C6OOH=>C-C6O2	1.00E+11	0.0	12491.6
604. 1-C5H10=>C2H5+C3H5	1.00E+16	0.0	70961.1	718. RM-C6OOH=>C-C6O2	1.00E+11	0.0	6401.1
605. 1-C5H10-OH=>P-C4H9+CH2O	1.00E+11	0.0	-3997.3	719. RL-C6OOH=>C-C6O2	1.00E+11	0.0	7499.8
606. 1-C5H10-OH=>C3H7CHO+CH3	1.00E+11	0.0	-3997.3	720. RB-C6OOH=>A-C6O2	1.00E+11	0.0	10365.9
607. 1-C5H10-O=>P-C4H9+CHO	1.00E+11	0.0	-1049.2	721. RC-C6OOH=>A-C6O2	1.00E+11	0.0	6592.1
608. 1-C5H10-O=>C3H7CO+CH3	1.00E+11	0.0	-1049.2	722. RA-C6OOH=>A-C6O2	1.00E+11	0.0	6592.1
609. 1-C5H10-HO2=>1C5OOH2	1.00E+11	0.0	10523.5	723. RD-C6OOH=>A-C6O2	1.00E+11	0.0	6998.2
610. 1-C5H10-HO2=>4C5OOH5	1.00E+11	0.0	10523.5	724. RE-C6OOH=>A-C6O2	1.00E+11	0.0	15978.8
611. 1-C5H10-CH3=>3CSH9-1+CH4	1.00E+12	0.0	7294.4	725. RS-C6OOH=>D-C6O2	1.00E+11	0.0	12491.6
612. 1-C5H10-OH=>3CSH9-1+H2O	3.00E+13	0.0	1229.1	726. RR-C6OOH=>D-C6O2	1.00E+11	0.0	6592.1
613. 1-C5H10-O=>3CSH9-1+OH	2.62E+11	0.5	11892.1	727. RQ-C6OOH=>D-C6O2	1.00E+11	0.0	7499.8
614. 1-C5H10-H=>3CSH9-1+H2	3.70E+13	0.0	3898.0	728. RP-C6OOH=>D-C6O2	1.00E+11	0.0	15978.8
615. 4M2TE=>2TE4YL+CH3	2.00E+16	0.0	70961.1	729. RG-C6OOH=>B-C6O2	1.00E+11	0.0	12491.6
616. 4M2TE+OH=>L-C4H9+CH3CHO	1.00E+11	0.0	-3997.3	730. RI-C6OOH=>B-C6O2	1.00E+11	0.0	12491.6
617. 4M2TE+OH=>IC3H7CHO-C2H5	1.00E+11	0.0	-3997.3	731. RH-C6OOH=>B-C6O2	1.00E+11	0.0	6592.1
618. 4M2TE+O=>1-C4H9+CH3CO	1.00E+11	0.0	-1049.2	732. RI-C6OOH=>B-C6O2	1.00E+11	0.0	6998.2
619. 4M2TE+O=>IC3H7CO+C2H5	1.00E+11	0.0	-1049.2	733. G-C6OOH=>B3C6H13O+OH	7.50E+15	0.0	42466.8
620. 4M2TE+HO2=>RK-C6O0H	1.00E+11	0.0	10523.5	734. F-C6OOH=>B1C6H13O+OH	7.50E+15	0.0	42466.8
621. 4M2TE+HO2=>RN-C6O0H	1.00E+11	0.0	10523.5	735. D-C6OOH=>A4C6H13O+OH	6.25E+15	0.0	41583.1
622. 4M2TE+CH3=>C5-C6H11+CH4	1.50E+12	0.0	7294.4	736. A-C6OOH=>A1C6H13O+OH	7.50E+15	0.0	42466.8
623. 4M2TE+CH3=>C2-C6H11+CH4	5.00E+13	0.0	7294.4	737. E-C6OOH=>A5C6H13O+OH	7.50E+15	0.0	42466.8
624. 4M2TE+OH=>C5-C6H11+H2O	4.50E+13	0.0	1229.1	738. B-C6OOH=>A2C6H13O+OH	3.75E+15	0.0	41511.4
625. 4M2TE+OH=>C2-C6H11+H2O	1.50E+13	0.0	1229.1	739. 2M1BE+HO2=>B-C5H11+O2	2.00E+11	0.0	19919.8
626. 4M2TE+O=>3-C5-C6H11+OH	3.92E+11	0.5	11892.1	740. 2M1BE+HO2=>A-C5H11+O2	2.00E+11	0.0	19919.8
627. 4M2TE+H=>C2-C6H11+OH	1.31E+11	0.5	11892.1	741. 2M1BE=>I-C4H7+CH3	1.00E+16	0.0	70961.1
628. 4M2TE+H=>C5-C6H11+H2	5.55E+13	0.0	3898.0	742. 2M1BE+OH=>S-C4H9+CH2O	1.00E+11	0.0	-3997.3
629. 4M2TE+O=>C2-C6H11+H2	1.85E+13	0.0	3898.0	743. 2M1BE+O=>S-C4H9+CHO	1.00E+11	0.0	-1049.2
630. RY-C6OOH+O2=>Y-C6O4H	5.00E+13	0.0	0.0	744. 2M1BE+HO2=>RE-C5OOH	1.00E+11	0.0	10523.5
631. RY-C6OOH+O2=>X-C6O4H	5.00E+13	0.0	0.0	745. 2M1BE+HO2=>RB-C5OOH	1.00E+11	0.0	10523.5
632. RT-C6OOH+O2=>V-C6O4H	5.00E+13	0.0	0.0	746. 2M1BE+CH3=>A3-C5H9+CH4	1.00E+12	0.0	7294.4
633. RU-C6OOH+O2=>W-C6O4H	5.00E+13	0.0	0.0	747. 2M1BE+CH3=>A2-C5H9+CH4	1.50E+12	0.0	7294.4
634. RZ-C6OOH+O2=>Z-C6O4H	5.00E+13	0.0	0.0	748. 2M1BE+OH=>A3-C5H9+H2O	3.00E+13	0.0	1229.1
635. RX-C6OOH+O2=>AA-C6O4H	5.00E+13	0.0	0.0	749. 2M1BE+OH=>A2-C5H9+H2O	4.50E+13	0.0	1229.1
636. RL-C6OOH+O2=>N-C6O4H	5.00E+13	0.0	0.0	750. 2M1BE+O=>A3-C5H9+OH	2.62E+11	0.5	11892.1
637. RM-C6OOH+O2=>O-C6O4H	5.00E+13	0.0	0.0	751. 2M1BE+O=>A2-C5H9+OH	3.92E+11	0.5	11892.1
638. RE-C6OOH+O2=>E-C6O4H	5.00E+13	0.0	0.0	752. 2M1BE+H=>A3-C5H9+H2	3.70E+13	0.0	3898.0
639. RD-C6OOH+O2=>D-C6O4H	5.00E+13	0.0	0.0	753. 2M1BE+H=>A2-C5H9+H2	5.55E+13	0.0	3898.0
640. RA-C6OOH+O2=>A-C6O4H	5.00E+13	0.0	0.0	754. NEOC5H11=>D-C5O2	2.00E+12	0.0	0.0
641. RC-C6OOH+O2=>C-C6O4H	5.00E+13	0.0	0.0	755. NEOC5H11=>I-C4H8+CH3	1.00E+13	0.0	29784.1
642. RB-C6OOH+O2=>B-C6O4H	5.00E+13	0.0	0.0	756. TC4H9CHO+CH3O=>M-C5H90+CH3O	1.15E+11	0.0	1279.3
643. RP-C6OOH+O2=>R-C6O4H	5.00E+13	0.0	0.0	757. TC4H9CHO+CH3O2=>N-C5H90+CH3O	1.81E+13	0.0	19368.0
644. RQ-C6OOH+O2=>S-C6O4H	5.00E+13	0.0	0.0	758. TC4H9CHO+CH3O2=>M-C5H90+CH3O	1.00E+12	0.0	9494.1
645. RR-C6OOH+O2=>T-C6O4H	5.00E+13	0.0	0.0	759. TC4H9CHO+CH3=>M-C5H90+CH4	1.70E+12	0.0	8433.6
646. RI-C6OOH+O2=>I-C6O4H	5.00E+13	0.0	0.0	760. TC4H9CHO+HO=>N-C5H90+H2O	8.28E+04	2.5	16468.4
647. RH-C6OOH+O2=>J-C6O4H	5.00E+13	0.0	0.0	761. TC4H9CHO+HO=>M-C5H90+H2O	2.80E+12	0.0	13590.3
648. RF-C6OOH+O2=>F-C6O4H	5.00E+13	0.0	0.0	762. TC4H9CHO+OH=>N-C5H90+H2O	1.58E+10	1.0	1585.0
649. RG-C6OOH+O2=>G-C6O4H	5.00E+13	0.0	0.0	763. TC4H9CHO+HO=>M-C5H90+H2O	2.69E+10	0.8	-339.9
650. RJ-C6OOH+O2=>K-C6O4H	5.00E+13	0.0	0.0	764. TC4H9CHO+O2=>M-C5H90+H2O	2.00E+13	0.5	42180.2
651. RN-C6OOH+O2=>P-C6O4H	5.00E+13	0.0	0.0	765. TC4H9CHO+O2=>M-C5H90+H2O	5.00E+12	0.0	1788.7
652. RK-C6OOH+O2=>L-C6O4H	5.00E+13	0.0	0.0	766. TC4H9CHO+H=>M-C5H90+H2	4.00E+13	0.0	4196.5
653. RS-C6OOH+O2=>U-C6O4H	5.00E+13	0.0	0.0	767. M-C5H90=>T-C4H9+CO	1.58E+13	0.0	17196.9
654. RO-C6OOH+O2=>Q-C6O4H	5.00E+13	0.0	0.0	768. 2-C5H11+O2=>4-C5O2	2.00E+12	0.0	0.0
655. Z28=>Z27+Z27	5.00E+13	0.0	0.0	769. 2-C5H11+O2=>C2H5+C3H6	2.00E+13	0.0	28566.0
656. Z31=>Z29+Z30	5.00E+13	0.0	0.0	770. 2-C5H11+O2=>C5H11	3.00E+11	0.0	21090.1
657. RY-C6OOH=>C-C6THF+OH	9.38E+09	0.0	6995.8	771. 2-C5H11+O2=>2-C5H10+H2O	5.00E+08	0.0	3898.0
658. RV-C6OOH=>C-C6THF+OH	9.38E+09	0.0	6995.8	772. 2-C5H11+O2=>1-C5H10+H2O	7.50E+08	0.0	6195.7
659. RT-C6OOH=>E-C6OXE+OH	7.50E+10	0.0	15240.8	773. J-C5H11+O2=>5-C5O2	2.00E+12	0.0	0.0
660. RU-C6OOH=>F-C6OXE+OH	7.50E+10	0.0	15240.8	774. 1-C5H11+O2=>N-C3H7+C2H4	2.00E+13	0.0	28566.0
661. RZ-C6OOH=>E-C6OXI+OH	6.00E+10	0.0	21985.8	775. I-C5H11+O2=>2-C5H11	2.00E+11	0.0	18071.1
662. RX-C6OOH=>B-C6OXI+OH	6.00E+10	0.0	21985.8	776. I-C5H11+O2=>1-C5H10+H2O	5.00E+08	0.0	3898.0
663. RL-C6OOH=>C-C6OXE+OH	9.38E+09	0.0	6995.8	777. I-C5O0H2+O2=>500SHP4	5.00E+13	0.0	0.0
665. RE-C6OOH=>A-C6THF+OH	1.17E+09	0.0	1798.7	778. I-C5O0H2+O2=>2POXI+OH	6.00E+11	0.0	21985.8
666. RD-C6OOH=>A-C6THF+OH	9.38E+09	0.0	6995.8	779. I-C5O0H2+O2=>1-C5H10+H2O	2.00E+13	0.0	20015.3
667. RA-C6OOH=>A-C6OXE+OH	7.50E+10	0.0	15240.8	780. I-C5O0H2+O2=>4-C5O2	1.00E+11	0.0	12491.6
668. RC-C6OOH=>B-C6OXE+OH	7.50E+10	0.0	15240.8	781. I-C5O0H5+O2=>4OOSH5P	5.00E+13	0.0	0.0
669. RB-C6OOH=>A-C6OXI+OH	6.00E+11	0.0	21985.8	782. I-C5O0H5+O2=>2POXI+OH	6.00E+11	0.0	21985.8
670. RP-C6OOH=>A-C6OXI+OH	6.00E+11	0.0	21985.8	783. I-C5O0H5+>1-C5H10+H2O	2.00E+13	0.0	20015.3
671. RJ-C6OOH=>2M1TE+H2O2	9.38E+09	0.0	6995.8	784. I-C5O0H5+>5-C5O2	1.00E+11	0.0	12491.6
672. RR-C6OOH=>2M1TE+H2O2	7.50E+10	0.0	15240.8	785. 3CSH9-1=C4H6+CH3	2.51E+13	0.0	29975.2
673. RJ-C6OOH=>B-C6THF+OH	9.38E+09	0.0	6995.8	786. TC3H6CHO+H=>IC3H7CHO	2.00E+14	0.0	0.0
674. RH-C6OOH=>C-C6OXE+OH	7.50E+10	0.0					

812. D-C6O4H=>D-C6202H	2.00E+11	0.0	14999.5	926. 2-C5H10+O=>2TE1YL+OH	3.92E+11	0.5	11892.1
813. A-C6O4H=>A-C6202H	2.00E+11	0.0	14593.5	927. 2-C5H10+O=>2TE4YL+OH	2.62E+11	0.5	11892.1
814. C-C6O4H=>C-C6202H	2.00E+11	0.0	14593.5	928. 2-C5H10+H=>2TE1YL+H2	5.55E+13	0.0	3898.0
815. B-C6O4H=>B-C6202H	2.00E+11	0.0	20493.0	929. 2-C5H10+H=>2TE4YL+H2	3.70E+13	0.0	3898.0
816. R-C6O4H=>L-C6202H	2.00E+11	0.0	23884.6	930. 5-C5O2=>4C5OOH5	5.96E+12	0.0	27880.5
817. S-C6O4H=>M-C6202H	2.00E+11	0.0	14999.5	931. 5-C5O2=>3C5OOH5	4.96E+11	0.0	22136.2
818. T-C6O4H=>N-C6202H	2.00E+11	0.0	14593.5	932. 5-C5O2=>2C5OOH5	4.12E+10	0.0	19337.0
819. K-C6O4H=>F-C6202H	1.00E+11	0.0	17005.8	933. 5-C5O2=>1C5OOH5	5.16E+09	0.0	23884.6
820. P-C6O4H=>J-C6202H	1.00E+11	0.0	17005.8	934. 5-C5O2-HO2=>5C5OOH+O2	1.75E+10	0.0	-3272.2
821. L-C6O4H=>G-C6202H	1.00E+11	0.0	17005.8	935. 5-C5O2-HO2=>5C5OOH+HO2	2.41E+12	0.0	9933.6
822. U-C6O4H=>O-C6202H	2.00E+11	0.0	20493.0	936. 5-C5O2+1-C8H18=>5C5OOH+Al-C8H17	9.00E+12	0.0	13996.4
823. Q-C6O4H=>K-C6202H	1.00E+11	0.0	17005.8	937. 5-C5O2+1-C8H18=>5C5OOH+DL-C8H17	6.00E+12	0.0	13996.4
824. Z2=>Z26	2.00E+11	0.0	20493.0	938. 5-C5O2+1-C8H18=>5C5OOH+Bl-C8H17	2.00E+12	0.0	11010.8
825. C-C6THF-HO2=>R-C6H11O+H2O2	6.00E+04	2.6	13900.8	939. 5-C5O2+1-C8H18=>5C5OOH+Cl-C8H17	1.00E+12	0.0	8001.3
826. C-C6THF-HO=>R-C6H11O+H2O	1.90E+08	1.6	-34.9	940. 5-C5O2+1-C8H18=>5C5OOH+1-C5H11	6.00E+12	0.0	13996.4
827. C-C6THF-HO2=>W-C6H11O+H2O2	6.00E+04	2.6	13900.8	941. 5-C5O2+1-C8H18=>5C5OOH+3-C5H11	2.00E+12	0.0	11010.8
828. C-C6THF-HO=>W-C6H11O+H2O	1.90E+08	1.6	-34.9	942. 5-C5O2+1-C8H18=>5C5OOH+2-C5H11	4.00E+12	0.0	11010.8
829. E-C6OXE-HO2=>U-C6H11O+H2O2	6.00E+04	2.6	13900.8	943. 5-C5O2+1-C8H12=>5C5OOH+D-C5H11	3.00E+12	0.0	13996.4
830. E-C6OXE-HO=>U-C6H11O+H2O	1.90E+08	1.6	-34.9	944. 5-C5O2+1-C8H12=>5C5OOH+A-C5H11	6.00E+12	0.0	13996.4
831. F-C6OXE-HO2=>V-C6H11O+H2O2	1.08E+04	2.5	10525.9	945. 5-C5O2+1-C8H12=>5C5OOH+C-C5H11	2.00E+12	0.0	11010.8
832. F-C6OXE-OH=>V-C6H11O+H2O	8.84E+09	1.0	-148.8	946. 5-C5O2+1-C8H12=>5C5OOH+B-C5H11	1.00E+12	0.0	8001.3
833. E-C6OXI-HO2=>S-C6H11O+H2O2	6.00E+04	2.6	13900.8	947. 5-C5O2+1-C8H1+O2	2.00E+15	0.0	28016.6
834. E-C6OXI-OH=>S-C6H11O+H2O	1.90E+08	1.6	-34.9	948. 400SHP=>4-CH5PH	2.00E+11	0.0	20493.0
835. E-C6OXI-HO2=>Q-C6H11O+H2O2	1.08E+04	2.5	10525.9	949. 500SHP=>4-CH5PH	1.00E+11	0.0	17005.8
836. E-C6OXI-OH=>Q-C6H11O+H2O	8.84E+09	1.0	-148.8	950. 400SHP=>4C5OOH+O2	5.00E+12	0.0	27945.0
837. A-C6THF-HO2=>H-C6H11O+H2O2	6.00E+04	2.6	13900.8	951. 500SHP=>1C5OOH+H2+O2	5.00E+12	0.0	27945.0
838. A-C6THF-HO=>H-C6H11O+H2O	1.90E+08	1.6	-34.9	952. 2POXI+HO2=>1-2C5O+H2O	6.00E+04	2.6	13900.8
839. A-C6THF-HO2=>C-C6H11O+H2O2	6.00E+04	2.6	13900.8	953. 2POXI+HO=>1-2C5O+H2O	1.90E+08	1.6	-34.9
840. A-C6THF-HO=>O-C6H11O+H2O	1.90E+08	1.6	-34.9	954. 2POXI+HO2=>2-IC5O+H2O	1.08E+04	2.5	10525.9
841. A-C6THF-HO2=>N-C6H11O+H2O2	1.08E+04	2.5	10525.9	955. 2POXI+HO=>2-IC5O+H2O	8.84E+09	1.0	-148.8
842. A-C6THF-HO=>N-C6H11O+H2O2	8.84E+09	1.0	-148.8	956. CH3OOH-CH3O+H	6.00E+14	0.0	42299.6
843. A-C6OXE-HO2=>K-C6H11O+H2O2	6.00E+04	2.6	13900.8	957. OH-CH3OOH-CH2+CH3O2	7.30E+11	0.0	-238.8
844. A-C6OXE-HO=>K-C6H11O+H2O2	1.90E+08	1.6	-34.9	958. O-CH3OOH-CH2+CH3O2	1.99E+13	0.0	4753.0
845. B-C6OXE-HO2=>M-C6H11O+H2O2	1.08E+04	2.5	10525.9	959. CH3O2+H2O=>CH3OOH+HO2	2.64E+12	0.0	9988.3
846. B-C6OXE-OH=>M-C6H11O+H2O	8.84E+09	1.0	-148.8	960. CH3O2+CH4-CH3OOH+CH3	1.81E+11	0.0	18582.2
847. A-C6OXI-HO2=>L-C6H11O+H2O2	6.00E+04	2.6	13900.8	961. CH3O2+CH3O-CH3OOH+CH2OH	1.81E+11	0.0	13781.4
848. A-C6OXI-HO2=>L-C6H11O+H2O	1.90E+08	1.6	-34.9	962. T-C6202H=>T-C6OHP+OH	1.00E+09	0.0	7499.8
849. A-C6THP-HO2=>D-C6H11O+H2O2	6.00E+04	2.6	13900.8	963. R-C6202H=>C6OHP+OH	1.00E+09	0.0	7499.8
850. A-C6THP-HO=>D-C6H11O+H2O	1.90E+08	1.6	-34.9	964. P-C6202H=>P-C6OHP+OH	1.00E+09	0.0	7499.8
851. D-C6OXE-HO2=>B-C6H11O+H2O2	1.08E+04	2.5	10525.9	965. Q-C6202H=>Q-C6OHP+OH	1.00E+09	0.0	7499.8
852. D-C6OXE-HO=>B-C6H11O+H2O	8.84E+09	1.0	-148.8	966. U-C6202H=>U-C6OHP+OH	1.00E+09	0.0	7499.8
853. B-C6THF-HO2=>C-C6H11O+H2O2	6.00E+04	2.6	13900.8	967. S-C6202H=>S-C6OHP+OH	1.00E+09	0.0	7499.8
854. B-C6THF-OH=>C-C6H11O+H2O	1.90E+08	1.6	-34.9	968. H-C6202H=>H-C6OHP+OH	1.00E+09	0.0	7499.8
855. C-C6OXE-HO2=>C-C6H11O+H2O2	6.00E+04	2.6	13900.8	969. I-C6202H=>I-C6OHP+OH	1.00E+09	0.0	7499.8
856. C-C6OXE-OH=>G-C6H11O+H2O	8.84E+09	1.0	-148.8	970. E-C6202H=>E-C6OHP+OH	1.00E+09	0.0	7499.8
857. B-C6OXI-HO2=>J-C6H11O+H2O2	1.08E+04	2.5	10525.9	971. D-C6202H=>D-C6OHP+OH	1.00E+09	0.0	7499.8
858. B-C6OXI-OH=>J-C6H11O+H2O2	8.84E+09	1.0	-148.8	972. A-C6202H=>A-C6OHP+OH	1.00E+09	0.0	7499.8
859. C-C6OXI-HO2=>I-C6H11O+H2O2	1.08E+04	2.5	10525.9	973. C-C6202H=>C-C6OHP+OH	1.00E+09	0.0	7499.8
860. C-C6OXI-OH=>I-C6H11O+H2O2	8.84E+09	1.0	-148.8	974. B-C6202H=>B-C6OHP+OH	1.00E+09	0.0	7499.8
861. C-C6OXI-HO2=>F-C6H11O+H2O2	1.08E+04	2.5	10525.9	975. L-C6202H=>L-C6OHP+OH	1.00E+09	0.0	7499.8
862. C-C6OXI-OH=>F-C6H11O+H2O2	8.84E+09	1.0	-148.8	976. M-C6202H=>M-C6OHP+OH	1.00E+09	0.0	7499.8
863. D-C6OXI-HO2=>E-C6H11O+H2O2	6.00E+04	2.6	13900.8	977. N-C6202H=>N-C6OHP+OH	1.00E+09	0.0	7499.8
864. D-C6OXI-OH=>E-C6H11O+H2O2	1.90E+08	1.6	-34.9	978. F-C6202H=>F-C6OHP+OH	1.00E+09	0.0	7499.8
865. D-C6OXI-HO2=>A-C6H11O+H2O2	1.08E+04	2.5	10525.9	979. J-C6202H=>J-C6OHP+OH	1.00E+09	0.0	7499.8
866. D-C6OXI-OH=>A-C6H11O+H2O2	8.84E+09	1.0	-148.8	980. G-C6202H=>G-C6OHP+OH	1.00E+09	0.0	7499.8
867. Z23+HO2=>Z21+H2O2	6.00E+04	2.6	13900.8	981. O-C6202H=>O-C6OHP+OH	1.00E+09	0.0	7499.8
868. Z23+OH=>Z21+H2O	1.90E+08	1.6	-34.9	982. K-C6202H=>K-C6OHP+OH	1.00E+09	0.0	7499.8
869. 23DM1BE=>A-C5H9+CH3	2.00E+10	0.0	70961.1	983. Z26=>Z25+OH	1.00E+09	0.0	7499.8
870. 23DM1BE+OH=>C-C5H11+CH2O	1.00E+11	0.0	-3997.3	984. G-C6H11O=>1C4H8+CH3CO	3.70E+13	0.0	28661.5
871. 23DM1BE-OH=>C-CSH11+CHO	1.00E+11	0.0	-1049.2	985. L-C6H11O=>IC3H5CHO+CH2S	3.70E+13	0.0	28661.5
872. 23DM1BE+HO2=>Z31	1.00E+11	0.0	10523.5	986. W-C6H11O=>TC3H6CHO+CH2	3.70E+13	0.0	28661.5
873. 23DM1BE+HO2=>Z28	1.00E+11	0.0	10523.5	987. U-C6H11O=>IC3H5CHO+CH2S	3.70E+13	0.0	28661.5
874. 23DM1BE+CH3=>Z20+CH4	5.00E+11	0.0	7294.4	988. V-C6H11O=>A-C5H8O+CH3	3.70E+13	0.0	28661.5
875. 23DM1BE+CH3=>Z19+CH4	1.50E+12	0.0	7294.4	989. W-C6H11O=>2M1BE+CHO	3.70E+13	0.0	28661.5
876. 23DM1BE+OH=>Z20+H2O	1.50E+13	0.0	1229.1	990. V-C6H11O=>B-C5H8O+CH3	7.40E+13	0.0	28661.5
878. 23DM1BE+O=>Z20+OH	1.31E+11	0.5	11892.1	992. C-C6H11O=>1C4H8+CH2CHO	3.70E+13	0.0	28661.5
879. 23DM1BE+O=>Z19+OH	3.92E+11	0.5	11892.1	993. S-C6H11O=>T-C4H9+CH2CO	4.00E+13	0.0	13709.8
880. 23DM1BE+H=>Z20+H2	1.85E+13	0.0	3898.0	994. P-C6H11O=>NEOC5H1+CO	1.58E+13	0.0	17196.9
881. 23DM1BE+H=>Z19+H2	5.55E+13	0.0	3898.0	995. Q-C6H11O=>E-C5H8O+CH3	1.11E+14	0.0	28661.5
882. RC-C4O0H=>C3H7CHO+OH	1.00E+09	0.0	7475.9	996. R-C6H11O=>4C4H8+CH2CHO	3.70E+13	0.0	28661.5
883. IC3OOH=>C2H5CHO+OH	1.00E+09	0.0	7475.9	997. R-C6H11O=>D-C5H8O+CH3	7.40E+13	0.0	28661.5
884. RB-C4O0H=>C3H7CHO+OH	1.00E+09	0.0	7475.9	998. O-C6H11O=>IC3H6CHO+CH2	3.70E+13	0.0	28661.5
885. RE-C4O0H=>C3H7CHO+OH	1.00E+09	0.0	7475.9	999. K-C6H11O=>N-C3H7+CH2CHO	3.70E+13	0.0	28661.5
886. 2C3OOH=>C2H5CHO+OH	1.00E+09	0.0	7475.9	1000. K-C6H11O=>1-C5H10+CHO	3.70E+13	0.0	28661.5
887. COOH=>CH20+OH	1.00E+09	0.0	7475.9	1001. M-C6H11O=>2-C5H10+CHO	3.70E+13	0.0	28661.5
888. C3COOH=>CH3CHO+OH	1.00E+09	0.0	7475.9	1002. G-C6H11O=>2-C5H10+CH3	3.70E+13	0.0	28661.5
890. C2H3COOH=>C2H5CHO+OH	1.00E+09	0.0	7475.9	1003. M-C6H11O=>C-S5H8O+CH3	3.70E+13	0.0	28661.5
891. C2H3COOH=>C2H5CHO+OH	1.00E+09	0.0	7475.9	1004. D-C6H11O=>4-CH24CHO+CH3H6	3.70E+13	0.0	28661.5
892. A3-C5H9=>B-C5H9	1.00E+20	0.0	0	1005. B-C6H11O=>3-TEAL+CH3	3.70E+13	0.0	28661.5
893. A3-C5H9=>C4H6+CH3	2.51E+13	0.0	29975.2	1006. B-C6H11O=>3-TEAL+CH3	7.40E+13	0.0	28661.5
894. A3-C5H9=>C2H5+CH3	2.51E+13	0.0	29975.2	1007. B-C6H11O=>3M1BE+CHO	3.70E+13	0.0	28661.5
895. 4-C5O2=>3C5OOH4	5.96E+12	0.0	27880.5	1008. N-C6H11O=>2C2H4CHO+CH3H6	3.70E+13	0.0	28661.5
896. 4-C5O2=>1C5H12=>4C5OOH+1-C5H11	8.94E+12	0.0	29679.0	1009. I-C6H11O=>1-C3H7+CH2CO	2.00E+13	0.0	13709.8
897. 4-C5O2=>2C5OOH4	4.96E+11	0.0	22136.2	1010. F-C6H11O=>2-C5H8O+CH3	2.00E+13	0.0	13709.8
898. 4-C5O2=>1C5H12=>4C5OOH+1-C5H11	6.18E+10	0.0	21085.3	1011. F-C6H11O=>2TE4ON+CH3	7.40E+13	0.0	28661.5
899. 4-C5O2+1-C5H12=>4C5OOH+2-C5H11+O2	1.75E+10	0.0	-3272.2	1012. H-C6H11O=>CH3COCH2+CH3H6	3.70E+13	0.0	28661.5
900. 4-C5O2+H2O2=>4C5OOH+H2O2	2.41E+12	0.0	9933.6	1			

Low pressure limit: 0.16500E+27 -0.33000E+01 0.00000E+00	Reverse Arrhenius coefficients:	5.18E+15 -0.3 57960.0
TROE centering: 0.49500E+00 0.23255E+04 0.10000E+02 0.00000E+00	HCO+O2=CO+HO2	7.58E+12 0.0 410.0
1029. CH3O2+CH2O=CH3OOH+CHO 1.30E+11 0.0 9004.5	Reverse Arrhenius coefficients:	9.03E+11 0.3 32930.0
1030. CH3O2+CH3=CH3O+CH3O 1.65E+13 0.0 -1194.2	HO2+H=OH+OH	7.08E+13 0.0 300.0
1031. CH3O2+HO2=CH3OOH+O2 2.40E+11 0.0 -1576.4	Reverse Arrhenius coefficients:	1.35E+14 -0.3 39570.0
1032. CH3O2+CH3O2=>CH2O+CH3OH+O2 2.80E+10 0.0 -788.2	HO2+H=H2+O2	1.66E+13 0.0 820.0
1033. CH3O2+CH3O2=>CH3O+CH3O+O2 2.70E+10 0.0 -788.2	Reverse Arrhenius coefficients:	9.14E+14 -0.3 58300.0
1034. HCO+OH=CO+H2O 1.02E+14 0.0 0.0	HO2+OH=H2O+O2	2.89E+13 0.0 -500.0
Reverse Arrhenius coefficients: 2.90E+15 0.0 105200.0	Reverse Arrhenius coefficients:	6.89E+15 -0.3 72140.0
1035. CO+OH=CO2+H 1.40E+05 1.9 -1347.0	H2O2+O2=HO2+HO2	5.35E+17 -0.7 53150.0
Reverse Arrhenius coefficients: 1.57E+07 1.9 20990.0	Reverse Arrhenius coefficients:	4.20E+14 0.0 11980.0
1036. H2+O2=O+OH 1.97E+14 0.0 16540.0	H2O2+H=H2O+OH	2.41E+13 0.0 3970.0
Reverse Arrhenius coefficients: 1.56E+13 0.0 425.0	Reverse Arrhenius coefficients:	7.75E+12 0.0 74710.0
1037. O+H2=H+OH 5.08E+04 2.7 6292.0	CH4+HO2=CH3+H2O2	3.42E+11 0.0 19290.0
Reverse Arrhenius coefficients: 2.23E+04 2.7 4197.0	Reverse Arrhenius coefficients:	3.36E+11 -0.3 2502.0
1038. O+H2O=OH+OH 2.97E+06 2.0 13400.0	CH2O+HO2=HCO+H2O2	6.40E-02 4.5 6557.0
Reverse Arrhenius coefficients: 3.01E+05 2.0 -3850.0	Reverse Arrhenius coefficients:	1.19E-02 4.2 4921.0
1039. OH+H2=H+H2O 2.16E+08 1.5 3430.0	HO+M=O+H+M	3.91E+22 -2.0 105300.0
Reverse Arrhenius coefficients: 9.35E+08 1.5 18580.0	Reverse Arrhenius coefficients:	4.72E+18 -1.0 0.0
1040. HCO+M=H+CO-M 1.86E+17 -1.0 17000.0	H2 Enhanced by 2.500E+00	
Reverse Arrhenius coefficients: 6.47E+13 0.0 -442.0	H2O Enhanced by 1.200E+01	
1041. H2O2+OH=H2O+HO2 1.00E+12 0.0 0.0	CO Enhanced by 1.900E+00	
Reverse Arrhenius coefficients: 1.68E+11 0.3 31460.0	CO2 Enhanced by 3.800E+00	
1042. C2H4+O=CH3+HCO 1.02E+07 1.9 179.0	1083. O2+M+O+M 6.47E+20 -1.5 121500.0	
Reverse Arrhenius coefficients: 2.85E+08 1.1 31770.0	Reverse Arrhenius coefficients: 6.17E+15 -0.5 0.0	
1043. H+C2H4(+M)=C2H5(+M) 1.08E+05 0.5 1822.0	H2 Enhanced by 2.500E+00	
Low pressure limit: 0.11120E+35 -0.50000E+01 0.44480E+04	H2O Enhanced by 1.200E+01	
TROE centering: 0.10000E+01 0.10000E-14 0.95000E+02 0.20000E+03	CO Enhanced by 1.900E+00	
H2 Enhanced by 2.000E+00	CO2 Enhanced by 3.800E+00	
H2O Enhanced by 5.000E+00		
CO Enhanced by 2.000E+00		
CO2 Enhanced by 3.000E+00		
1044. CH3OH(+M)=CH3-OH(+M) 1.90E+16 0.0 91730.0	1084. H2+M=H+H+M 4.57E+19 -1.4 104400.0	
Low pressure limit: 0.29500E+45 -0.73500E+01 0.95460E+05	Reverse Arrhenius coefficients: 2.42E+15 -0.4 -3040.0	
TROE centering: 0.41400E+00 0.27900E+03 0.54590E+04 0.10000E+11	H2 Enhanced by 2.500E+00	
H2 Enhanced by 2.000E+00	H2O Enhanced by 1.200E+01	
H2O Enhanced by 1.600E+01	CO Enhanced by 1.900E+00	
CO Enhanced by 2.000E+00	CO2 Enhanced by 3.800E+00	
CO2 Enhanced by 3.000E+00		
1045. C2H6+H=C2H5+H2 5.54E+02 3.5 5167.0	1085. C2H3+H(+M)=C2H4(+M) 6.10E+12 0.3 280.0	
Reverse Arrhenius coefficients: 1.36E-01 4.1 8857.0	Low pressure limit: 0.98000E+30 -0.38600E+01 0.33200E+04	
1046. CH3OH+HO2=CH2O+H2O2 3.98E+13 0.0 19400.0	TROE centering: 0.78200E+00 0.20800E+03 0.26630E+04 0.60950E+04	
Reverse Arrhenius coefficients: 3.13E+15 -0.9 10750.0	H2 Enhanced by 2.500E+00	
1047. C2H5+O2=C2H4+H2O 1.22E+30 -5.8 10100.0	H2O Enhanced by 1.200E+01	
Reverse Arrhenius coefficients: 1.26E+30 -5.6 22310.0	CO Enhanced by 1.900E+00	
1048. C2H6+OH=C2H5+H2O 5.12E+06 2.1 855.0	CO2 Enhanced by 3.800E+00	
Reverse Arrhenius coefficients: 1.01E+07 -2.1 29880.0		
1049. C2H6+O=C2H5+OH 1.13E+14 0.0 7850.0	1087. C2H2+H(+M)=C2H3(+M) 3.11E+11 0.6 2589.0	
Reverse Arrhenius coefficients: 2.08E+13 0.0 127200.0	Low pressure limit: 0.22540E+41 -0.72690E+01 0.65770E+04	
1050. CH3+HO2=CH3+OH 1.10E+13 0.0 0.0	TROE centering: 0.10000E+01 0.10000E-14 0.67500E+03 0.10000E+16	
Reverse Arrhenius coefficients: 4.78E+14 -0.3 24550.0	H2 Enhanced by 2.000E+00	
1051. CO+HO2=CO2+OH 3.01E+13 0.0 23000.0	H2O Enhanced by 5.000E+00	
Reverse Arrhenius coefficients: 6.44E+15 -0.3 84610.0	CO Enhanced by 2.000E+00	
1052. CH3+CH3(+M)=C2H6(+M) 9.21E+16 -1.2 635.8	CO2 Enhanced by 3.000E+00	
Low pressure limit: 0.11350E+37 -0.52460E+01 0.17050E+04	1088. C2H4+H=C2H3+H2 8.42E-03 4.6 2583.0	
TROE centering: 0.40500E+00 0.11200E+04 0.69600E+02 0.10000E+16	Reverse Arrhenius coefficients: 5.72E-01 3.8 3233.0	
H2 Enhanced by 2.000E+00	1089. C2H4+H=C2H3+H2O 2.02E+13 0.0 5955.0	
H2O Enhanced by 5.000E+00	Reverse Arrhenius coefficients: 1.02E+13 0.0 20220.0	
CO Enhanced by 2.000E+00	1090. C2H3-O2=C2H2+HO2 5.19E-15 -1.3 3310.0	
CO2 Enhanced by 3.000E+00	Reverse Arrhenius coefficients: 2.73E-16 -0.9 11400.0	
1053. H2O+M=H+OH+M 1.84E+27 -3.0 122600.0	Declared duplicate reaction..	
Reverse Arrhenius coefficients: 2.25E+22 -2.0 0.0	1091. C2H2+M=C2H+H-M 4.20E+16 0.0 107000.0	
H2 Enhanced by 2.500E+00	Reverse Arrhenius coefficients: 7.13E+07 2.1 -28910.0	
H2O Enhanced by 1.200E+01	1092. C2H2+O2=HCCO+OH 2.00E+08 1.5 30100.0	
CO Enhanced by 1.900E+00	Reverse Arrhenius coefficients: 2.23E+05 1.5 25400.0	
CO2 Enhanced by 3.800E+00	1093. C2H2+O2=CO+H2O 7.28E+19 -2.5 1809.0	
1054. H+O2(+M)=HO2(+M) 1.62E+11 0.6 0.0	Reverse Arrhenius coefficients: 8.51E+20 -2.5 179800.0	
Low pressure limit: 0.35000E+17 -0.41000E+00 -0.11160E+04	1094. C2H2+O2=CH+H2O 3.37E+07 2.0 14000.0	
TROE centering: 0.50000E+00 0.10000E-29 0.10000E+31 0.10000E+11	Reverse Arrhenius coefficients: 4.67E+03 3.1 685.0	
H2 Enhanced by 2.500E+00	1095. O+C2H2-C2H+OH 3.16E+15 -0.6 15000.0	
H2O Enhanced by 5.000E+00	Reverse Arrhenius coefficients: 4.44E+10 0.5 -1570.0	
CO Enhanced by 2.000E+00	1096. C2H2O+O=CH2+CO 6.12E+06 2.0 52570.0	
CO2 Enhanced by 3.000E+00	Reverse Arrhenius coefficients: 1.15E+06 2.0 52570.0	
1055. CO+O(+M)=CO2(+M) 1.80E+10 0.0 2384.0	1097. C2H2+O2=HCO+CO 2.41E+12 0.0 0.0	
Low pressure limit: 0.13500E+25 -0.27880E+01 0.41910E+04	Reverse Arrhenius coefficients: 1.33E+16 -1.1 154100.0	
TROE centering: 0.50000E+00 0.10000E-29 0.10000E+31 0.10000E+11	1098. C2H+O=CO+CH 1.81E+13 0.0 0.0	
H2 Enhanced by 2.500E+00	Reverse Arrhenius coefficients: 7.48E+16 -1.1 82130.0	
H2O Enhanced by 1.200E+01	1099. CH2+O2=HCO+OH 1.29E+20 -3.3 284.0	
CO Enhanced by 1.900E+00	Reverse Arrhenius coefficients: 5.31E+19 -3.3 73170.0	
CO2 Enhanced by 3.800E+00	Reverse Arrhenius coefficients: 5.00E+13 0.0 0.0	
1056. CO+O2=CO2+O 1.07E-15 7.1 13320.0	Reverse Arrhenius coefficients: 0.00E+00 0.0 0.0	
Reverse Arrhenius coefficients: 9.44E-15 7.1 19540.0	1100. CH2+O+CO+H-H 1.00E+18 -1.6 0.0	
1057. HCO+H=CO+H2 7.34E+13 0.0 0.0	Reverse Arrhenius coefficients: 7.03E+17 -1.6 2990.0	
Reverse Arrhenius coefficients: 4.81E+14 0.0 90000.0	1102. CH2+OH=CH+H2O 1.13E+07 2.0 3000.0	
1058. HCO+O=CO+OH 3.02E+13 0.0 0.0	Reverse Arrhenius coefficients: 3.44E+07 2.0 21150.0	
Reverse Arrhenius coefficients: 8.70E+13 0.0 87900.0	1103. CH2+O2=CO+H+H 3.29E+21 -3.3 2868.0	
1059. CH2O+M=HCO+H-M 6.28E+29 -3.6 93200.0	Reverse Arrhenius coefficients: 0.00E+00 0.0 0.0	
Reverse Arrhenius coefficients: 2.66E+24 -2.6 427.0	1104. CH+O2=HCO+O 4.40E+13 0.0 71990.0	
1060. CH2O+OH=HCO+H2O 3.09E+10 1.2 -447.0	Reverse Arrhenius coefficients: 7.10E+06 1.8 -596.0	
Reverse Arrhenius coefficients: 1.19E+09 1.2 29380.0	1105. CH3OH+OH=CH2OH+H2O 3.29E+01 3.5 22720.0	
1061. CH2O+H=HCO+H2 9.33E+08 1.5 2976.0	Reverse Arrhenius coefficients: 3.60E+12 0.0 6095.0	
Reverse Arrhenius coefficients: 7.45E+07 1.5 17650.0	Reverse Arrhenius coefficients: 7.47E+12 0.0 7825.0	
1062. CH2O+O=HCO+OH 4.16E+11 0.6 2762.0	Reverse Arrhenius coefficients: 1.44E+13 0.0 6095.0	
Reverse Arrhenius coefficients: 1.46E+10 0.6 15340.0	1107. CH3OH+H=CH2OH+H2 1.54E+07 1.7 14250.0	
1063. CH3+OH=CH2O+H2 2.25E+13 0.0 4300.0	Reverse Arrhenius coefficients: 3.19E+01 3.2 7172.0	
Reverse Arrhenius coefficients: 6.76E+14 0.0 76030.0	1108. CH3OH+CH=CH2OH+CH4 8.93E-04 4.8 15810.0	
1064. CH3+O=CH2O+H 8.00E+13 0.0 0.0	Reverse Arrhenius coefficients: 3.88E+05 2.5 3080.0	
Reverse Arrhenius coefficients: 1.06E+15 0.0 69630.0	1109. CH3OH+O=CH2OH+OH 4.96E-03 2.5 8781.0	
1065. CH3+O2=CH3+O 2.00E+18 -1.6 29210.0	Reverse Arrhenius coefficients: 3.81E+06 2.0 1641.0	
Reverse Arrhenius coefficients: 3.58E+18 -1.6 -1631.0	Reverse Arrhenius coefficients: 1.77E+11 0.7 24180.0	
1066. CH2O+CH3-HCO+CH4 3.64E-06 5.4 998.0	1111. CH2OH(+M)=CH2O+H(-M) 2.80E+14 -0.7 32820.0	
Reverse Arrhenius coefficients: 7.58E-04 5.4 16150.0	Low pressure limit: 0.60100E+34 -0.53900E+01 0.36200E+05	
1067. HCO+CH3=CH4+CO 1.21E+14 0.0 0.0	TROE centering: 0.96000E+00 0.67600E+02 0.18550E+04 0.75430E+04	
Reverse Arrhenius coefficients: 2.07E+16 0.0 90480.0	1112. C2H3+O2=C2H2+H2O 2.12E-06 6.0 9484.0	
1068. CH3O(+M)=CH2O+H(-M) 5.45E+13 0.0 13500.0	Reverse Arrhenius coefficients: 1.11E-07 6.3 17570.0	
Low pressure limit: 0.23440E+26 -0.27000E+01 0.30600E+05	Declared duplicate reaction..	
1069. C2H4(+M)=C2H2+H2(+M) 1.80E+13 0.0 76000.0	1113. H2O2+O=OH+H2O 9.55E+06 2.0 3970.0	
Low pressure limit: 0.15000E+16 0.00000E+00 0.55443E+05	Reverse Arrhenius coefficients: 2.54E+07 1.7 19850.0	
1070. HO2+O=OH+O2 3.25E+13 0.0 0.0	1114. C2H2+O=HCCO+H 1.43E+07 2.0 1900.0	
Reverse Arrhenius coefficients: 7.86E+14 -0.3 55390.0	Reverse Arrhenius coefficients: 2.02E+05 2.0 13310.0	
1071. HCO+HO2=CH2O+O2 2.97E+10 0.3 -3861.0	1115. C2H2+OH=CH2CO+H 2.19E-04 4.5 -1000.0	
Reverse Arrhenius coefficients: 2.05E+13 0.0 38950.0	Reverse Arrhenius coefficients: 2.16E-03 4.5 19670.0	
1072. CH3+O2=CH2O+H2O2 6.05E+10 0.0 2424.0	1116. CH2CO+H=CH3+CO 1.10E+13 0.0 34000.0	
Reverse Arrhenius coefficients: 1.32E+09 0.3 31390.0	Reverse Arrhenius coefficients: 2.40E+12 0.0 40200.0	
1073. CH3+HO2=CH4+O2 3.24E+12 0.0 0.0	1117. CH2CO+O=CH2+CO2 1.75E+12 0.0 1350.0	
	Reverse Arrhenius coefficients: 3.74E+12 0.0 53690.0	
	1118. CH2+O2=CH2O+O 3.29E+21 -3.3 2868.0	
	Reverse Arrhenius coefficients: 3.86E+22 -3.3 63180.0	
	Low pressure limit: 0.36000E+16 0.00000E+00 0.59270E+05	

1120. CH2CO+O=HCCO+OH	1.00E+13	0.0	8000.0		2.28E+14	-0.6	28400.0
Reverse Arhenius coefficients:	1.43E+10	0.0	-1255.0	Reverse Arhenius coefficients:	4.10E+11	0.0	7204.0
1121. CH2CO+OH=HCCO+H2O	1.00E+13	0.0	2000.0	N-C3H7-H+C3H6	2.67E+15	-0.6	36820.0
Reverse Arhenius coefficients:	1.41E+11	0.0	9995.0	Reverse Arhenius coefficients:	1.00E+13	0.0	2500.0
1122. CH2CO+H=HCCO+H2	2.00E+14	0.0	8000.0	N-C3H7+O2=C3H6+H2O	3.00E+11	0.0	3000.0
Reverse Arhenius coefficients:	6.52E+11	0.0	840.0	Reverse Arhenius coefficients:	2.00E+11	0.0	17500.0
1123. HCCO+OH=HCO+HCO	1.00E+13	0.0		C2H4+CH3O-C2H3+CH3OH	1.20E+11	0.0	6750.0
Reverse Arhenius coefficients:	4.82E+13	0.0	40360.0	Reverse Arhenius coefficients:	1.00E+10	0.0	9000.0
1124. HCCO+H=CH2(S)+CO	1.10E+14	0.0	0.0	C3H6-OH-T-C3H5+H2O	1.11E+06	2.0	1451.0
Reverse Arhenius coefficients:	6.66E+13	0.0	39260.0	Reverse Arhenius coefficients:	3.28E+03	2.7	12310.0
1125. HCCO+O-H=CO+CO	8.00E+13	0.0	0.0	C3H6-O-A-C3H5+OH	5.24E+11	0.7	5884.0
Reverse Arhenius coefficients:	0.00E+00	0.0		Reverse Arhenius coefficients:	1.06E+11	0.7	20820.0
1126. C2H6+O2=C2H5+H2O2	4.00E+13	0.0	50900.0	C3H6-O-S-C3H5+OH	1.20E+11	0.7	8959.0
Reverse Arhenius coefficients:	3.00E+11	0.0		Reverse Arhenius coefficients:	1.57E+08	1.2	460.0
1127. C2H6+H-O2=C2H5+H2O2	1.70E+13	0.0	20460.0	C3H6-O-T-C3H5+OH	6.03E+10	0.7	7632.0
Reverse Arhenius coefficients:	1.07E+11	0.2	7842.0	Reverse Arhenius coefficients:	1.80E+07	1.4	1243.0
1128. CH2-O2+CO2+H2	1.01E+21	-3.3	1508.0	C3H6-H-A-C3H5+H2	1.73E+05	2.5	2492.0
Reverse Arhenius coefficients:	3.05E+23	-3.3	186700.0	Reverse Arhenius coefficients:	7.93E+04	2.5	19520.0
1129. CH3+CH2+CH4+C2H2	3.92E+11	0.0	0.0	C3H6-O2-S-C3H5+H2O	2.00E+12	0.0	62900.0
Reverse Arhenius coefficients:	2.96E+13	0.0	66050.0	Reverse Arhenius coefficients:	1.08E+08	0.8	984.0
1130. CH3+CH2+CH4+C2H4	1.95E+13	-0.5	0.0	C3H6-H-C2H4+CH3	4.85E+33	-5.8	18500.0
Reverse Arhenius coefficients:	2.90E+16	-0.7	70170.0	Reverse Arhenius coefficients:	2.31E+33	-5.9	31620.0
1131. CH3OH+CH2O=CH3O+CH3O	3.84E+13	0.1	84720.0	I-C3H7+H-C3H6	8.57E+18	-1.6	40340.0
Reverse Arhenius coefficients:	6.03E+13	0.0		Reverse Arhenius coefficients:	1.30E+13	0.0	1560.0
1132. CH2O+CH3O=CH3O+HCO	1.15E+11	0.0	1280.0	I-C3H7+H-C2H5+CH3	2.00E+13	0.0	0.0
Reverse Arhenius coefficients:	3.02E+11	0.0	18160.0	Reverse Arhenius coefficients:	4.82E+09	0.7	12090.0
1133. CH4+CH3O=CH3+CH3OH	1.57E+11	0.0	8842.0	I-C3H7+O2=C3H6+H2O	4.50E+11	0.0	5020.0
Reverse Arhenius coefficients:	1.05E+09	0.0	50000.0	Reverse Arhenius coefficients:	2.00E+11	0.0	17500.0
1134. C2H6+CH3O=C2H5+CH3OH	3.00E+11	0.0	7000.0	C3H8-M-C3H2+M	7.90E+22	-1.8	88630.0
Reverse Arhenius coefficients:	1.71E+10	0.0	50000.0	Reverse Arhenius coefficients:	3.66E+14	-0.4	989.0
1135. C2H3+H-C2H2+H2	2.00E+13	0.0	2500.0	C3H8-O2-L-C3H7+H2O	4.00E+13	0.0	47500.0
Reverse Arhenius coefficients:	1.33E+13	0.0	68080.0	Reverse Arhenius coefficients:	2.08E+12	0.0	0.0
1136. CH3O+CH3OH=CH2OH+CH3OH	3.00E+11	0.0	4074.0	Reverse Arhenius coefficients:	1.30E+06	2.4	4471.0
Reverse Arhenius coefficients:	1.55E+05	1.7	10500.0	Reverse Arhenius coefficients:	4.71E+05	2.1	12180.0
1137. CH3OH+OH=CH3O+H2O	1.00E+08	2.1	496.7	C3H8-H2-L-C3H7	1.88E+05	2.8	6280.0
Reverse Arhenius coefficients:	8.98E+06	2.1	17380.0	Reverse Arhenius coefficients:	2.76E+01	3.4	9530.0
1138. C2H5+H=CH3+CH3	3.61E+13	0.0	0.0	C3H8-O-L-C3H7+OH	2.81E+13	0.0	5200.0
Reverse Arhenius coefficients:	5.45E+16	-1.0	16980.0	Reverse Arhenius coefficients:	1.87E+12	0.0	9607.0
1139. C2H3+O2=CH2O+HCO	1.70E+29	-5.3	6500.0	Reverse Arhenius coefficients:	1.13E+14	0.0	7850.0
Reverse Arhenius coefficients:	1.66E+29	-5.3	93050.0	Reverse Arhenius coefficients:	7.53E+12	0.0	12260.0
1140. C2H6+C2H5+H	2.78E+21	-1.6	103800.0	C3H8-OH-N-C3H7+H2O	1.05E+10	1.0	1586.0
Reverse Arhenius coefficients:	3.61E+13	0.0	0.0	Reverse Arhenius coefficients:	6.93E+09	1.0	23250.0
1141. P-C2H4OH=C2H4+OH	1.29E+12	-0.4	26850.0	I-C3H7+O-L-C3H7+H2O	4.67E+07	1.6	-35.0
Reverse Arhenius coefficients:	9.93E+11	0.0	-960.0	Reverse Arhenius coefficients:	3.07E+07	1.6	21630.0
1142. S-C2H4OH+M=CHCCHO+H+M	1.00E+14	0.0	25000.0	C3H8-H2-O2-L-C3H7+H2O2	5.60E+12	0.0	17700.0
Reverse Arhenius coefficients:	4.71E+08	0.0	-3630.0	Reverse Arhenius coefficients:	4.16E+11	0.0	7426.0
1143. C2H4+CH3=C2H3+CH4	6.62E+00	3.7	9500.0	C3H8+H2-O2=N-C3H7+H2O2	1.68E+13	0.0	20430.0
Reverse Arhenius coefficients:	1.44E+00	0.0	5472.0	Reverse Arhenius coefficients:	2.33E+12	0.0	9826.0
1144. CH3CO(+M)=CH3-CO(+M)	3.00E+12	0.0	16720.0	C3H8+CH3-C2H4+L-C3H7	3.98E+11	0.0	9500.0
Low pressure limit: 0.12000E+16	0.00000E+00	0.0	12518E+05	Reverse Arhenius coefficients:	1.58E+12	0.0	16480.0
1145. CH3CHO=CH3+HCO	2.61E+15	0.1	80550.0	Reverse Arhenius coefficients:	1.29E+12	0.0	11600.0
Reverse Arhenius coefficients:	2.00E+13	0.0	0.0	Reverse Arhenius coefficients:	5.13E+12	0.0	18580.0
1146. CH3CHO+O2=CH3CO+H2O	3.01E+13	0.0	39150.0	Reverse Arhenius coefficients:	3.00E+10	0.0	12900.0
Reverse Arhenius coefficients:	8.55E+10	0.3	-1940.0	Reverse Arhenius coefficients:	1.00E+11	0.0	10400.0
1147. CH3CHO+OH=CH3CO+H2O	2.00E+00	1.8	1300.0	Reverse Arhenius coefficients:	1.31E+11	0.0	17800.0
Reverse Arhenius coefficients:	1.35E+06	1.8	32850.0	Reverse Arhenius coefficients:	1.00E+11	0.0	10400.0
1148. CH3CHO+H=CH3CO+H2	1.34E+13	0.0	3300.0	C2H3+CH3-C2H4+L-C3H7	1.00E+11	0.0	16480.0
Reverse Arhenius coefficients:	2.10E+12	0.0	19690.0	Reverse Arhenius coefficients:	1.31E+11	0.0	17800.0
1149. CH3CHO+O=CH3CO+OH	5.94E+12	0.0	1868.0	C2H3+CH3-C2H4+H-C3H7	1.00E+11	0.0	10400.0
Reverse Arhenius coefficients:	4.08E+11	0.0	16170.0	Reverse Arhenius coefficients:	1.31E+11	0.0	17800.0
1150. CH3CHO+H2O=CH3CO+H2O2	3.01E+12	0.0	11930.0	Reverse Arhenius coefficients:	1.00E+11	0.0	10400.0
Reverse Arhenius coefficients:	1.21E+13	-0.3	12010.0	Reverse Arhenius coefficients:	3.63E+10	0.0	9934.0
1151. CH3CHO+CH3=CH3CO+CH4	2.61E+06	1.8	5911.0	Reverse Arhenius coefficients:	1.00E+11	0.0	10400.0
Reverse Arhenius coefficients:	1.07E+07	1.8	22790.0	Reverse Arhenius coefficients:	3.98E+10	0.0	16100.0
1152. S-C3H5=C2H2+CH3	9.60E+39	-8.2	42030.0	Reverse Arhenius coefficients:	1.00E+10	0.0	9700.0
Reverse Arhenius coefficients:	1.61E+40	-8.6	20330.0	I-C3H8+CH3-H-C3H6	7.94E+11	0.0	20500.0
1153. C2H2+CH3-P-C3H4+H	1.21E+17	-1.2	16680.0	Reverse Arhenius coefficients:	1.00E+11	0.0	9800.0
Reverse Arhenius coefficients:	1.00E+14	0.0	4000.0	I-C3H8+CH3-N-C3H7+CH3H	3.00E+11	0.0	7000.0
1154. A-C3H5=C2H2+CH3	2.40E+48	-9.9	82080.0	Reverse Arhenius coefficients:	1.22E+10	0.0	9182.0
Reverse Arhenius coefficients:	2.61E+46	-9.8	36950.0	Reverse Arhenius coefficients:	3.00E+11	0.0	7000.0
1155. C3H6-C2H3+CH3	2.73E+02	-13.3	123200.0	Reverse Arhenius coefficients:	1.22E+10	0.0	9182.0
Reverse Arhenius coefficients:	4.71E+59	-13.2	29540.0	Reverse Arhenius coefficients:	1.23E+47	-9.7	74260.0
1156. C2H2+CH3-A-C3H4+H	6.74E+19	-2.1	31590.0	Reverse Arhenius coefficients:	3.02E+41	-8.7	26620.0
Reverse Arhenius coefficients:	1.15E+16	-0.7	15790.0	Reverse Arhenius coefficients:	1.92E+66	-14.2	128100.0
1157. I-C4H8-T-C3H5-1-C4H7+C3H6	7.94E+11	0.0	20500.0	Reverse Arhenius coefficients:	2.09E+59	-13.2	29530.0
Reverse Arhenius coefficients:	5.59E+20	-1.3	80170.0	Reverse Arhenius coefficients:	2.76E+55	-11.5	114300.0
1158. I-C4H8-T-C3H5-1-C4H7+C3H6	7.94E+11	0.0	20500.0	Reverse Arhenius coefficients:	3.30E+52	-11.1	24460.0
Reverse Arhenius coefficients:	5.59E+20	-1.3	82170.0	Reverse Arhenius coefficients:	6.89E+06	1.9	20100.0
1159. C3H6-A-C3H5+H	2.01E+61	-13.3	118500.0	Reverse Arhenius coefficients:	1.21E+11	0.7	7633.0
Reverse Arhenius coefficients:	4.89E+56	-12.2	28080.0	Reverse Arhenius coefficients:	1.07E+12	0.1	23150.0
1160. C3H6+OH-A-C2H2+CH3+H	2.50E+07	1.8	76.0	Reverse Arhenius coefficients:	5.20E+06	2.0	-298.0
Reverse Arhenius coefficients:	1.00E+00	0.0	0.0	Reverse Arhenius coefficients:	4.56E+08	1.4	32470.0
1161. C3H6+O-C2H2+HCO	1.58E+07	1.8	-1216.0	Reverse Arhenius coefficients:	1.58E+07	1.8	-1216.0
Reverse Arhenius coefficients:	1.40E+05	1.9	26510.0	Reverse Arhenius coefficients:	1.75E+09	0.5	27580.0
1162. C3H6+O-C3HCO+H+H	2.50E+07	-1.8	76.0	Reverse Arhenius coefficients:	6.00E+00	0.0	0.0
Reverse Arhenius coefficients:	0.00E+00	0.0		Reverse Arhenius coefficients:	1.34E+15	-0.5	38320.0
1163. C3H6-S-C3H5+H	7.71E+69	-16.1	140000.0	Reverse Arhenius coefficients:	1.75E+11	0.0	7600.0
Reverse Arhenius coefficients:	1.22E+63	-14.6	26160.0	Reverse Arhenius coefficients:	1.20E+14	0.0	49300.0
1164. C3H6+H2O2-A-C3H5+H2O2	1.50E+11	0.0	14190.0	Reverse Arhenius coefficients:	4.00E+13	0.0	1300.0
Reverse Arhenius coefficients:	5.87E+05	1.3	9759.0	Reverse Arhenius coefficients:	1.00E+11	0.0	37000.0
1165. C3H6+H2O2-S-C3H5+H2O2	7.50E+09	0.0	12570.0	Reverse Arhenius coefficients:	5.00E+10	0.0	7000.0
Reverse Arhenius coefficients:	2.31E+04	1.3	-13420.0	Reverse Arhenius coefficients:	1.00E+11	0.0	15900.0
1166. C3H6+H2O2-T-C3H5+H2O2	3.00E+09	0.0	9930.0	Reverse Arhenius coefficients:	1.23E+11	0.0	15000.0
Reverse Arhenius coefficients:	9.23E+03	1.3	-14060.0	Reverse Arhenius coefficients:	1.23E+11	0.0	46720.0
1167. C3H6+OH-A-C3H5+H2O	2.81E+06	2.0	-298.0	Reverse Arhenius coefficients:	1.60E+12	0.0	0.0
Reverse Arhenius coefficients:	6.19E+06	2.0	31880.0	Reverse Arhenius coefficients:	1.60E+12	0.0	0.0
1168. C3H6+OH-S-C3H5+H2O	2.11E+06	2.0	2778.0	Reverse Arhenius coefficients:	2.35E+12	0.0	0.0
Reverse Arhenius coefficients:	1.72E+04	2.5	11530.0	Reverse Arhenius coefficients:	1.60E+12	0.0	0.0
1169. C4H6-C2H3+C2H3	4.03E+19	-1.0	98150.0	Reverse Arhenius coefficients:	8.00E+12	0.0	0.0
Reverse Arhenius coefficients:	1.26E+13	0.0	0.0	Reverse Arhenius coefficients:	7.05E+13	0.0	57280.0
1170. C4H6+OH-C2H5+CH2CO	1.00E+12	0.0	0.0	Reverse Arhenius coefficients:	1.00E+11	0.0	
Reverse Arhenius coefficients:	3.73E+12	0.0	30200.0	Reverse Arhenius coefficients:	1.00E+11	0.0	
1171. C4H6+OH=CH2O+A-C3H5	1.00E+12	0.0	0.0	Reverse Arhenius coefficients:	1.00E+11	0.0	
Reverse Arhenius coefficients:	3.50E+06	0.0	71060.0	Reverse Arhenius coefficients:	1.00E+11	0.0	
1172. C4H6+OH-C2H3+CH3CHO	1.00E+12	0.0	0.0	Reverse Arhenius coefficients:	1.00E+11	0.0	
Reverse Arhenius coefficients:	5.44E+11	0.0	18550.0	Reverse Arhenius coefficients:	1.00E+11	0.0	
1173. C4H6+O-C2H4+CH2CO	1.00E+12	0.0	0.0	Reverse Arhenius coefficients:	1.00E+11	0.0	
Reverse Arhenius coefficients:	6.38E+11	0.0	94340.0	Reverse Arhenius coefficients:	1.00E+11	0.0	
1174. C4H6+O-C2H2+O-C3H4	1.00E+12	0.0	0.0	Reverse Arhenius coefficients:	1.00E+11	0.0	
Reverse Arhenius coefficients:	1.08E+12	0.0	79050.0	Reverse Arhenius coefficients:	1.00E+11	0.0	
1175. C2H4+O2=C2H3+H2O2	4.00E+13	0.0	58200.0	Reverse Arhenius coefficients:	1.00E+11	0.0	
Reverse Arhenius coefficients:	4.94E+13	-0.5	1368.0	Reverse Arhenius coefficients:	1.00E+11	0.0	
1176. CH2O+M=CO+H2+M	1.83E+32	-4.4	87120.0	Reverse Arhen			

1234. A-C3H5+C4H7=C3H6+C4H6	6.31E+12	0.0	0.0
Reverse Arrhenius coefficients:			
1235. C4H7-O2-C4H6-HO2	1.00E+09	0.0	0.0
Reverse Arrhenius coefficients:			
1236. H+C4H7-C4H6+H2	3.16E+13	0.0	0.0
Reverse Arrhenius coefficients:			
1237. C2H5+C4H7=C4H6+C2H6	1.07E+13	0.0	56810.0
Reverse Arrhenius coefficients:			
1238. C2H5+C4H7=C2H4+-1-C4H8	3.98E+12	0.0	49840.0
Reverse Arrhenius coefficients:			
1239. C2H5+C4H7=C2H4+-2-C4H8	3.21E+12	0.0	924E-06 1.5 -962.0
Reverse Arrhenius coefficients:			
1240. C2H3+C4H7=C2H4+C4H6	7.81E+02	2.9	50960.0
Reverse Arrhenius coefficients:			
1241. C2H3+C4H7=C2H4+C4H6	5.00E+11	0.0	5.00E-11 0.0 0.0
Reverse Arrhenius coefficients:			
1242. C2-C4H8+OH-C2H5+CH3CHO	8.48E+11	0.0	56330.0
Reverse Arrhenius coefficients:			
1243. C2-C4H8+OH-C2H5+CH3CHO	3.98E+12	0.0	0.0
Reverse Arrhenius coefficients:			
1244. C2-C4H8+OH-C2H5+CH3CHO	1.16E+13	0.0	57710.0
Reverse Arrhenius coefficients:			
1245. C2-C4H8+O-L-C3H7+HCO	4.11E+18	-1.0	97350.0
Reverse Arrhenius coefficients:			
1246. C2-C4H8+OH-C4H7+CH4	5.00E+13	0.0	0.0
Reverse Arrhenius coefficients:			
1247. C2-C4H8+OH-C4H7+CH4	1.00E+11	0.0	82000.0
Reverse Arrhenius coefficients:			
1248. C2-C4H8+OH-C4H7+H2	6.00E+11	0.0	18760.0
Reverse Arrhenius coefficients:			
1249. C2-C4H8+OH-C4H7+H2	5.00E+13	0.0	3800.0
Reverse Arrhenius coefficients:			
1250. C2-C4H8+O-C2H4-CH3CHO	3.16E+13	0.0	22300.0
Reverse Arrhenius coefficients:			
1251. C2-C4H8+O-C2H3+C2H5	2.60E+13	0.0	0.0
Reverse Arrhenius coefficients:			
1252. C2-C4H8+O-H-C4H4	2.43E+13	0.0	19930.0
Reverse Arrhenius coefficients:			
1253. C2-C4H8+CH3-C4H7+CH4	2.79E+06	2.1	-1775.0
Reverse Arrhenius coefficients:			
1254. C2-C4H8+O2-C4H7+H2O2	1.05E+05	2.1	24040.0
Reverse Arrhenius coefficients:			
1255. C2-C4H8+O2-C4H7+H2O2	3.90E+13	0.0	2217.0
Reverse Arrhenius coefficients:			
1256. C2-C4H8+O-C3H5-C4H7+C3H6	4.77E+12	0.0	26470.0
Reverse Arrhenius coefficients:			
1257. C2-C4H8+O2-C4H7+H2O2	4.64E+04	2.1	-1775.0
Reverse Arrhenius coefficients:			
1258. C2-C4H8+O2-C4H7+H2O2	7.40E+01	2.1	82480.0
Reverse Arrhenius coefficients:			
1259. C2-C4H8+O2-C4H7+H2O2	3.20E+12	0.0	14900.0
Reverse Arrhenius coefficients:			
1260. C2-C4H8+O2-C4H7+H2O2	1.58E+11	0.0	47000.0
Reverse Arrhenius coefficients:			
1261. C2-C4H8+O2-C4H7+H2O2	8.00E+13	0.0	35400.0
Reverse Arrhenius coefficients:			
1262. C2-C4H8+O2-C4H7+H2O2	3.00E+11	0.0	71000.0
Reverse Arrhenius coefficients:			
1263. C2-C4H8+O2-C4H7+H2O2	5.00E+12	0.0	0.0
Reverse Arrhenius coefficients:			
1264. C2-C4H8+O2-C4H7+H2O2	1.00E+19	-1.0	96770.0
Reverse Arrhenius coefficients:			
1265. C2-C4H8+O2-C4H7+H2O2	9.00E+12	0.0	0.0
Reverse Arrhenius coefficients:			
1266. C2-C4H8+O2-C4H7+H2O2	4.11E+18	-1.0	97350.0
Reverse Arrhenius coefficients:			
1267. C2-C4H8+O2-C4H7+H2O2	5.00E+13	0.0	0.0
Reverse Arrhenius coefficients:			
1268. C2-C4H8+O2-C4H7+H2O2	1.00E+11	0.0	73000.0
Reverse Arrhenius coefficients:			
1269. C2-C4H8+O2-C4H7+H2O2	6.00E+11	0.0	17860.0
Reverse Arrhenius coefficients:			
1270. C2-C4H8+O2-C4H7+H2O2	5.00E+13	0.0	39000.0
Reverse Arrhenius coefficients:			
1271. C2-C4H8+O2-C4H7+H2O2	5.00E+13	0.0	40970.0
Reverse Arrhenius coefficients:			
1272. C2-C4H8+O2-C4H7+H2O2	1.00E+13	0.0	12000.0
Reverse Arrhenius coefficients:			
1273. C2-C4H8+O2-C4H7+H2O2	4.50E+19	0.0	50200.0
Reverse Arrhenius coefficients:			
1274. C2-C4H8+O2-C4H7+H2O2	2.00E+19	0.0	17500.0
Reverse Arrhenius coefficients:			
1275. C2-C4H8+O2-C4H7+H2O2	3.00E+11	0.0	30230.0
Reverse Arrhenius coefficients:			
1276. C2-C4H8+O2-C4H7+H2O2	3.30E+11	0.0	7200.0
Reverse Arrhenius coefficients:			
1277. C2-C4H8+O2-C4H7+H2O2	5.20E+20	-2.4	39720.0
Reverse Arrhenius coefficients:			
1278. C2-C4H8+O2-C4H7+H2O2	1.00E+13	0.0	2900.0
Reverse Arrhenius coefficients:			
1279. C2-C4H8+O2-C4H7+H2O2	3.59E+20	-2.1	40970.0
Reverse Arrhenius coefficients:			
1280. C2-C4H8+O2-C4H7+H2O2	1.00E+13	0.0	12000.0
Reverse Arrhenius coefficients:			
1281. C2-C4H8+O2-C4H7+H2O2	4.50E+19	0.0	50200.0
Reverse Arrhenius coefficients:			
1282. C2-C4H8+O2-C4H7+H2O2	2.00E+19	0.0	17500.0
Reverse Arrhenius coefficients:			
1283. C2-C4H8+O2-C4H7+H2O2	3.00E+11	0.0	3000.0
Reverse Arrhenius coefficients:			
1284. C2-C4H8+O2-C4H7+H2O2	2.00E+19	0.0	17500.0
Reverse Arrhenius coefficients:			
1285. C2-C4H8+O2-C4H7+H2O2	3.90E+37	-7.4	38670.0
Reverse Arrhenius coefficients:			
1286. C2-C4H8+O2-C4H7+H2O2	1.59E+34	-7.1	18030.0
Reverse Arrhenius coefficients:			
1287. C2-C4H8+O2-C4H7+H2O2	5.98E+32	-6.2	40070.0
Reverse Arrhenius coefficients:			
1288. C2-C4H8+O2-C4H7+H2O2	1.61E+29	-5.2	6265.0
Reverse Arrhenius coefficients:			
1289. C2-C4H8+O2-C4H7+H2O2	1.50E+19	0.0	20000.0
Reverse Arrhenius coefficients:			
1290. C2-C4H8+O2-C4H7+H2O2	2.00E+03	0.0	17500.0
Reverse Arrhenius coefficients:			
1291. C2-C4H8+O2-C4H7+H2O2	1.91E+84	-20.5	45370.0
Reverse Arrhenius coefficients:			
1292. C2-C4H8+O2-C4H7+H2O2	5.24E+09	-20.2	46440.0
Reverse Arrhenius coefficients:			
1293. C2-C4H8+O2-C4H7+H2O2	9.85E+95	-23.1	147600.0
Reverse Arrhenius coefficients:			
1294. C2-C4H8+O2-C4H7+H2O2	8.68E+89	-22.1	44410.0
Reverse Arrhenius coefficients:			
1295. C2-C4H8+O2-C4H7+H2O2	1.26E+14	0.0	7300.0
Reverse Arrhenius coefficients:			
1296. C2-C4H8+O2-C4H7+H2O2	1.00E+12	0.0	16000.0
Reverse Arrhenius coefficients:			
1297. C2-C4H8+O2-C4H7+H2O2	1.00E+14	0.0	8400.0
Reverse Arrhenius coefficients:			
1298. C2-C4H8+O2-C4H7+H2O2	3.20E+12	0.0	15700.0
Reverse Arrhenius coefficients:			
1299. C2-C4H8+O2-C4H7+H2O2	1.00E+11	0.0	21000.0
Reverse Arrhenius coefficients:			
1300. C2-C4H8+O2-C4H7+H2O2	8.20E+12	0.0	14200.0
Reverse Arrhenius coefficients:			
1301. C2-C4H8+O2-C4H7+H2O2	2.00E+11	0.0	15000.0
Reverse Arrhenius coefficients:			
1302. C2-C4H8+O2-C4H7+H2O2	5.73E+10	0.5	63.0
Reverse Arrhenius coefficients:			
1303. C2-C4H8+O2-C4H7+H2O2	1.17E+11	0.5	21600.0
Reverse Arrhenius coefficients:			
1304. C2-C4H8+O2-C4H7+H2O2	2.00E+19	0.0	2900.0
Reverse Arrhenius coefficients:			
1305. C2-C4H8+O2-C4H7+H2O2	3.00E+10	0.0	12400.0
Reverse Arrhenius coefficients:			
1306. C2-C4H8+O2-C4H7+H2O2	1.00E+10	0.0	14900.0
Reverse Arrhenius coefficients:			
1307. C2-C4H8+O2-C4H7+H2O2	3.00E+12	0.0	12300.0
Reverse Arrhenius coefficients:			
1308. C2-C4H8+O2-C4H7+H2O2	1.00E+11	0.0	12920.0
Reverse Arrhenius coefficients:			
1309. C2-C4H8+O2-C4H7+H2O2	1.00E+12	0.0	11040.0
Reverse Arrhenius coefficients:			
1310. C2-C4H8+O2-C4H7+H2O2	7.12E+10	0.0	9917.0
Reverse Arrhenius coefficients:			
1311. C2-C4H8+O2-C4H7+H2O2	1.00E+12	0.0	18000.0
Reverse Arrhenius coefficients:			
1312. C2-C4H8+O2-C4H7+H2O2	2.57E+12	0.0	25380.0
Reverse Arrhenius coefficients:			
1313. C2-C4H8+O2-C4H7+H2O2	8.00E+11	0.0	16400.0
Reverse Arrhenius coefficients:			
1314. C2-C4H8+O2-C4H7+H2O2	2.05E+12	0.0	24180.0
Reverse Arrhenius coefficients:			
1315. C2-C4H8+O2-C4H7+H2O2	2.19E+11	0.0	11400.0
Reverse Arrhenius coefficients:			
1316. C2-C4H8+O2-C4H7+H2O2	5.56E+12	0.0	18560.0
Reverse Arrhenius coefficients:			
1317. C2-C4H8+O2-C4H7+H2O2	2.19E+11	0.0	9600.0
Reverse Arrhenius coefficients:			
1318. C2-C4H8+O2-C4H7+H2O2	3.43E+12	0.0	16460.0
Reverse Arrhenius coefficients:			
1319. C2-C4H8+O2-C4H7+H2O2	1.88E+05	2.8	6280.0
Reverse Arrhenius coefficients:			
1320. C2-C4H8+O2-C4H7+H2O2	2.81E+01	3.4	10000.0
Reverse Arrhenius coefficients:			
1321. C2-C4H8+O2-C4H7+H2O2	2.60E+06	2.4	4471.0
Reverse Arrhenius coefficients:			
1322. C2-C4H8+O2-C4H7+H2O2	1.20E+06	2.1	12700.0
Reverse Arrhenius coefficients:			
1323. C2-C4H8+O2-C4H7+H2O2	1.05E+10	1.0	15860.0
Reverse Arrhenius coefficients:			
1324. C2-C4H8+O2-C4H7+H2O2	6.82E+06	1.7	20460.0
Reverse Arrhenius coefficients:			
1325. C2-C4H8+O2-C4H7+H2O2	9.34E+07	1.6	-35.0
Reverse Arrhenius coefficients:			
1326. C2-C4H8+O2-C4H7+H2O2	1.87E+08	1.4	23350.0
Reverse Arrhenius coefficients:			
1327. C2-C4H8+O2-C4H7+H2O2	1.13E+14	0.0	7850.0
Reverse Arrhenius coefficients:			
1328. C2-C4H8+O2-C4H7+H2O2	1.48E+13	0.0	12240.0
Reverse Arrhenius coefficients:			
1329. C2-C4H8+O2-C4H7+H2O2	5.62E+13	0.0	5200.0
Reverse Arrhenius coefficients:			
1330. C2-C4H8+O2-C4H7+H2O2	7.35E+12	0.0	9590.0
Reverse Arrhenius coefficients:			
1331. C2-C4H8+O2-C4H7+H2O2	1.70E+13	0.0	20460.0
Reverse Arrhenius coefficients:			
1332. C2-C4H8+O2-C4H7+H2O2	4.58E+12	0.0	9809.0
Reverse Arrhenius coefficients:			
1333. C2-C4H8+O2-C4H7+H2O2	1.12E+13	0.0	17700.0
Reverse Arrhenius coefficients:			
1334. C2-C4H8+O2-C4H7+H2O2	1.63E+12	0.0	7409.0
Reverse Arrhenius coefficients:			
1335. C2-C4H8+O2-C4H7+H2O2	3.00E+11	0.0	7000.0
Reverse Arrhenius coefficients:			
1336. C2-C4H8+O2-C4H7+H2O2	1.22E+10	0.0	50000.0
Reverse Arrhenius coefficients:			
1337. C2-C4H8+O2-C4H7+H2O2	9.19E+13	0.4	73040.0
Reverse Arrhenius coefficients:			
1338. C2-C4H8+O2-C4H7+H2O2	1.80E+13	0.0	0.0
Reverse Arrhenius coefficients:			
1339. C2-C4H8+O2-C4H7+H2O2	3.00E+12	0.0	0.0
Reverse Arrhenius coefficients:			
1340. C2-C4H8+O2-C4H7+H2O2	2.06E+21	-2.3	25730.0
Reverse Arrhenius coefficients:			
1341. C2-C4H8+O2-C4H7+H2O2	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:			
1342. C2-C4H8+O2-C4H7+H2O2	2.05E+21	-1.5	-6372.0
Reverse Arrhenius coefficients:			
1343. C2-C4H8+O2-C4H7+H2O2	3.86E+08	1.5	-6372.0
Reverse Arrhenius coefficients:			
1344. C2-C4H8+O2-C4H7+H2O2	5.32E+14	-0.4	17580.0
Reverse Arrhenius coefficients:			
1345. C2-C4H8+O2-C4H7+H2O2	7.50E+13	0.0	29000.0
Reverse Arrhenius coefficients:			
1346. C2-C4H8+O2-C4H7+H2O2	9.19E+13	0.4	73040.0
Reverse Arrhenius coefficients:			
1347. C2-C4H8+O2-C4H7+H2O2	1.80E+14	0.0	0.0
Reverse Arrhenius coefficients:			
1348. C2-C4H8+O2-C4H7+H2O2	3.50E+10	0.0	-3275.0
Reverse Arrhenius coefficients:			
1349. C2-C4H8+O2-C4H7+H2O2	2.62E+06	2.1	916.

1348. O+CH2OH<=>OH+CH2O	4.20E+13	0.0	0.0
Reverse Arrhenius coefficients:	5.44E+11	0.7	73340.0
1349. CH2O+CH3OH<=>CH2OH+CH2OH	6.50E+12	0.7	68460.0
Reverse Arrhenius coefficients:	3.00E+12	0.0	0.0
1350. CH2OH+HO2<=>HOCH2O+OH	1.00E+13	0.0	0.0
Reverse Arrhenius coefficients:	8.17E+13	0.0	33470.0
1351. OCH2O2H<=>CH2O+HO2	1.28E+18	-1.8	10460.0
Reverse Arrhenius coefficients:	1.50E+11	0.0	11900.0
1352. OCH2O2H<=>HOCH2O2	3.00E+11	0.0	8600.0
Reverse Arrhenius coefficients:	4.24E+08	0.9	26200.0
1353. HOCH2O2+HO2<=>HOCH2O2H+O2	3.50E+10	0.0	-3275.0
Reverse Arrhenius coefficients:	1.05E+14	-0.8	34870.0
1354. HOCH2O2H<=>HOCH2O+OH	1.02E+21	-1.9	42490.0
Reverse Arrhenius coefficients:	1.00E+13	0.0	0.0
1355. CH3OH(-M)<=>CH2OH(H+M)	2.69E+16	-0.1	98940.0
Low pressure limit: 0.23400E+41 -0.63300E+01 0.10310E+06			
TROE centering: 0.77300E+00 0.69300E+03 0.53330E+04 0.10000E+11			
1356. CH3OH+O2<=>CH2OH+HO2	2.05E+13	0.0	44900.0
Reverse Arrhenius coefficients:	1.24E+12	-0.2	-3501.0
1357. CH4+CH2<=>CH3+CH3	2.46E+06	2.0	8270.0
Reverse Arrhenius coefficients:	1.74E+06	1.9	12980.0
1358. CH3+OH<=>CH2S+H2O	4.51E+17	-1.3	1417.0
Reverse Arrhenius coefficients:	1.65E+16	-0.9	1039.0
1359. CH3+OH<=>CH3O+H	6.94E+09	1.3	11200.0
Reverse Arrhenius coefficients:	1.50E+12	0.5	-110.0
1360. CH3+OH<=>CH2OH+H2	3.09E+07	1.6	4506.0
Reverse Arrhenius coefficients:	1.65E+11	0.7	-284.0
1361. CH3+OH<=>CH2+H2O	5.60E+07	1.6	5420.0
Reverse Arrhenius coefficients:	9.22E+05	2.1	14060.0
1362. CH3+O2<=>CH2O+OH	2.64E+00	3.3	8105.0
Reverse Arrhenius coefficients:	5.28E-01	3.5	59920.0
1363. CH3O2+CH2O<=>CH3O2H+HCO	1.99E+12	0.0	11660.0
Reverse Arrhenius coefficients:	1.32E+14	-0.9	9259.0
1364. CH4+CH3O2<=>CH3+CH3O2H	1.81E+11	0.0	18480.0
Reverse Arrhenius coefficients:	2.23E+12	-0.7	-655.0
1365. CH3OH+CH3O2<=>CH2OH+CH3O2H	1.81E+12	0.0	13710.0
Reverse Arrhenius coefficients:	2.35E+14	-0.0	2404.0
1366. CH3O2+HO2<=>CH3O2H+O2	2.47E+11	0.0	-1570.0
Reverse Arrhenius coefficients:	5.30E+10	-0.8	35520.0
1367. CH3O2+H<=>CH3O+OH	9.60E+13	0.0	0.0
Reverse Arrhenius coefficients:	1.72E+09	1.0	40780.0
1368. CH3O2+O<=>CH3O+O2	3.60E+13	0.0	0.0
Reverse Arrhenius coefficients:	2.23E+11	0.6	57520.0
1369. CH3O2+OH<=>CH3OH+O2	6.00E+13	0.0	0.0
Reverse Arrhenius coefficients:	1.54E+13	0.4	59160.0
1370. CH3O2H+O2<=>CH3O+OH	6.31E+14	0.0	42300.0
Reverse Arrhenius coefficients:	2.51E+06	1.9	-2875.0
1371. CH2(S)+<=>CH2	1.00E+13	0.0	0.0
Reverse Arrhenius coefficients:	4.49E+12	0.0	90200.0
1372. CH2(S)+CH4<=>CH3+CH3	1.60E+13	0.0	-570.0
Reverse Arrhenius coefficients:	5.07E+12	-0.1	13160.0
1373. CH2(S)+O2<=>CO+OH+H	7.00E+13	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1374. CH2(S)+H2<=>CH3+H	7.00E+13	0.0	0.0
Reverse Arrhenius coefficients:	2.02E+16	-0.6	15270.0
1375. CH2(S)+H<=>CH2+H	3.00E+13	0.0	0.0
Reverse Arrhenius coefficients:	1.35E+13	0.0	90200.0
1376. CH2(S)+H<=>CH+H2	3.00E+13	0.0	0.0
Reverse Arrhenius coefficients:	6.95E+13	-0.3	12480.0
1377. CH2(S)+O<=>CO+H+H	3.00E+13	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1378. CH2(S)+OH<=>CH2O+H	3.00E+13	0.0	0.0
Reverse Arrhenius coefficients:	1.15E+18	-0.8	85230.0
1379. CH2(S)+CO2<=>CH2O+CO	3.00E+12	0.0	0.0
Reverse Arrhenius coefficients:	4.37E+10	0.4	59810.0
1380. CH2+O2(-M)<=>CH3(+M)	2.50E+16	-0.8	0.0
Low pressure limit: 0.32000E+28 -0.31400E+01 0.12300E+04			
TROE centering: 0.68000E+00 0.78000E+02 0.1950E+04 0.55900E+04			
H2 Enhanced by 2.000E+00			
H2O Enhanced by 6.000E+00			
AR Enhanced by 7.000E-01			
CO Enhanced by 1.500E+00			
CO2 Enhanced by 2.000E+00			
CH4 Enhanced by 2.000E+00			
C2H6 Enhanced by 3.000E+00			
HE Enhanced by 7.000E-01			
1381. CH2+O2<=>CO+OH+H	5.00E+12	0.0	1500.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1382. C+OH<=>CO+H	5.00E+13	0.0	0.0
Reverse Arrhenius coefficients:	1.36E+15	0.0	154300.0
1383. C+O2<=>CO+O	5.00E+13	0.0	0.0
Reverse Arrhenius coefficients:	1.07E+14	0.0	138200.0
1384. CH+H<=>C+H2	5.00E+13	0.0	0.0
Reverse Arrhenius coefficients:	2.04E+14	0.0	23820.0
1385. CH+O<=>CO+H	5.70E+13	0.0	0.0
Reverse Arrhenius coefficients:	2.7E+15	0.0	176000.0
1386. CH+OH<=>HCO+H	3.00E+13	0.0	0.0
Reverse Arrhenius coefficients:	5.07E+14	0.0	88110.0
1387. CH+H2O<=>H+CH2O	1.71E+13	0.0	-755.0
Reverse Arrhenius coefficients:	8.37E+14	0.0	57520.0
1388. CH+CO2<=>HCO+CO	1.70E+12	0.0	685.0
Reverse Arrhenius coefficients:	2.56E+11	0.0	66460.0
1389. CH5+(H+M)<=>C2H6(+M)	5.21E+10	-1.0	1580.0
Low pressure limit: 0.1990E+42 -0.70800E+01 0.66850E+04			
TROE centering: 0.84200E+00 0.12500E+03 0.22190E+04 0.68820E+04			
H2 Enhanced by 2.000E+00			
H2O Enhanced by 6.000E+00			
AR Enhanced by 7.000E-01			
CO Enhanced by 1.500E+00			
CO2 Enhanced by 2.000E+00			
CH4 Enhanced by 2.000E+00			
C2H6 Enhanced by 3.000E+00			
HE Enhanced by 7.000E-01			
1390. C2H6+CH3O2<=>C2H5+CH3O2H	1.94E+01	3.6	17100.0
Reverse Arrhenius coefficients:	2.02E+01	3.2	17340.0
1391. C2H6+CH<=>C2H5+CH2	1.10E+14	0.0	-260.0
Reverse Arrhenius coefficients:	1.97E+09	0.9	-1490.0
1392. CH2(S)+C2H6<=>CH3+CH2H5	1.20E+14	0.0	0.0
Reverse Arrhenius coefficients:	3.20E+12	0.1	17500.0
1393. H2+CH3O2<=>H+CH3O2H	1.50E+14	0.0	26030.0
Reverse Arrhenius coefficients:	1.69E+18	-1.1	8434.0
1394. H2+C2H5O2<=>H+C2H5O2H	1.50E+14	0.0	26030.0
Reverse Arrhenius coefficients:	1.69E+18	-1.1	8438.0
1395. C2H5+H<=>C2H4+H2	2.00E+12	0.0	0.0
Low pressure limit: 0.32000E+28 -0.31400E+01 0.12300E+04			
TROE centering: 0.68000E+00 0.78000E+02 0.1950E+04 0.55900E+04			
H2 Enhanced by 2.000E+00			
H2O Enhanced by 6.000E+00			
AR Enhanced by 7.000E-01			
CO Enhanced by 1.500E+00			
CO2 Enhanced by 2.000E+00			
CH4 Enhanced by 2.000E+00			
C2H6 Enhanced by 3.000E+00			
HE Enhanced by 7.000E-01			
1396. C2H5+O<=>CH3CHO+H	4.44E+11	0.4	68070.0
Reverse Arrhenius coefficients:	1.10E+14	0.0	0.0
1397. C2H5+HO2<=>C2H5O+OH	1.03E+17	-0.5	77420.0
Reverse Arrhenius coefficients:	1.10E+13	0.0	0.0
1398. CH3O2+CH3H<=>CH3O+CH3H5O	9.68E+15	-0.7	27650.0
Reverse Arrhenius coefficients:	8.00E+12	0.0	-1000.0
1399. C2H5O+O2<=>CH3CHO+HO2	4.40E+14	-0.4	30890.0
Reverse Arrhenius coefficients:	4.28E+10	0.0	1097.0
1400. C2H5O=>CH3+CH2O	1.32E+08	0.6	34130.0
Reverse Arrhenius coefficients:	3.00E+11	0.0	6336.0
1401. C2H5O=>CH3CHO+H	5.43E+15	-0.7	22230.0
Reverse Arrhenius coefficients:	8.00E+12	0.0	6400.0
1402. C2H5O2<=>C2H5+O2	1.31E+62	-14.8	49180.0
Reverse Arrhenius coefficients:	2.88E+56	-13.8	14620.0
1403. C2H5O2+CH2O<=>C2H5O2H+HCO	1.99E+12	0.0	11660.0
Reverse Arrhenius coefficients:	1.32E+14	-0.9	9263.0
1404. CH4+C2H5O2<=>CH3+CH2H5O2H	1.81E+11	0.0	18480.0
Reverse Arrhenius coefficients:	2.24E+12	-0.7	-651.0
1405. CH3O+CH2H5O2<=>CH2O+CH2H5O2H	1.81E+12	0.0	13710.0
Reverse Arrhenius coefficients:	2.35E+14	-1.0	2408.0
1406. C2H5O2+HO2<=>C2H5O2H+O2	1.75E+10	0.0	-3275.0
Reverse Arrhenius coefficients:	3.76E+13	-0.8	33820.0
1407. C2H6+C2H5O2<=>C2H5O+CH2H5O2H	8.60E+00	3.8	17200.0
Reverse Arrhenius coefficients:	8.96E+00	3.5	1838.0
1408. C2H5O2H<=>C2H5O+OH	6.31E+14	0.0	42300.0
Reverse Arrhenius coefficients:	5.66E+08	1.0	-1705.0
1409. C2H4O2H<=>C2H5+O2	4.37E+47	-12.1	31020.0
Reverse Arrhenius coefficients:	1.81E+45	-11.5	14600.0
1410. C2H5+O2<=>C2H4O1+2+OH	1.63E+11	-0.3	6150.0
Reverse Arrhenius coefficients:	3.63E+13	-0.6	39840.0
1411. C2H5+O2<=>CH3CHO+OH	8.26E+02	2.4	5285.0
Reverse Arrhenius coefficients:	2.25E+03	2.3	65970.0
1412. C2H5O2H<=>C2H4O2H	2.28E+39	-8.5	45170.0
Reverse Arrhenius coefficients:	1.20E+36	-8.1	27020.0
1413. C2H5O2H<=>CH3CHO+OH	2.52E+41	-10.2	43710.0
Reverse Arrhenius coefficients:	1.50E+36	-9.3	69840.0
1414. C2H5O2H<=>C2H4+HO2	1.82E+38	-8.4	37890.0
Reverse Arrhenius coefficients:	4.63E+32	-7.4	16700.0
1415. C2H5O2H<=>C2H4O1+2+OH	4.00E+43	-10.5	45580.0
Reverse Arrhenius coefficients:	1.96E+40	9.8	44710.0
1416. C2H4O2H<=>C2H4O1+2+OH	8.85E-30	-6.1	20660.0
Reverse Arrhenius coefficients:	8.20E+30	-5.8	37930.0
1417. C2H4O2H<=>C2H4+HO2	3.98E+34	-7.2	23250.0
Reverse Arrhenius coefficients:	1.92E+32	-6.6	20210.0
1418. C2H4O2H<=>CH3CHO+OH	1.19E+34	-9.0	29210.0
Reverse Arrhenius coefficients:	1.34E+32	-8.5	73480.0
1419. C2H4O1+2<=>CH3+HCO	3.63E+13	0.0	57200.0
Reverse Arrhenius coefficients:	1.01E+04	1.5	-2750.0
1420. C2H4O1+2<=>CH3CHO+H	7.41E+12	0.0	53800.0
Reverse Arrhenius coefficients:	9.01E+10	0.2	80800.0
1421. C2H4O1+2+OH<=>C2H3O1+2+H2O	1.78E+13	0.0	3610.0
Reverse Arrhenius coefficients:	1.35E+10	0.7	24740.0
1422. C2H4O1+2-H<=>C2H3O1+2+H2	8.00E+13	0.0	9680.0
Reverse Arrhenius coefficients:	5.71E+09	0.8	15920.0
1423. C2H4O1+2-HO2<=>C2H3O1+2+H2O	1.13E+13	0.0	30430.0
Reverse Arrhenius coefficients:	4.67E+11	0.1	20670.0
1424. C2H4O1+2-CH3O2<=>C2H3O1+2+CH3O2H	1.13E+13	0.0	30430.0
Reverse Arrhenius coefficients:	9.08E+12	-0.3	19070.0
1425. C2H4O1+2-C2H5O2<=>C2H3O1+2-C2H5O2H	1.13E+13	0.0	30430.0
Reverse Arrhenius coefficients:	9.09E+12	-0.3	19080.0
1426. C2H4O1+2-CH3<=>C2H3O1+2+CH4	1.07E+12	0.0	11830.0
Reverse Arrhenius coefficients:	6.97E+10	0.4	19610.0
1427. C2H4O1+2-CH3O<=>C2H3O1+2-CH3OH	1.20E+11	0.0	6750.0
Reverse Arrhenius coefficients:	1.84E+08	0.6	13220.0
1428. C2H3O1+2<=>CH3CO	8.50E+14	0.0	14000.0
Reverse Arrhenius coefficients:	1.00E+14	0.0	48710.0
1429. C2H3O1+2<=>CH2CHO	1.00E+14	0.0	14000.0
Reverse Arrhenius coefficients:	1.24E+15	-0.4	44010.0
1430. CH3CHO+CH3C03<=>CH3O2H+CH3CO3H	3.01E+12	0.0	11920.0
Reverse Arrhenius coefficients:	2.34E+13	-0.5	828.0
1431. CH3CHO+CH3C03<=>CH3CO+CH3C03H	3.01E+12	0.0	11920.0
Reverse Arrhenius coefficients:	1.92E+12	0.0	12650.0
1432. CH3CHO+OH<=>CH3+CH3OCHO	3.00E+15	-1.1	0.0
Reverse Arrhenius coefficients:	2.37E+16	-1.3	23750.0
1433. CH3CHO+OH<=>CH2CHO+H2O	1.72E+05	2.4	815.0
Reverse Arrhenius coefficients:	1.33E+05	2.5	24950.0
1434. CH3CO+H<=>CH2CO+H2	2.00E+13	0.0	0.0
Reverse Arrhenius coefficients:	1.04E+13	0.2	60560.0
1435. CH3CO+O<=>CH2CO+OH	2.00E+13	0.0	0.0
Reverse Arrhenius coefficients:			

Reverse Arrhenius coefficients:	1.62E+15	0.0	69060.0	Reverse Arrhenius coefficients:	1.30E+11	0.3	5391.0	
1453. CH+HCCO<=>CO+C2H2	5.00E+13	0.0	0.0	1508. C2H3CHO-C2H3<=>C2H3CO+C2H4	1.74E+12	0.0	8440.0	
Reverse Arrhenius coefficients:	1.72E+17	0.0	164600.0	Reverse Arrhenius coefficients:	1.00E+13	0.0	28000.0	
1454. C2H4+O<=>CH2CHO+H	4.99E+06	1.9	183.0	1509. C2H3CHO-CH3O<=>C2H3CO+CH3OH	1.00E+12	0.0	3300.0	
Reverse Arrhenius coefficients:	1.54E+09	1.2	18780.0	Reverse Arrhenius coefficients:	5.30E+10	0.4	22910.0	
1455. C2H4+CH3O2<=>C2H3+CH3O2H	2.23E+12	0.0	17190.0	1510. C2HSCHO<=>C2H5+HCO	1.50E+27	-3.2	87040.0	
Reverse Arrhenius coefficients:	7.93E+12	-0.6	-8167.0	Reverse Arrhenius coefficients:	1.81E+13	0.0	0.0	
1456. C2H4+C2H5O2<=>C2H3+C2H5O2H	2.23E+12	0.0	17190.0	1511. C2HSCHO-H<=>C2H5CO+H2	4.00E+13	0.0	4200.0	
Reverse Arrhenius coefficients:	7.94E+12	-0.6	-8163.0	Reverse Arrhenius coefficients:	2.38E+10	0.7	18130.0	
1457. C2H4+CH3CO3<=>C2H3+CH3CO3H	1.13E+13	0.0	30430.0	1512. C2H5CHO-O<=>C2H5CO+OH	5.00E+12	0.0	1790.0	
Reverse Arrhenius coefficients:	3.30E+12	-0.1	9440.0	Reverse Arrhenius coefficients:	1.54E+09	0.6	14310.0	
1458. C2H4+CH3O2<=>C2H4O1-2+CH3O	2.82E+12	0.0	17110.0	1513. C2HSCHO-OH<=>C2H5CO+H2O	2.69E+10	0.8	-340.0	
Reverse Arrhenius coefficients:	3.38E+13	-0.1	41660.0	Reverse Arrhenius coefficients:	1.70E+08	1.3	28480.0	
1459. C2H4+C2H5O2<=>C2H4O1-2+C2H5O	2.82E+12	0.0	17110.0	1514. C2HSCHO-CH3<=>C2H5CO+CH4	2.61E+06	1.8	5911.0	
Reverse Arrhenius coefficients:	7.64E+15	-0.9	42830.0	Reverse Arrhenius coefficients:	1.41E+06	2.0	21380.0	
1460. C2H4+HO2<=>C2H4O1-2+OH	2.23E+12	0.0	17190.0	1515. C2HSCHO-HO2<=>C2H5CO+H2O2	2.80E+12	0.0	13600.0	
Reverse Arrhenius coefficients:	4.28E+14	-0.4	37500.0	Reverse Arrhenius coefficients:	9.63E+11	0.0	11530.0	
1461. CH-CH4<=>C2H4-H	6.00E+13	0.0	0.0	1516. C2HSCHO-CH3O<=>C2H5CO+CH3OH	1.00E+12	0.0	3300.0	
Reverse Arrhenius coefficients:	3.57E+14	0.0	55480.0	Reverse Arrhenius coefficients:	1.28E+10	0.4	17460.0	
1462. CH2(S)-CH3<=>C2H4+H	2.00E+13	0.0	0.0	1517. C2HSCHO-CH3O2<=>C2H5CO+CH3O2H	3.01E+12	0.0	11920.0	
Reverse Arrhenius coefficients:	6.13E+19	-1.2	73050.0	Reverse Arrhenius coefficients:	2.01E+13	-0.5	8260.0	
1463. C2H3+O2<=>C2H2CHO+O	5.50E+14	-0.6	5260.0	1518. C2HSCHO-C2H3<=>C2H5CO+C2H6	1.00E+12	0.0	8000.0	
Reverse Arrhenius coefficients:	3.00E+18	-1.4	16300.0	Reverse Arrhenius coefficients:	6.43E+12	0.0	19700.0	
1464. C2H3-OH<=>C2H2+H2O	5.00E+12	0.0	0.0	1519. C2HSCHO-C2H50H<=>C2HSCHO+C2H50H	6.03E+11	0.0	3300.0	
Reverse Arrhenius coefficients:	5.18E+13	0.1	84130.0	Reverse Arrhenius coefficients:	3.02E+11	0.0	18160.0	
1465. C2H2+OH<=>CH3-CO	4.83E+04	4.0	-2000.0	1520. C2HSCHO-C2H502<=>C2H5CO+C2H5O2H	3.01E+12	0.0	11920.0	
Reverse Arrhenius coefficients:	3.49E+06	4.6	52120.0	Reverse Arrhenius coefficients:	2.02E+13	-0.5	8264.0	
1466. OH+C2H2<=>HCCOH	5.04E+05	2.3	13500.0	1521. C2HSCHO-C2H2<=>C2H5CO+H2O	1.00E+13	0.0	40700.0	
Reverse Arrhenius coefficients:	3.85E+09	1.4	4382.0	Reverse Arrhenius coefficients:	3.13E+10	0.3	-58.0	
1467. H-HCCOH<=>H+CH2CO	1.00E+13	0.0	0.0	1522. C2HSCHO+CH3CO3<=>C2H5CO+CH3CO3H	3.01E+12	0.0	11920.0	
Reverse Arrhenius coefficients:	9.30E+13	-0.3	31110.0	Reverse Arrhenius coefficients:	1.65E+12	0.0	12630.0	
1468. C2H50H+O2<=>PC2H4OH+HO2	2.00E+13	0.0	52800.0	1523. C2HSCHO-C2H3<=>C2H5CO+C2H4	1.70E+12	0.0	8440.0	
Reverse Arrhenius coefficients:	2.19E+10	0.3	443.0	Reverse Arrhenius coefficients:	3.20E+12	0.1	30130.0	
1469. C2H50H+O2<=>SC2H4OH+HO2	1.50E+13	0.0	50150.0	1524. C2HSCHO<=>C2H5+CO	2.46E+23	-3.2	17550.0	
Reverse Arrhenius coefficients:	1.95E+11	0.1	4879.0	Reverse Arrhenius coefficients:	1.51E+11	0.0	4810.0	
1470. C2H50H+OH<=>PC2H4OH+H2O	1.81E+11	0.4	717.0	1525. CH3OCH3(+M)<=>CH3+CH3(+M)	7.25E+21	-0.9	80250.0	
Reverse Arrhenius coefficients:	4.01E+08	0.9	17940.0	Low pressure limit: 0.3500E+61 -0.1150E+02 0.10100E+06	TROE centering: 0.18300E+00 0.13000E+01 0.13000E+05 0.67100E+10			
1471. C2H50H+OH<=>SC2H4OH+H2O	5.56E+10	0.5	-380.0	1526. CH3OCH3+OH<=>CH3OCH2+H2O	6.32E+06	2.0	-651.7	
Reverse Arrhenius coefficients:	1.46E+09	0.8	23930.0	Reverse Arrhenius coefficients:	7.85E+04	2.2	21210.0	
1472. C2H50H+H<=>PC2H4OH+H2	1.88E+03	3.2	7150.0	1527. CH3OCH3+H<=>CH3OCH2+H2	7.72E+06	2.1	3384.0	
Reverse Arrhenius coefficients:	3.93E-01	3.8	9484.0	Reverse Arrhenius coefficients:	9.04E+03	2.4	10360.0	
1473. C2H50H+H<=>SC2H4OH+H2	1.79E+05	2.5	3420.0	1528. CH3OCH3+O<=>CH3OCH2+OH	7.75E+08	1.4	2250.0	
Reverse Arrhenius coefficients:	4.43E+02	3.0	12840.0	Reverse Arrhenius coefficients:	4.71E+05	1.7	7810.0	
1474. C2H50H+HO2<=>PC2H4OH+H2O2	2.38E+04	2.5	16490.0	1529. CH3OCH3+HO2<=>CH3OCH2+H2O2	1.68E+13	0.0	17690.0	
Reverse Arrhenius coefficients:	2.88E+03	2.5	28270.	Reverse Arrhenius coefficients:	1.14E+13	-0.4	8657.0	
1475. C2H50H+HO2<=>SC2H4OH+H2O2	6.00E+12	0.0	16000.0	1530. CH3OCH3+CH3O2<=>CH3OCH2+CH3O2H	1.68E+13	0.0	17690.0	
Reverse Arrhenius coefficients:	8.59E+12	-0.3	9419.0	Reverse Arrhenius coefficients:	2.22E+14	-0.8	7062.0	
1476. C2H50H+CH3O2<=>PC2H4OH+CH3O2H	1.23E+04	2.5	15750.0	1531. CH3OCH3+CH3<=>CH3OCH2+CH4	1.44E+06	5.7	5700.0	
Reverse Arrhenius coefficients:	2.89E+04	2.0	488.0	Reverse Arrhenius coefficients:	1.54E-06	5.6	14210.0	
1477. C2H50H+CH3O2<=>SC2H4OH+CH3O2H	8.20E+03	2.5	10750.0	1532. CH3OCH3+O2<=>CH3OCH2+H2O	4.10E+13	0.0	44910.0	
Reverse Arrhenius coefficients:	2.38E+05	1.8	2574.0	Reverse Arrhenius coefficients:	2.52E+11	0.0	2806.0	
1478. C2H50H-CH3O2<=>C2H50+CH3O2H	2.50E+12	0.0	24000.0	1533. CH3OCH3+CH3O<=>CH3OCH2+CH3OH	6.02E+11	0.0	4074.0	
Reverse Arrhenius coefficients:	1.30E+15	-0.9	6187.0	Reverse Arrhenius coefficients:	7.38E+10	-0.3	10260.0	
1479. C2H50H+O<=>PC2H4OH+OH	9.69E+02	3.2	4658.0	1534. CH3OCH3+CH3OCH202<=>CH3OCH2+CH3OCH202H	5.00E+12	0.0	0	
Reverse Arrhenius coefficients:	1.05E-01	3.8	5580.0	1576.0	Reverse Arrhenius coefficients:	6.43E+13	-0.8	7258.0
1480. C2H50H+O<=>SC2H4OH+OH	1.45E+05	2.5	876.0	1535. CH3OCH3+O2CHO<=>CH3OCH2+H2OCHO	4.42E+04	2.6	0	
Reverse Arrhenius coefficients:	1.86E+02	2.9	8884.0	1591.0	Reverse Arrhenius coefficients:	1.72E+06	1.7	5832.0
1481. C2H50H+CH3<=>PC2H4OH+CH4	3.30E+02	3.3	12290.0	1536. CH3OCH3+O-CHO<=>CH3OCH2+HOCHO	1.00E+13	0.0	17690.0	
Reverse Arrhenius coefficients:	6.27E+01	3.5	1616.0	Reverse Arrhenius coefficients:	7.20E+12	-0.3	33130.0	
1482. C2H50H+CH3<=>SC2H4OH+CH4	1.99E+01	3.4	7634.0	1537. CH3OCH2<=>CH2O+CH3	1.60E+13	0.0	25500.0	
Reverse Arrhenius coefficients:	4.50E+01	3.4	18590.0	Reverse Arrhenius coefficients:	2.60E+05	1.9	16670.0	
1483. C2H50H+CH25<=>PC2H4OH+C2H6	5.00E+10	0.0	13400.0	1538. CH3OCH2-CH3O<=>CH3OCH3+CH2O	2.41E+13	0.0	0.0	
Reverse Arrhenius coefficients:	7.00E+10	0.0	26990.0	Reverse Arrhenius coefficients:	1.25E+14	0.3	78540.0	
1484. C2H50H+CH25<=>SC2H4OH+C2H6	5.00E+10	0.0	10400.0	1539. CH3OCH2-CH2O<=>CH3OCH3+HCO	5.49E+03	2.8	5862.0	
Reverse Arrhenius coefficients:	7.00E+10	0.0	2.4	1530. CH3OCH2-CH3O<=>CH3OCH3+CH3CO	1.26E+12	0.0	8499.0	
1485. PC2H4OH<=>C2H4+OH	1.05E+25	-4.0	30390.0	Reverse Arrhenius coefficients:	7.75E+11	0.3	16980.0	
Reverse Arrhenius coefficients:	4.17E+20	-2.8	1240.0	1541. CH3OCH2O2<=>CH3OCH2+O2	4.44E+19	-1.6	36240.0	
1486. SC2H4OH+M<=>CH3CHO+H+M	1.00E+14	0.0	25000.0	Reverse Arrhenius coefficients:	2.00E+12	0.0	0.0	
Reverse Arrhenius coefficients:	2.74E+12	0.5	-470.0	1542. CH3OCH2+CH3O<=>CH3OCH2+H2O+HCO	1.00E+12	0.0	0.0	
1487. O2CH2+OH<=>PC2H4OH+O2	3.90E+16	-1.0	30000.0	1166.0	Reverse Arrhenius coefficients:	6.48E+13	-0.8	9455.0
Reverse Arrhenius coefficients:	1.20E+11	0.0	-1100.0	1543. CH3OCH2+CH3OCH202<=>CH3OCH2+CH3OCH202H	2.80E+12	0.0	0	
1488. O2CH2+OH<=>OH+CH2+H2O	3.12E+09	0.0	18900.0	1560.0	Reverse Arrhenius coefficients:	1.00E+12	0.0	10000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	1544. CH3OCH202+CH3OCH202<=>O2+CH3OCH20+CH3OCH20	2.21E+23	-4.5	0.0	
1489. SC2H4OH+O2<=>CH3CHO+HO2	3.81E+06	2.0	1641.0	Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
Reverse Arrhenius coefficients:	2.19E+05	2.4	25040.0	1545. CH3OCH202+CH3OCH202<=>CH3OCH20+H2O	2.11E+22	-2.1	43830.0	
1490. CH3COCH3(+M)<=>CH3CO+CH3(-M)	7.11E+21	-1.6	84680.0	Reverse Arrhenius coefficients:	2.00E+13	0.0	0.0	
Low pressure limit: 0.70130E+90 -0.20380E+02 0.10715E+06	TROE centering: 0.8630E+00 0.10000E+11 0.41640E+03 0.32900E+10	1546. CH3OCH202+CH3OCH202<=>O2+CH3OCH20+CH3OCH20	2.11E+22	-2.1	43830.0			
1491. CH3COCH3+OH<=>CH3COCH2+H2O	1.25E+05	2.5	445.0	Reverse Arrhenius coefficients:	2.00E+13	0.0	0.0	
Reverse Arrhenius coefficients:	8.62E+04	2.3	24710.0	1547. CH3OCH202+CH3OCH2+H2O<=>CH3OCH20+H2O	1.00E+11	0.0	1190.0	
Reverse Arrhenius coefficients:	6.37E+04	2.4	14530.0	Reverse Arrhenius coefficients:	1.25E+12	0.1	8218.0	
1493. CH3COCH3+O<=>CH3COCH2+OH	5.31E+11	0.2	4890.0	1548. CH3OCH20+CH3O<=>CH3OCHO+H	1.00E+13	0.0	7838.0	
Reverse Arrhenius coefficients:	1.73E+10	0.1	12850.0	Reverse Arrhenius coefficients:	6.00E+10	0.0	2158.0	
1494. CH3COCH3+CH3<=>CH3COCH2+CH4	3.96E+11	0.0	9784.0	Reverse Arrhenius coefficients:	1.25E+12	-0.8	11120.0	
Reverse Arrhenius coefficients:	2.35E+13	-0.5	20690.0	1549. CH3OCH202+CH3O<=>CH2OCH2O2H	1.00E+11	0.0	20760.0	
1495. CH3COCH3+CH3O<=>CH3COCH2+CH3O	4.34E+11	0.0	6460.0	Reverse Arrhenius coefficients:	1.00E+11	0.0	0.0	
Reverse Arrhenius coefficients:	6.06E+11	-0.3	16060.0	1551. O2CH2OCH202+CH2O<=>CH2OCH2O2+H2O	1.92E+19	-1.6	36270.0	
1496. CH3COCH3+O2<=>CH3COCH2+H2O	6.03E+13	0.0	48500.0	Reverse Arrhenius coefficients:	1.09E+10	0.0	46480.0	
Reverse Arrhenius coefficients:	2.06E+13	-0.4	3181.0	1552. CH3OCH20+CH3O<=>CH3OCHO+H	6.06E+12	0.1	8218.0	
1497. CH3COCH3+HO2<=>CH3COCH2+H2O2	1.70E+13	0.0	20460.0	Reverse Arrhenius coefficients:	1.00E+13	0.0	0.0	
Reverse Arrhenius coefficients:	6.40E+14	-0.8	13830.0	1553. O2CH2OCH202+CH2O<=>O2+CH2OCH2O+H2O	4.00E+10	0.0	18580.0	
1498. CH3COCH3+CH3O2<=>CH3COCH2+CH3O2H	1.70E+13	0.0	0.0	Reverse Arrhenius coefficients:	5.04E+03	1.4	59640.0	
2046.0	Reverse Arrhenius coefficients:	1.24E+16	-1.2	12230.0	1554. O2CH2OCH202+CH2O<=>O2+CH2OCH2O+H2O	2.00E+16	0.0	40500.0
1499. CH3COCH2<=>CH2CO+CH3	1.00E+14	0.0	31000.0	Reverse Arrhenius coefficients:	1.18E+08	1.9	-3952.0	
Reverse Arrhenius coefficients:	1.00E+11	0.0	6000.0	1555. OCH2CHO<=>HOCH2OCHO	2.90E+19	-2.2	31850.0	
1500. CH3COCH202<=>CH3COCH2+O2	2.02E+15	-1.0	24460.0	Reverse Arrhenius coefficients:	1.25E+11	0.0	11900.0	
Reverse Arrhenius coefficients:	1.20E+11	0.0	-1100.0	1556. HOCH2OCHO<=>HOCH2O+CO	1.00E+11	0.0	14000.0	
1501. CH3COCH3+CH3COCH202<=>CH3COCH2+CH3OCH2O2H	1.00E+11	0.0	5000.0	Reverse Arrhenius coefficients:	1.57E+09			

1561.	CH ₃ CHOH<=>CH ₃ O+HCO	5.37E+16	0.0	97090.0	
	Reverse Arhenius coefficients:	3.00E+13	0.0	0.0	
1562.	CH ₃ CHOH<=>CH ₃ -OCHO	3.21E+17	-0.5	79970.0	
	Reverse Arhenius coefficients:	1.00E+13	0.0	0.0	
1563.	CH ₃ CHOH+O2<=>CH ₃ CO+H ₂ O	1.00E+13	0.0	49700.0	
	Reverse Arhenius coefficients:	2.98E+10	0.3	1.0	
1564.	CH ₃ CHOH+O2<=>CH ₂ CHO+H ₂ O	2.05E+13	0.0	52000.0	
	Reverse Arhenius coefficients:	2.14E+10	0.4	331.0	
1565.	CH ₃ CHOH+O2<=>CH ₃ OCO+H ₂ O	1.58E+07	1.8	934.0	
	Reverse Arhenius coefficients:	9.52E+04	2.4	20820.0	
1566.	CH ₃ CHOH+O2<=>CH ₂ CHO+H ₂ O	5.27E+09	1.0	1586.0	
	Reverse Arhenius coefficients:	1.11E+07	1.6	19500.0	
1567.	CH ₃ CHOH+H ₂ O2<=>CH ₃ CO+H ₂ O ₂	4.82E+03	2.6	13910.0	
	Reverse Arhenius coefficients:	1.58E+06	2.6	2899.0	
1568.	CH ₃ CHOH+H ₂ O2<=>CH ₂ CHO+H ₂ O ₂	2.38E+04	2.5	16490.0	
	Reverse Arhenius coefficients:	2.75E+03	2.6	3513.0	
1569.	CH ₃ CHOH+O<=>CH ₃ OCO+OH	2.76E+05	2.5	2830.0	
	Reverse Arhenius coefficients:	8.13E+01	3.1	6408.0	
1570.	CH ₃ CHOH+O<=>CH ₂ CHO+OH	9.80E+05	2.4	4750.0	
	Reverse Arhenius coefficients:	1.01E+02	3.1	6358.0	
1571.	CH ₃ CHOH+H<=>CH ₃ OCO+H ₂	6.50E+05	2.4	4471.0	
	Reverse Arhenius coefficients:	3.69E+02	3.1	9461.0	
1572.	CH ₃ CHOH+H<=>CH ₂ CHO+H ₂	6.65E+05	2.5	6756.0	
	Reverse Arhenius coefficients:	1.33E+02	3.2	9776.0	
1573.	CH ₃ CHOH+CH<=>CH ₃ OCO+CH ₄	7.55E-01	3.5	5481.0	
	Reverse Arhenius coefficients:	3.91E-01	3.7	12010.0	
1574.	CH ₃ CHOH+CH<=>CH ₂ CHO+CH ₄	4.52E-01	3.6	7154.0	
	Reverse Arhenius coefficients:	8.22E-02	3.9	11710.0	
1575.	CH ₃ CHOH+CH ₃ O<=>CH ₃ OCO+CH ₃ OH	5.48E+11	0.0	5000.0	
	Reverse Arhenius coefficients:	6.68E+09	0.5	10220.0	
1576.	CH ₃ CHOH+CH ₃ O<=>CH ₂ CHO+CH ₃ OH	2.17E+11	0.0	6458.0	
	Reverse Arhenius coefficients:	9.29E+08	0.5	9705.0	
1577.	CH ₃ CHOH+CH ₃ O2<=>CH ₃ OCO+CH ₃ O ₂	4.82E+03	2.6	13910.0	
	Reverse Arhenius coefficients:	3.08E+04	2.1	1304.0	
1578.	CH ₃ CHOH+CH ₃ O2<=>CH ₂ CHO+CH ₃ O ₂ H	2.38E+04	2.5	16490.0	
	Reverse Arhenius coefficients:	5.34E+04	2.1	1918.0	
1579.	CH ₃ CHOH+HCO<=>CH ₃ OCO+CH ₂ O	5.40E+06	1.9	17010.0	
	Reverse Arhenius coefficients:	5.20E+05	2.3	6860.0	
1580.	CH ₃ CHOH+HCO<=>CH ₂ CHO+CH ₂ O	1.02E+05	2.5	18430.0	
	Reverse Arhenius coefficients:	3.46E+03	2.9	6261.0	
1581.	CH ₃ CHOH<=>CH ₃ OCO	2.62E+11	0.0	38180.0	
	Reverse Arhenius coefficients:	1.63E+12	-0.2	40670.0	
1582.	CH ₃ OCO<=>CH ₃ C ₂ O	3.59E+14	-0.2	16100.0	
	Reverse Arhenius coefficients:	4.76E+07	1.5	34700.0	
1583.	CH ₃ OCO<=>CH ₃ -CO	1.43E+15	0.0	23770.0	
	Reverse Arhenius coefficients:	1.55E+06	2.0	5730.0	
1584.	CH ₃ OCO<=>CH ₂ H+HCO	4.66E+12	0.1	27440.0	
	Reverse Arhenius coefficients:	1.50E+11	0.0	11900.0	
1585.	CH ₃ H<=>N-C ₃ H ₇ +H	3.75E+17	-0.4	101200.0	
	Reverse Arhenius coefficients:	1.00E+14	0.0	0.0	
1586.	CH ₃ H<=>C3H7H	2.38E+18	-0.7	98680.0	
	Reverse Arhenius coefficients:	1.00E+14	0.0	0.0	
1587.	CH ₃ H<=>C3H5-A<=>N-C ₃ H7+C ₃ H6	7.94E+11	0.0	20500.0	
	Reverse Arhenius coefficients:	5.37E+16	-1.3	13400.0	
1588.	CH ₃ H<=>C3H5-A<=>L-C ₃ H7+C ₃ H6	7.94E+11	-0.1	16200.0	
	Reverse Arhenius coefficients:	5.37E+16	-1.3	9095.0	
1589.	CH ₃ O2+C ₃ H8<=>CH ₃ O2H+N-C ₃ H7	8.10E+04	2.5	16690.0	
	Reverse Arhenius coefficients:	9.72E+04	2.0	1435.0	
1590.	CH ₃ O2+C ₃ H8<=>CH ₃ O2H+I-C ₃ H7	5.88E+04	2.5	14860.0	
	Reverse Arhenius coefficients:	1.11E+04	2.3	2147.0	
1591.	CH ₃ O2+C ₃ H8<=>CH ₃ O2H+N-C ₃ H7	8.10E+04	2.5	16690.0	
	Reverse Arhenius coefficients:	9.74E+04	2.0	1439.0	
1592.	CH ₃ O2+C ₃ H8<=>CH ₃ O2H+I-C ₃ H7	5.88E+04	2.5	14860.0	
	Reverse Arhenius coefficients:	1.12E+04	2.3	2151.0	
1593.	NC ₃ H7O2+C ₃ H8<=>NC ₃ H7O2H+N-C ₃ H7	1.70E+13	0.0	20460.0	
	Reverse Arhenius coefficients:	2.09E+13	-0.5	5000.0	
1594.	NC ₃ H7O2+C ₃ H8<=>NC ₃ H7O2H+I-C ₃ H7	2.00E+12	0.0	17000.0	
	Reverse Arhenius coefficients:	3.87E+11	-0.2	4080.0	
1595.	IC ₃ H7O2+C ₃ H8<=>IC ₃ H7O2H+N-C ₃ H7	1.70E+13	0.0	20460.0	
	Reverse Arhenius coefficients:	2.09E+13	-0.5	5000.0	
1596.	IC ₃ H7O2+C ₃ H8<=>IC ₃ H7O2H+I-C ₃ H7	2.00E+12	0.0	17000.0	
	Reverse Arhenius coefficients:	3.88E+11	-0.2	4080.0	
1597.	CH ₃ H<=>CH ₃ COS<=>C3H7+CH ₃ CO ₃ H	2.00E+12	0.0	17000.0	
	Reverse Arhenius coefficients:	3.10E+10	0.3	8650.0	
1598.	CH ₃ H<=>CH ₃ COS<=>N-C ₃ H7+CH ₃ CO ₃ H	1.70E+13	0.0	20460.0	
	Reverse Arhenius coefficients:	1.67E+12	0.0	9570.0	
1599.	CH ₃ H<=>CH ₂ O<=>N-C ₃ H7+H ₂ CO ₂ CHO	5.52E+04	2.5	16480.0	
	Reverse Arhenius coefficients:	1.19E-08	5.5	-1920.0	
1600.	CH ₃ H<=>CH ₂ O<=>I-C ₃ H7+H ₂ CO ₂ CHO	1.48E-04	2.6	13910.0	
	Reverse Arhenius coefficients:	7.84E-06	4.7	-30.0	
1601.	I-C ₃ H7+OH<=>C3H5-H+H2O	2.41E+13	0.0	0.0	
	Reverse Arhenius coefficients:	2.98E+12	0.6	38320.0	
1602.	I-C ₃ H7+OH<=>CH ₃ COCH ₃ +H	4.82E+13	0.0	0.0	
	Reverse Arhenius coefficients:	1.20E+16	-0.2	79380.0	
1603.	I-C ₃ H7+OH<=>CH ₃ CO+CH ₃	4.82E+13	0.0	0.0	
	Reverse Arhenius coefficients:	1.28E+11	0.8	86480.0	
1604.	C2H5CHO+N-C ₃ H7<=>C2H5CO+C ₃ H8	1.70E+12	0.0	8440.0	
	Reverse Arhenius coefficients:	1.90E+14	0.0	18790.0	
1605.	C2H5CHO-I-C ₃ H7<=>C2H5CO+C ₃ H8	1.70E+12	0.0	8440.0	
	Reverse Arhenius coefficients:	1.90E+14	0.0	18790.0	
1606.	C2H5CHO+CH ₃ A<->C2H5CO+C ₃ H6	1.70E+12	0.0	8440.0	
	Reverse Arhenius coefficients:	1.00E+13	0.0	28000.0	
1607.	C3H6<=>C3H5-A+H	2.01E+61	-13.3	118500.0	
	Reverse Arhenius coefficients:	2.04E+61	-13.5	30610.0	
1608.	C3H6<=>C3H5-S+H	7.71E+69	-16.1	140000.0	
	Reverse Arhenius coefficients:	2.55E+67	-15.9	28690.0	
1609.	C3H6<=>C3H5-T+H	5.62E+71	-16.6	139300.0	
	Reverse Arhenius coefficients:	4.26E+68	-16.2	30080.0	
1610.	C3H6+O<=>C3H5-A+OH	5.24E+11	0.7	5884.0	
	Reverse Arhenius coefficients:	1.10E+11	0.7	20150.0	
1611.	C3H6+O<=>C3H5-S+OH	1.20E+11	0.7	8959.0	
	Reverse Arhenius coefficients:	8.24E+07	1.2	-207.0	
1612.	C3H6+O<=>C3H5-T+OH	6.03E+10	0.7	7632.0	
	Reverse Arhenius coefficients:	9.48E+06	1.4	576.0	
1613.	C3H6+OH<=>C3H5-A+H2O	3.12E+06	2.0	-298.0	
	Reverse Arhenius coefficients:	1.34E+07	1.9	30270.0	
1614.	C3H6+OH<=>C3H5-S+H2O	2.11E+06	2.0	2778.0	
	Reverse Arhenius coefficients:	2.96E+04	2.4	9916.0	
1615.	C3H6+OH<=>C3H5-T+H2O	1.11E+06	2.0	1451.0	
	Reverse Arhenius coefficients:	3.56E+03	2.6	10700.0	
1616.	C3H6+H2O<=>C3H5-A+H2O2	2.70E+04	2.5	12340.0	
	Reverse Arhenius coefficients:	6.34E+06	1.8	12010.0	
1617.	C3H6+H2O<=>C3H5-S+H2O2	1.80E+04	2.5	27620.0	
	Reverse Arhenius coefficients:	1.80E+04	2.5	27620.0	
	Reverse Arhenius coefficients:	1.38E+04	2.3	3864.0	
	Reverse Arhenius coefficients:	1.58E+03	2.5	23590.0	
	Reverse Arhenius coefficients:	1.58E+03	2.5	1940.0	
	Reverse Arhenius coefficients:	1.73E+05	-2.5	2492.0	
	Reverse Arhenius coefficients:	1.70E+04	2.5	18170.0	
	Reverse Arhenius coefficients:	1.80E+04	2.5	12280.0	
	Reverse Arhenius coefficients:	1.06E+03	3.0	4526.0	
	Reverse Arhenius coefficients:	4.05E+05	2.5	9794.0	
	Reverse Arhenius coefficients:	1.23E+02	3.2	4150.0	
	Reverse Arhenius coefficients:	1.22E+02	3.5	39900.0	
	Reverse Arhenius coefficients:	8.51E+12	-0.3	887.0	
	Reverse Arhenius coefficients:	2.00E+12	0.0	62900.0	
	Reverse Arhenius coefficients:	1.39E+10	0.2	459.0	
	Reverse Arhenius coefficients:	1.40E+12	0.0	60700.0	
	Reverse Arhenius coefficients:	2.22E+09	0.3	369.0	
	Reverse Arhenius coefficients:	2.21E+00	3.5	5675.0	
	Reverse Arhenius coefficients:	8.18E+02	3.1	22890.0	
	Reverse Arhenius coefficients:	1.35E+00	3.5	12850.0	
	Reverse Arhenius coefficients:	1.63E+00	3.6	6635.0	
	Reverse Arhenius coefficients:	2.32E-01	3.7	7552.0	
	Reverse Arhenius coefficients:	1.00E+10	0.0	9800.0	
	Reverse Arhenius coefficients:	5.37E+05	1.3	16440.0	
	Reverse Arhenius coefficients:	1.629C3H3O<=>C3H5-A+CH3CO3H	3.24E+11	0.0	14900.0
	Reverse Arhenius coefficients:	2.00E+10	0.0	15000.0	
	Reverse Arhenius coefficients:	1.630C3H3S<=>C3H5-A+CH3O2H	3.24E+11	0.0	14900.0
	Reverse Arhenius coefficients:	2.00E+10	0.0	15000.0	
	Reverse Arhenius coefficients:	1.631C3H6OH<=>C3H6O2+H	1.29E+12	0.0	14900.0
	Reverse Arhenius coefficients:	9.93E+11	0.0	-960.0	
	Reverse Arhenius coefficients:	2.87E+19	-1.9	34290.0	
	Reverse Arhenius coefficients:	1.20E+11	0.0	-1100.0	
	Reverse Arhenius coefficients:	1.637C3H6OH<=>CH3CHO+CH2-OH	1.25E+10	0.0	18900.0
	Reverse Arhenius coefficients:	0.00E+00	0.0	0.0	
	Reverse Arhenius coefficients:	2.61E+46	-9.6	36590.0	
	Reverse Arhenius coefficients:	4.19E+13	0.2	61930.0	
	Reverse Arhenius coefficients:	2.40E+11	0.7	3007.0	
	Reverse Arhenius coefficients:	1.60E+12	0.1	11660.0	
	Reverse Arhenius coefficients:	1.641C3H5-A+CH3O2<=>C3H5O+CH3O	7.00E+12	0.0	-1000.0
	Reverse Arhenius coefficients:	1.99E+15	-0.7	17020.0	
	Reverse Arhenius coefficients:	2.82E+00	3.8	47220.0	
	Reverse Arhenius coefficients:	1.633C3H5-A+CH3-C<CH3-A+CH4	1.00E+11	0.0	0.0
	Reverse Arhenius coefficients:	4.92E+12	0.1	47780.0	
	Reverse Arhenius coefficients:	1.644C3H5-A+CH2-C<CH2+C3H4-A	4.00E+11	0.0	0.0
	Reverse Arhenius coefficients:	1.80E+12	0.1	40330.0	
	Reverse Arhenius coefficients:	1.645C3H5-A+CH2-C<CH2+C3H4-C3H6	4.00E+11	0.0	0.0
	Reverse Arhenius coefficients:	6.94E+14	-1.3	52800.0	
	Reverse Arhenius coefficients:	1.646C3H5-A+CH2-C<CH2+C3H4-A+H2	1.00E+12	0.1	48190.0
	Reverse Arhenius coefficients:	1.62E+13	0.1	47780.0	
	Reverse Arhenius coefficients:	1.647C3H4-A+CH3-C<CH3-A+CH5-A+CH3	4.75E+08	0.7	28700.0
	Reverse Arhenius coefficients:	8.43E+10	0.0	-2620.0	
	Reverse Arhenius coefficients:	1.648C3H5-A+O2-C<CH3-A+H2O	2.18E+21	-2.9	30760.0
	Reverse Arhenius coefficients:	2.61E+19	-2.4	20710.0	
	Reverse Arhenius coefficients:	1.649C3H5-A+O2-C<CH2CHO+CH2O	7.14E+15	-1.2	21050.0
	Reverse Arhenius coefficients:	4.94E+16	-1.4	88620.0	
	Reverse Arhenius coefficients:	1.599E+13	-0.6	75140.0	
	Reverse Arhenius coefficients:	9.72E+29	-5.7	21450.0	
	Reverse Arhenius coefficients:	0.00E+00	0.0	0.0	
	Reverse Arhenius coefficients:	9.60E+39	-8.2	42030.0	
	Reverse Arhenius coefficients:	1.61E+40	-8.6	20330.0	
	Reverse Arhenius coefficients:	1.653C3H5-S<=>C3H4-P+H	4.19E+15	-0.7	37480.0
	Reverse Arhenius coefficients:	5.80E+12	0.0	3100.0	
	Reverse Arhenius coefficients:	4.34E+12	0.0	0.0	
	Reverse Arhenius coefficients:	1.61E+17	-1.3	96530.0	
	Reverse Arhenius coefficients:	3.33E+12	0.0	0.0	
	Reverse Arhenius coefficients:	7.98E+12	0.1	68860.0	
	Reverse Arhenius coefficients:	1.00E+11	0.0	0.0	
	Reverse Arhenius coefficients:	6.25E+12	0.1	69340.0	
	Reverse Arhenius coefficients:	2.16E+40	-8.3	45110.0	
	Reverse Arhenius coefficients:	1.61E+40	-8.6	20330.0	
	Reverse Arhenius coefficients:	3.51E+14	-0.4	40890.0	
	Reverse Arhenius coefficients:	8.50E+12	0.0	20000.0	
	Reverse Arhenius coefficients:	1.08E+12	0.1	38490.0	
	Reverse Arhenius coefficients:	6.50E+12	0.0	20000.0	
	Reverse Arhenius coefficients:	1.89E+30	-5.6	15540.0	
	Reverse Arhenius coefficients:	3.04E+31	-5.6	26810.0	
	Reverse Arhenius coefficients:	3.81E+17	-1.4	5580.0	
	Reverse Arhenius coefficients:	2.00E+11	0.0	17500.0	
	Reverse Arhenius coefficients:	3.71E+25	-4.0	7043.0	
	Reverse Arhenius coefficients:	1.87E+27	-4.4	101200.0	
	Reverse Arhenius coefficients:	3.33E+12	0.0	0.0	
	Reverse Arhenius coefficients:	2.14E+16	-0.9	71050.0	
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Reverse Arrhenius coefficients:	5.06E-02	3.8	24210.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1675. C3H4-A+C3HS->>C3H3+C3H6	2.00E+11	0.0	7700.0		1731. H2+NC3H7O2<>H+NC3H7O2H	3.01E+13	0.0	26030.0
Reverse Arrhenius coefficients:	2.64E+19	-2.7	42140.0		1732. H2+IC3H7O2<>H+IC3H7O2H	3.01E+13	0.0	26030.0
1676. C3H4-A+C2H<>C3H3+C2H2	1.00E+13	0.0	0.0		Reverse Arrhenius coefficients:	4.80E+13	0.0	7950.0
Reverse Arrhenius coefficients:	1.42E+16	-1.4	53820.0		1733. IC3H7O2+C2H6<>IC3H7O2H+C2H5	1.70E+13	0.0	20460.0
1677. C3H4-P-M<>C3H3+H+M	1.14E+17	0.0	70000.0		Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0
Reverse Arrhenius coefficients:	6.71E+11	0.6	6420.0		1734. NC3H7O2-C2H6<>NC3H7O2H+C2H5	1.70E+13	0.0	20460.0
1678. C3H4-P->>C2H+CH3	4.20E+16	0.0	100000.0		Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0
Reverse Arrhenius coefficients:	1.02E+12	0.6	1600.0		1735. IC3H7O2+C2H5CHO<>IC3H7O2H+C2H5CO	2.00E+11	0.0	9500.0
1679. C3H4-P+O2<>HCCO+OH+CH2	1.00E+07	1.5	30100.0		Reverse Arrhenius coefficients:	5.00E+09	0.0	10000.0
Reverse Arrhenius coefficients:	1.00E+00	0.0	0.0		1736. NC3H7O2-C2H5CHO<>NC3H7O2H+C2H5CO	2.00E+11	0.0	9500.0
1680. C3H4-P+O2<>C3H3+HO2	2.00E+13	0.0	41600.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	6.37E+11	-0.2	10210.0		1737. IC3H7O2+C2H5O2<>IC3H7O2H+C2H5O-O2	1.40E+16	-1.6	1860.0
1681. C3H4-P+HO2<>C2H4+CO+OH	3.00E+12	0.0	19000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	1.00E+00	0.0	0.0		1738. NC3H7O2-C2H5O2<>NC3H7O2H+C2H5O+O2	1.40E+16	-1.6	1860.0
1682. C3H4-P+OH<>>C3H3+H2O	1.00E+07	2.0	1000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	6.44E+05	2.0	30000.0		1739. IC3H7O2+C2H5O2<>IC3H7O2H+C2H5O	1.40E+16	-1.6	1860.0
1683. C3H4-P+OH<>>C2H2CO+CH3	5.00E-04	4.5	-1000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	1.08E-02	4.1	31280.0		1740. NC3H7O2-C2H5O2<>NC3H7O2H+C2H5O+O2	1.40E+16	-1.6	1860.0
1684. C3H4-P-O=>C2H3+HCO	3.20E-12	0.0	2010.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	2.55E+12	-0.4	32350.0		1741. IC3H7O2+IC3H7O2<>O2+IC3H7O+IC3H7O	1.40E+16	-1.6	1860.0
1685. C3H4-P-O=>HCCO-CH2+H	9.60E+08	1.0	0.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	1.43E+04	1.8	26990.0		1742. NC3H7O2+NC3H7O2<>O2+NC3H7O+NC3H7O	1.40E+16	-1.6	1860.0
1686. C3H4-P-O=>HCCO-CH2+H	3.20E-19	0.0	2010.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	1.00E-30	0.0	0.0		1743. IC3H7O2+NC3H7O2<>IC3H7O+NC3H7O+O2	1.40E+16	-1.6	1860.0
1687. C3H4-P-O=>C3H3+OH	7.65E+08	1.5	8600.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	2.18E+08	1.3	22470.0		1744. IC3H7O2+CH3=>IC3H7O+CH3O	7.00E+12	0.0	-1000.0
1688. C3H4-P-H=>C3H3+H2	2.00E+07	2.0	5000.0		Reverse Arrhenius coefficients:	1.14E+11	0.7	26720.0
Reverse Arrhenius coefficients:	1.22E+05	2.1	19110.0		1745. IC3H7O2+C2H5=>IC3H7O+C2H5O	7.00E+12	0.0	-1000.0
1689. C3H4-P+CH3=>C3H3+CH4	1.50E+03	3.5	5600.0		Reverse Arrhenius coefficients:	1.63E+13	0.1	29130.0
Reverse Arrhenius coefficients:	8.31E+00	3.2	21250.0		1746. IC3H7O2+IC3H7=>IC3H7O+IC3H7O	7.00E+12	0.0	-1000.0
1690. C3H4-P+C2H=>C3H3+C2H2	1.00E+12	0.0	0.0		Reverse Arrhenius coefficients:	2.78E+13	0.3	29800.0
Reverse Arrhenius coefficients:	5.30E+11	-0.4	49630.0		1747. IC3H7O2+N-C3H7=>IC3H7O+NC3H7O	7.00E+12	0.0	-1000.0
1691. C3H4-P+C2H3=>C3H3+C2H4	1.00E+12	0.0	7700.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	9.54E+11	-0.2	52450.0		1748. IC3H7O2+CH3=>IC3H7O+CH3O	7.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	4.93E+16	-1.7	37950.0		Reverse Arrhenius coefficients:	1.64E+13	0.1	27800.0
1693. C3H3+O=>CH2O+C2H	1.00E+13	0.0	0.0		1749. NC3H7O2+CH3=>NC3H7O+CH3O	7.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	5.45E+14	0.0	31610.0		Reverse Arrhenius coefficients:	5.30E+12	0.0	26920.0
1694. C3H3+OH=>C2H2+H2O	1.00E+13	-0.0	0.0		1750. NC3H7O2-C2H5=>NC3H7O+C2H5O	7.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	1.34E+15	0.0	15680.0		Reverse Arrhenius coefficients:	1.14E+14	-0.6	29330.0
1695. C3H3+O2=>CH2CO+HCO	3.01E+10	0.0	2870.0		1751. NC3H7O2+L-C3H7=>NC3H7O+IC3H7O	7.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	4.88E+11	0.0	59470.0		Reverse Arrhenius coefficients:	1.29E+15	-0.4	30000.0
1696. C3H3+CH3=>C2H5+C2H	4.30E+15	-0.8	45630.0		1752. NC3H7O2+N-C3H7=>NC3H7O+NC3H7O	7.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	1.81E+13	0.0	0.0		Reverse Arrhenius coefficients:	7.61E+14	-0.6	28000.0
1697. C3H2+O2=>HCO-HCCO	5.00E+13	0.0	0.0		1753. NC3H7O2+CH35-A=>NC3H7O+C3H5O	7.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	2.33E+14	-3.2	77190.0		Reverse Arrhenius coefficients:	1.96E+11	0.2	14340.0
1698. C3H4-H+HO2=>C2H4+CO+OH	1.00E+12	0.0	14000.0		1754. NC3H7O2H=>NC3H7O+OH	1.50E+16	0.0	42500.0
Reverse Arrhenius coefficients:	1.00E+00	0.0	0.0		Reverse Arrhenius coefficients:	1.14E+08	-1.7	-4034.0
1699. C3H4-A+HO2=>C3H3+H2O2	3.00E+13	0.0	14000.0		1755. IC3H7O2H=>IC3H7O+OH	9.45E+15	0.0	42600.0
Reverse Arrhenius coefficients:	1.55E+16	-1.4	44000.0		Reverse Arrhenius coefficients:	1.55E+06	2.4	-4132.0
1700. C2H2+CH3=>C3H4-P+H	4.23E+08	1.1	12090.0		1756. NC3H7O2+>C2H5+CH2O	2.72E+21	-2.4	15700.0
Reverse Arrhenius coefficients:	1.00E+00	0.0	40000.0		Reverse Arrhenius coefficients:	1.00E+11	0.0	3496.0
1701. C2H2+CH3=>C3H4-A+H	6.74E+19	-2.1	31590.0		1757. NC3H7O2H=>C2H5CHO+H	8.90E+10	0.7	19800.0
Reverse Arrhenius coefficients:	6.41E+25	-3.3	21770.0		Reverse Arrhenius coefficients:	4.00E+12	0.0	6260.0
1702. C3H3+H=>C3H2+H2	5.00E+13	0.0	0.0		1758. IC3H7O2+CH3+CH3CHO	5.33E+19	-1.7	17140.0
Reverse Arrhenius coefficients:	6.00E+07	1.4	4110.0		Reverse Arrhenius coefficients:	1.00E+11	0.0	9256.0
1703. C3H2-OH=>C2H2+HCO	5.00E+13	0.0	0.0		1759. IC3H7O2+CH3COCH3+H	8.66E+14	-0.5	20080.0
Reverse Arrhenius coefficients:	2.28E+16	-0.3	75020.0		Reverse Arrhenius coefficients:	2.00E+12	0.0	7270.0
1704. C3H2+O2=>HCCO+CO+H	5.00E+13	0.0	0.0		1760. IC3H7O2+>C3HCOCH3+HO2	9.09E+09	0.0	390.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		Reverse Arrhenius coefficients:	1.00E+11	0.0	32000.0
1705. CH3CHCO+OH=>C2H5+C2O2	1.73E+12	0.0	-1010.0		1761. NC3H7O2+>C3H6OOH1-2	6.00E+11	0.0	26850.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		Reverse Arrhenius coefficients:	1.12E+08	0.6	11720.0
1706. CH3CHCO-OH=>C2H4+HCO+CO	2.00E+12	0.0	-1010.0		1762. NC3H7O2+>C3H6OOH1-3	1.12E+11	0.0	24400.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		Reverse Arrhenius coefficients:	2.72E+11	-0.5	8936.0
1707. CH3CHCO+O=>C3H3CO+CO	3.20E+12	0.0	-437.0		1763. IC3H7O2+>C3H6OOH2-1	1.80E+12	0.0	29400.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		Reverse Arrhenius coefficients:	1.12E+10	0.1	11810.0
1708. N-C3H7+HO2=>NC3H7O+OH	7.00E+12	0.0	-1000.0		1764. IC3H7O2+>C3H6OOH2-2	1.23E+35	-7.1	44940.0
Reverse Arrhenius coefficients:	6.22E+15	-0.7	25100.0		Reverse Arrhenius coefficients:	2.38E+34	-7.1	44940.0
1710. I-C3H7+HO2=>IC3H7+OH	7.00E+12	0.0	-1000.0		1765. C3H6OOH1-2=>C3H6OOH2+2-OH	6.00E+11	0.0	22000.0
Reverse Arrhenius coefficients:	1.05E+16	-0.6	27320.0		Reverse Arrhenius coefficients:	1.15E+11	0.5	38370.0
1711. CH3O2-N-C3H7=>CH3O+NC3H7O	7.00E+12	0.0	-1000.0		1766. C3H6OOH1-3=>C3H6OOH1-3+OH	7.50E+10	0.0	15250.0
Reverse Arrhenius coefficients:	3.89E+14	-0.4	29550.0		Reverse Arrhenius coefficients:	1.19E+06	1.8	28710.0
1712. CH3O2+L-C3H7=>C3H3+IC3H7O	7.00E+12	0.0	-1000.0		1767. C3H6OOH2+>C3H6OOH2+2-OH	6.00E+11	0.0	22000.0
Reverse Arrhenius coefficients:	6.57E+14	-0.3	31560.0		Reverse Arrhenius coefficients:	2.78E+08	1.2	36090.0
1713. NC3H7O2=>N-C3H7+O2	2.40E+20	-1.6	35960.0		1768. C3H6OOH1-3=>C3H6OOH1-2+O2	7.83E+15	-1.3	15950.0
Reverse Arrhenius coefficients:	4.52E+12	0.0	0.0		Reverse Arrhenius coefficients:	1.00E+11	0.0	11000.0
1714. IC3H7O2=>L-C3H7+O2	3.13E+22	-2.2	381600.0		1769. C3H6OOH2=>C3H6OOH2+2-OH	3.24E+18	-2.0	18970.0
Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0		Reverse Arrhenius coefficients:	1.00E+11	0.0	11750.0
1715. NC3H7O2+CH2O=>NC3H7O2H+HCO	5.60E+12	0.0	13600.0		1770. C3H6OOH1-3=>OH+CH2O+C2H4	3.04E+15	-0.8	27400.0
Reverse Arrhenius coefficients:	8.00E+11	0.0	10000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1716. NC3H7O2+CH3CHO=>NC3H7O2H+CH3CO	5.60E+12	0.0	13600.0		1771. C3H6OOH2-1=>C2H3OOH+CH3	6.54E+27	-5.1	38320.0
Reverse Arrhenius coefficients:	1.00E+12	0.0	10000.0		Reverse Arrhenius coefficients:	4.46E+22	-4.2	10630.0
1717. IC3H7O2+CH2O=>IC3H7O2H+HCO	5.60E+12	0.0	13600.0		1772. C3H6OOH1-2=>C2H4+CH2O+OH	1.31E+33	-7.0	48120.0
Reverse Arrhenius coefficients:	8.00E+11	0.0	10000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1718. IC3H7O2+CH3CHO=>IC3H7O2H+CH3CO	2.80E+12	0.0	13600.0		1773. C3H6OOH2-2=>C3H3COCH3+OH	9.00E+14	1.0	1500.0
Reverse Arrhenius coefficients:	1.00E+12	0.0	10000.0		Reverse Arrhenius coefficients:	1.02E+14	0.3	36750.0
1719. NC3H7O2+HO2=>NC3H7O2H+O2	1.75E+10	0.0	-3275.0		1774. C3H6OOH1-202=>C3H6OOH1-2+O2	2.39E+25	-2.9	40100.0
Reverse Arrhenius coefficients:	3.84E+13	-0.8	33610.0		Reverse Arrhenius coefficients:	5.00E+12	0.0	0.0
1720. IC3H7O2+HO2=>C3H7O2H+O2	1.75E+10	0.0	-3275.0		1775. C3H6OOH1-302=>C3H6OOH1-3+O2	2.85E+20	-1.6	35690.0
Reverse Arrhenius coefficients:	3.86E+13	-0.8	33610.0		Reverse Arrhenius coefficients:	4.52E+12	0.0	0.0
1721. C2H4+NC3H7O2=>C2H3+NC3H7O2H	1.13E+13	0.0	30430.0		1776. C3H6OOH2-102=>C3H6OOH2-1+O2	5.23E+22	-2.2	37820.0
Reverse Arrhenius coefficients:	3.00E+12	0.0	11500.0		Reverse Arrhenius coefficients:	4.52E+12	0.0	0.0
1722. C2H4+IC3H7O2=>C2H3+IC3H7O2H	1.13E+13	0.0	30430.0		1777. C3H6OOH1-202=>C3KET12+OH	6.00E+11	0.0	26400.0
Reverse Arrhenius coefficients:	3.00E+12	0.0	11500.0		Reverse Arrhenius coefficients:	9.25E+04	1.3	48920.0
1723. CH3OH+NC3H7O2=>CH2OH+IC3H7O2H	6.30E+12	0.0	19360.0		1778. C3H6OOH1-302=>C3KET13+OH	7.50E+10	0.0	21400.0
Reverse Arrhenius coefficients:	1.00E+09	0.0	10000.0		Reverse Arrhenius coefficients:	4.10E+03	1.5	44740.0
1724. CH3OH+IC3								

1786. C3KET13<=>CH2O+CH2CHO+OH	1.00E+16	0.0	43000.0				
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0				
1787. C3KET21<=>CH2O+CH3CO+OH	1.00E+16	0.0	43000.0				
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0				
1788. AC3H5OOH<=>C3H5O+OH	3.88E+19	-1.5	45370.0				
Reverse Arrhenius coefficients:	2.00E+13	0.0	0.0				
1789. C3H5O<=>C2H3CHO+H	1.00E+14	-0.2	29100.0				
Reverse Arrhenius coefficients:	1.68E+14	0.0	19690.0				
1790. C3H5O<=>C2H3+CH2O	1.46E+20	-2.0	35090.0				
Reverse Arrhenius coefficients:	1.50E+11	0.0	10600.0				
1791. C3H5O+O2<=>C2H3CHO+HO2	1.00E+12	0.0	6000.0				
Reverse Arrhenius coefficients:	1.29E+11	0.0	32000.0				
1792. C2H3OOH<=>CH2CHO+OH	8.40E+14	0.0	43000.0				
Reverse Arrhenius coefficients:	1.00E+11	0.0	0.0				
1793. C3H6O1-2<=>C2H4+CH2O	6.00E+14	0.0	60000.0				
Reverse Arrhenius coefficients:	2.97E+11	1.0	31080.0				
1794. C3H6O1-2+OH<=>CH2O+C2H3+H2O	5.00E+12	0.0	0.0				
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0				
1795. C3H6O1-2+H<=>CH2O+C2H3+H2	2.63E+07	2.0	5000.0				
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0				
1796. C3H6O1-2+O<=>CH2O+C2H3+OH	8.43E+13	0.0	5200.0				
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0				
1797. C3H6O1-2+HO2<=>CH2O+C2H3+H2O2	1.00E+13	0.0	15000.0				
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0				
1798. C3H6O1-2+CH3O2<=>CH2O+C2H3+CH3O2H	1.00E+13	0.0	19000.0				
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0				
1799. C3H6O1-2+CH3<=>CH2O+C2H3+CH4	2.00E+11	0.0	10000.0				
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0				
1800. C3H6O1-3<=>C2H4+CH2O	6.00E+14	0.0	60000.0				
Reverse Arrhenius coefficients:	2.97E+11	0.0	31080.0				
1801. C3H6O1-3+OH<=>CH2O+C2H3+H2O	5.00E+12	0.0	0.0				
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0				
1802. C3H6O1-3+O<=>CH2O+C2H3+OH	8.43E+13	0.0	5200.0				
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0				
1803. C3H6O1-3+H<=>CH2O+C2H3+H2	2.63E+07	2.0	5000.0				
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0				
1804. C3H6O1-3+CH3O2<=>CH2O+C2H3+CH3O2H	1.00E+13	0.0	19000.0				
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0				
1805. C3H6O1-3+HO2<=>CH2O+C2H3+H2O2	1.00E+13	0.0	15000.0				
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0				
1806. C3H6O1-3+CH3<=>CH2O+C2H3+CH4	2.00E+11	0.0	10000.0				
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0				
1807. IC 3H7O2<=>C3H6+HO2	1.01E+43	-9.4	41490.0				
Reverse Arrhenius coefficients:	1.95E+33	-7.3	16670.0				
1808. NC3H7O2<=>C3H6+HO2	5.04E+38	-8.1	40490.0				
Reverse Arrhenius coefficients:	1.20E+30	-6.2	20420.0				
1809. C4H10+(M)<=>C2H5-C2H5(-M)	2.72E+15	0.0	75610.0				
Low pressure limit: 0.47200E+19 0.00000E+00 0.49576E+05							
TROE centering: 0.72000E+00 0.15000E+04 0.10000E+11							
1810. C4H10(+M)<=>C-N-C3H5+(M)	4.28E+14	0.0	69900.0				
Low pressure limit: 0.53400E+18 0.00000E+00 0.42959E+05							
TROE centering: 0.72000E+00 0.15000E+04 0.10000E+11							
1811. C4H10+C3H5-A<=>P-C4H9+C3H6	7.94E+11	0.0	20500.0				
Reverse Arrhenius coefficients:	1.00E+12	0.0	20000.0				
1812. C4H10+C3H5-A<=>S-C4H9+C3H6	3.16E+11	0.0	16400.0				
Reverse Arrhenius coefficients:	1.00E+12	0.0	20000.0				
1813. C4H10+C2F50<=>P-C4H9+C2H5OH	3.00E+11	0.0	7000.0				
Reverse Arrhenius coefficients:	1.00E+10	0.0	9000.0				
1814. C4H10+C2H5O<=>S-C4H9+C2H5OH	6.00E+11	0.0	7000.0				
Reverse Arrhenius coefficients:	1.00E+10	0.0	9000.0				
1815. C4H10-P-C4H9<=>S-C4H9+C4H10	1.00E+11	0.0	10400.0				
Reverse Arrhenius coefficients:	1.50E+11	0.0	12300.0				
1816. C4H10-CH3CO3<=>P-C4H9+CH3CO3H	1.70E+13	0.0	20460.0				
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0				
1817. C4H10-CH3CO3<=>C4H9+CH3CO3H	1.12E+13	0.0	17700.0				
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0				
1818. C4H10-O2CHO<=>P-C4H9+HO2CHO	1.68E+13	0.0	20440.0				
Reverse Arrhenius coefficients:	3.68E+00	3.0	2505.0				
1819. C4H10-O2CHO<=>S-C4H9+HO2CHO	1.12E+13	0.0	17690.0				
Reverse Arrhenius coefficients:	7.60E+03	2.1	4266.0				
1820. CH3O2+C4H10<=>CH3O2H-P-C4H9	1.39E+00	4.0	18280.0				
Reverse Arrhenius coefficients:	1.68E+00	3.5	3016.0				
1821. CH3O2-C4H10<=>CH3O2H-S-C4H9	2.04E+01	3.6	14810.0				
Reverse Arrhenius coefficients:	1.68E+00	3.4	2050.0				
1822. C2H5O2+C4H10<=>C2H5O2H-P-C4H9	4.08E+01	3.6	17160.0				
Reverse Arrhenius coefficients:	4.94E+01	3.1	18990.0				
1823. C2H5O2+C4H10<=>C2H5O2H-S-C4H9	1.26E+02	3.4	13720.0				
Reverse Arrhenius coefficients:	1.04E+01	3.2	967.0				
1824. NC3H7O2+C4H10<=>NC3H7O2H+P-C4H9	1.70E+13	0.0	20460.0				
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0				
1825. NC3H7O2+C4H10<=>NC3H7O2H+S-C4H9	1.12E+13	0.0	17700.0				
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0				
1826. IC3H7O2-C4H10<=>IC3H7O2H+P-C4H9	1.70E+13	0.0	20460.0				
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0				
1827. IC3H7O2-C4H10<=>IC3H7O2H+S-C4H9	1.12E+13	0.0	17700.0				
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0				
1828. PC4H9O2+C3H8<=>PC4H9O2H+N-C3H7	1.70E+13	0.0	20460.0				
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0				
1829. PC4H9O2+C3H8<=>PC4H9O2H+I-C3H7	2.00E+12	0.0	17000.0				
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0				
1830. PC4H9O2+C4H10<=>PC4H9O2H+P-C4H9	1.70E+13	0.0	20460.0				
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0				
1831. PC4H9O2+C4H10<=>PC4H9O2H+S-C4H9	1.12E+13	0.0	17700.0				
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0				
1832. SC4H9O2-C3H8<=>SC4H9O2H+N-C3H7	1.70E+13	0.0	20460.0				
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0				
1833. SC4H9O2-C3H8<=>SC4H9O2H+I-C3H7	2.00E+12	0.0	17000.0				
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0				
1834. SC4H9O2+C4H10<=>SC4H9O2H+P-C4H9	1.70E+13	0.0	20460.0				
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0				
1835. SC4H9O2+C4H10<=>SC4H9O2H+S-C4H9	1.12E+13	0.0	17700.0				
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0				
1836. P-C4H9+O2<=>C4H8-1+H	2.62E+12	0.3	35700.0				
Reverse Arrhenius coefficients:	2.50E+11	0.5	2620.0				
1837. S-C4H9<=>C4H8-2+H	2.84E+11	0.3	35520.0				
Reverse Arrhenius coefficients:	2.50E+11	0.5	2620.0				
1838. S-C4H9<=>C4H8-1+H	3.03E+11	0.6	36820.0				
Reverse Arrhenius coefficients:	4.24E+11	0.5	1230.0				
1839. P-C4H9+O2<=>C4H8-1+H02	2.00E+18	0.0	5000.0				
Reverse Arrhenius coefficients:	2.00E-19	0.0	17500.0				
1840. S-C4H9+O2<=>C4H8-1+H02	2.00E+18	0.0	5000.0				
Reverse Arrhenius coefficients:	2.00E-19	0.0	17500.0				
1841. S-C4H9+O2<=>C4H8-2+H02	2.00E+18	0.0	5000.0				
Reverse Arrhenius coefficients:	2.00E-19	0.0	17500.0				
1842. C4H8-1<=>C3H5-A+C3H3	5.08E+19	-1.3	76510.0				
Reverse Arrhenius coefficients:	1.35E+13	0.0	0.0				
1843. C4H8-1<=>C2H3+C2H5	2.88E+23	-2.0	101600.0				
Reverse Arrhenius coefficients:	9.00E+12	0.0	0.0				
1844. C4H8-1<=>H+C4H7-1-3	3.72E+14	-0.1	85200.0				
Reverse Arrhenius coefficients:	5.00E+13	0.0	0.0				
1845. C4H8-1+O2<=>C4H7-1-3+HO2	2.00E+13	0.0	37190.0				
Reverse Arrhenius coefficients:	4.65E+12	0.1	-168.0				
1846. C4H8-1+H<=>C4H7-1+H2	7.81E+05	2.5	12290.0				
Reverse Arrhenius coefficients:	2.21E+05	2.4	6469.0				
1847. C4H8-1+H<=>C4H7-1+H2+H	3.90E+05	2.5	5821.0				
Reverse Arrhenius coefficients:	2.56E+04	2.5	2125.0				
1848. C4H8-1+H<=>C4H7-1-3+H2	3.38E+05	2.4	207.0				
Reverse Arrhenius coefficients:	4.32E+06	2.1	20330.0				
1849. C4H8-1+H<=>C4H7-1+H2+H2	6.65E+05	2.5	6756.0				
Reverse Arrhenius coefficients:	3.04E+04	2.5	11030.0				
1850. C4H8-1+HO<=>C4H7-1-1+H20	2.14E+06	2.0	2778.0				
Reverse Arrhenius coefficients:	2.62E+06	1.9	12120.0				
1851. C4H8-1+OH<=>C4H7-1-2+H20	2.22E+06	2.0	1451.0				
Reverse Arrhenius coefficients:	6.30E+05	2.0	12910.0				
1852. C4H8-1+OH<=>C4H7-1-3+H2O	2.76E+04	2.6	-1919.0				
Reverse Arrhenius coefficients:	1.53E+06	2.4	3360.0				
1853. C4H8-1+OH<=>C4H7-1-4+H20	5.27E+09	1.0	1586.0				
Reverse Arrhenius coefficients:	1.04E+09	1.0	21010.0				
1854. C4H8-1+CH3<=>C4H7-1-3+CH4	3.69E+00	3.3	4002.0				
Reverse Arrhenius coefficients:	1.23E+03	3.0	24610.0				
1855. C4H8-1+CH3<=>C4H7-1+CH4	4.52E-01	3.6	7154.0				
Reverse Arrhenius coefficients:	5.40E-01	3.6	11910.0				
1856. C4H8-1+HO2<=>C4H7-1-3+H2O2	4.82E+03	2.5	10530.0				
Reverse Arrhenius coefficients:	1.59E+06	2.0	14350.0				
1857. C4H8-1+HO2<=>C4H7-1-4+H2O2	2.38E+03	2.5	16490.0				
Reverse Arrhenius coefficients:	2.80E+03	2.2	4460.0			</	

1899. C4H71-3+CH3O<=>C4H8-1+CH2O	2.41E+13	0.0	0.0
Reverse Arrhenius coefficients:	2.48E+12	0.3	66330.0
1900. C4H71-3+O<=>C2H3CHO+CH3	6.03E+13	0.0	0.0
Reverse Arrhenius coefficients:	3.38E+15	-0.8	81630.0
1901. C4H71-3+HO2<=>C4H70+OH	9.64E+12	0.0	0.0
Reverse Arrhenius coefficients:	7.29E+15	-1.1	15530.0
1902. C4H71-3+CH3O2<=>C4H70+CH3O	9.64E+12	0.0	0.0
Reverse Arrhenius coefficients:	7.12E+17	-1.7	20290.0
1903. C3H5-A+C4H71-3<=>C3H6+C4H6	6.31E+12	0.0	0.0
Reverse Arrhenius coefficients:	1.00E+10	0.0	50000.0
1904. C4H71-3+O2<=>C4H6+HO2	1.00E+09	0.0	0.0
Reverse Arrhenius coefficients:	1.00E+11	0.0	17000.0
1905. H+C4H71-3<=>C4H6+H2	3.16E+13	0.0	0.0
Reverse Arrhenius coefficients:	1.07E+13	0.0	56810.0
1906. C2H5+C4H71-3<=>C4H6+C2H6	3.98E+12	0.0	0.0
Reverse Arrhenius coefficients:	3.21E+12	0.0	49840.0
1907. C2H3+C4H71-3<=>C2H4+C4H6	3.98E+12	0.0	0.0
Reverse Arrhenius coefficients:	1.16E+13	0.0	57710.0
1908. C4H71-3+CH3O2<=>C4H70+C2H5O	3.80E+12	0.0	-1200.0
Reverse Arrhenius coefficients:	2.00E+10	0.0	0.0
1909. IC3H7O2+C4H71-3<=>C3H7O+C4H7O	3.80E+12	0.0	-1200.0
Reverse Arrhenius coefficients:	2.00E+10	0.0	0.0
1910. NC3H7O2+C4H71-3<=>NC3H7O+C4H7O	3.80E+12	0.0	-1200.0
Reverse Arrhenius coefficients:	2.00E+10	0.0	0.0
1911. C4H70<=>CH3CHO+C2H3	7.94E+14	0.0	19000.0
Reverse Arrhenius coefficients:	1.00E+10	0.0	20000.0
1912. C4H70<=>C2H3CHO+C3H3	7.94E+14	0.0	19000.0
Reverse Arrhenius coefficients:	1.00E+10	0.0	20000.0
1913. C4H6+OH<=>C2H0+C3H5-A	1.00E+12	0.0	0.0
Reverse Arrhenius coefficients:	3.50E+06	0.0	71060.0
1914. C4H6-O<=>C2H0-C3H4-A	1.00E+12	0.0	0.0
Reverse Arrhenius coefficients:	1.08E+12	0.0	79050.0
1915. C2H3+C2H4<=>C4H+H	5.00E+11	0.0	7300.0
Reverse Arrhenius coefficients:	1.00E+13	0.0	4700.0
1916. C4H801-2+OH<=>C2H0+C3H5-A+H2O	5.00E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1917. C4H801-2+H<=>C2H0-C3H5-A+H2	5.00E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1918. C4H801-2+O<=>C2H0-C3H5-A+OH	5.00E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1919. C4H801-2+HO2<=>C2H0-C3H5-A+H2O2	1.00E+13	0.0	15000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1920. C4H801-2+CH3O2<=>C2H0+C3H5-A+CH3O2H	1.00E+13	0.0	0.0
19000.0			
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1921. C4H801-2+CH3<=>C2H0-C3H5-A+C4H	2.00E+11	0.0	10000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1922. C4H801-3+OH<=>C2H0+C3H5-A+H2O	5.00E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1923. C4H801-3+H<=>C2H0-C3H5-A+H2	5.00E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1924. C4H801-3+O<=>C2H0-C3H5-A+OH	5.00E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1925. C4H801-3+HO2<=>C2H0-C3H5-A+H2O2	1.00E+13	0.0	15000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1926. C4H801-3+CH3O2<=>C2H0+C3H5-A+CH3O2H	1.00E+13	0.0	0.0
19000.0			
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1927. C4H801-3+CH3<=>C2H0-C3H5-A+C4H	2.00E+11	0.0	10000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1928. C4H801-4+OH<=>C2H0+C3H5-A+H2O	5.00E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1929. C4H801-4+H<=>C2H0-C3H5-A+H2	5.00E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1930. C4H801-4+O<=>C2H0-C3H5-A+OH	5.00E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1931. C4H801-4+HO2<=>C2H0-C3H5-A+H2O2	1.00E+13	0.0	15000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1932. C4H801-4+CH3O2<=>C2H0+C3H5-A+CH3O2H	1.00E+13	0.0	0.0
19000.0			
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1933. C4H801-4+CH3<=>C2H0-C3H5-A+C4H	2.00E+11	0.0	10000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1934. C4H802-3+OH<=>C2H0+C3H5-A+H2O	5.00E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1935. C4H802-3+H<=>C2H0-C3H5-A+H2	5.00E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1936. C4H802-3+O<=>C2H0-C3H5-A+OH	5.00E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1937. C4H802-3+HO2<=>C2H0-C3H5-A+H2O2	1.00E+13	0.0	15000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1938. C4H802-3+CH3O2<=>C2H0+C3H5-A+CH3O2H	1.00E+13	0.0	0.0
19000.0			
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1939. C4H802-3+CH3<=>C2H0+C3H5-A+C4H	2.00E+11	0.0	10000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1940. PC4H902->>PC4H9+O2	2.85E+20	-1.6	35930.0
Reverse Arrhenius coefficients:	4.52E+12	0.0	0.0
1941. SC4H902->>S-C4H9+O2	4.33E+22	-2.2	38160.0
Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0
1942. SC4H902+CH2O<=>SC4H902H+HCO	5.60E+12	0.0	13600.0
Reverse Arrhenius coefficients:	8.00E+11	0.0	10000.0
1943. SC4H902+CH3CHO<=>SC4H902H+CH3CO	2.80E+12	0.0	13600.0
Reverse Arrhenius coefficients:	1.00E+12	0.0	10000.0
1944. SC4H902+HO2<=>SC4H902H+O2	1.75E+10	-0.0	-3275.0
Reverse Arrhenius coefficients:	3.86E+13	-0.8	33620.0
1945. IC3H7O2+P-C4H9->IC3H7O+PC4H9O	7.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	2.28E+13	0.1	27480.0
1946. IC3H7O2+S-C4H9->IC3H7O+SC4H9O	7.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	3.94E+15	-0.4	29190.0
1947. NC3H7O2+P-C4H9->NC3H7O+PC4H9O	7.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	1.06E+15	-0.6	26780.0
1948. NC3H7O2+S-C4H9->NC3H7O+SC4H9O	7.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	1.82E+17	-1.1	29390.0
1949. SC4H902+SC4H9O2<=>O2+SC4H9O+SC4H9O	1.40E+16	-1.6	1860.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1950. SC4H902+NC3H7O2<=>SC4H9O+NC3H7O+O2	1.40E+16	-1.6	1860.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1951. SC4H902+IC3H7O2<=>SC4H9O+IC3H7O+O2	1.40E+16	-1.6	1860.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1952. SC4H902+C2H5O2<=>SC4H9O+C2H5O+O2	1.40E+16	-1.6	1860.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1953. SC4H902+CH3O2<=>SC4H9O+CH3O+O2	1.40E+16	-1.6	1860.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1954. SC4H902+CH3CO3<=>SC4H9O+CH3CO2+O2	1.40E+16	-1.6	1860.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1955. PC4H902+HO2<=>PC4H9O+OH+O2	1.40E+14	-1.6	1860.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1956. SC4H902+HO2<=>SC4H9O+OH+O2	1.40E+14	-1.6	1860.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1957. H2+PC4H9O2<=>H+PC4H9O2H	3.01E+13	0.0	26030.0
Reverse Arrhenius coefficients:	4.80E+13	0.0	7950.0
1958. H2+SC4H9O2<=>H+SC4H9O2H	3.01E+13	0.0	26030.0
Reverse Arrhenius coefficients:	4.80E+13	0.0	7950.0
1959. C2H6+PC4H9O2<=>C2H5+PC4H9O2H	1.70E+13	0.0	20460.0
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0
1960. C2H6+SC4H9O2<=>C2H5+SC4H9O2H	1.70E+13	0.0	20460.0
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0
1961. PC4H9O2+C2H5CHO<=>PC4H9O2H+C2H5CO	2.00E+11	0.0	9500.0
Reverse Arrhenius coefficients:	5.00E+09	0.0	10000.0
1962. SC4H9O2+C2H5CHO<=>SC4H9O2H+C2H5CO	2.00E+11	0.0	9500.0
Reverse Arrhenius coefficients:	5.00E+09	0.0	10000.0
1963. SC4H9O2+CH3<=>SC4H9O+CH3O	7.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	1.18E+13	0.1	26110.0
1964. SC4H9O2+C2H5<=>SC4H9O+C2H5O	7.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	1.67E+15	-0.5	28520.0
1965. SC4H9O2+I-C3H7<=>SC4H9O+IC3H7O	7.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	2.85E+15	-0.4	29190.0
1966. SC4H9O2+N-C3H7<=>SC4H9O+NC3H7O	7.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	1.69E+15	-0.5	27190.0
1967. SC4H9O2+P-C4H9<=>SC4H9O+PC4H9O	7.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	2.34E+15	-0.6	26870.0
1968. SC4H9O2+S-C4H9<=>SC4H9O+SC4H9O	7.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	4.05E+17	-1.0	28580.0
1969. SC4H9O2+C3H5-A<=>SC4H9O+C3H5O	7.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	4.36E+11	0.2	15350.0
1970. PC4H9O2+CH2O<=>PC4H9O2H+HCO	5.60E+12	0.0	13600.0
Reverse Arrhenius coefficients:	8.00E+11	0.0	10000.0
1971. PC4H9O2+CH3CHO<=>PC4H9O2H+CH3CO	2.80E+12	0.0	13600.0
Reverse Arrhenius coefficients:	1.00E+12	0.0	10000.0
1972. PC4H9O2+HO2<=>PC4H9O2H+O2	1.75E+10	0.0	-3275.0
Reverse Arrhenius coefficients:	4.36E+13	-0.8	33630.0
1973. C2H6+PC4H9O2<=>C3H5-A+PC4H9O2H	3.24E+11	0.0	14900.0
Reverse Arrhenius coefficients:	2.00E+10	0.0	15000.0
1974. C3H6+SC4H9O2<=>C3H5-A+SC4H9O2H	3.24E+11	0.0	14900.0
Reverse Arrhenius coefficients:	3.00E+12	0.0	11500.0
1976. C2H4+SC4H9O2<=>C2H3+SC4H9O2H	1.13E+13	0.0	30430.0
Reverse Arrhenius coefficients:	3.00E+12	0.0	11500.0
1977. C2H3+SC4H9O2<=>C2H2H+PC4H9O2H	6.30E+12	0.0	19360.0
Reverse Arrhenius coefficients:	1.00E+09	0.0	10000.0
1978. C2H3+SC4H9O2<=>C2H2H+SC4H9O2H	6.30E+12	0.0	19360.0
Reverse Arrhenius coefficients:	1.00E+09	0.0	10000.0
1979. C2H3CHO+PC4H9O2<=>C2H3CO+PC4H9O2H	2.80E+12	0.0	13600.0
Reverse Arrhenius coefficients:	1.00E+12	0.0	10000.0
1980. C2H3CHO+SC4H9O2<=>C2H3CO+SC4H9O2H	2.80E+12	0.0	10000.0
Reverse Arrhenius coefficients:	1.00E+12	0.0	10000.0
1981. CH4+PC4H9O2<=>CH3+PC4H9O2H	1.12E+13	0.0	24640.0
Reverse Arrhenius coefficients:	7.43E+11	0.0	5500.0
1982. CH4+SC4H9O2<=>CH3+SC4H9O2H	1.12E+13	0.0	24640.0
Reverse Arrhenius coefficients:	7.43E+11	0.0	5500.0
1983. C4H71-3+PC4H9O2<=>C4H70+PC4H9O	7.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	1.19E+14	-0.8	16100.0
1984. C4H71-3+SC4H9O2<=>C4H70+SC4H9O	7.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	2.25E+14	-0.7	1580.0
1985. H2O2+PC4H9O2<=>H2+PC4H9O2H	2.40E+12	0.0	10000.0
Reverse Arrhenius coefficients:	2.40E+12	0.0	10000.0
1986. H2O2+SC4H9O2<=>H2+SC4H9O2H	2.40E+12	0.0	10000.0
Reverse Arrhenius coefficients:	2.40E+12	0.0	10000.0
1987. PC4H9O2+PC4H9O2<=>PC4H9O+PC4H9O	1.40E+16	-1.6	1860.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1988. PC4H9O2+SC4H9O2<=>PC4H9O+SC4H9O+O2	1.40E+16	-1.6	1860.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1989. PC4H9O2+NC3H7O2<=>PC4H9O+NC3H7O+O2	1.40E+16	-1.6	1860.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1990. PC4H9O2+IC3H7O2<=>PC4H9O+IC3H7O+O2	1.40E+16	-1.6	1860.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
1991. PC4H9O2+C2H5O2<=>PC4H9O+C2H5O+O2	1.40E+16	-1.6	1860.0
Reverse Arrhenius coefficients:			

2009. SC4H9O<=>C2H5+CH3CHO	5.49E+22	-2.8	12650.0	
Reverse Arhenius coefficients:	3.33E+10	0.0	6397.0	
2010. PC4H9O2<=>C4H8OOH1-2	2.00E+11	0.0	26850.0	
Reverse Arhenius coefficients:	5.60E+08	0.3	11970.0	
2011. PC4H9O2<=>C4H8OOH1-3	2.50E+10	0.0	20850.0	
Reverse Arhenius coefficients:	3.23E+09	-0.1	7871.0	
2012. PC4H9O2<=>C4H8OOH1-4	4.69E+09	0.0	22350.0	
Reverse Arhenius coefficients:	1.27E+10	-0.5	6900.0	
2013. SC4H9O2<=>C4H8OOH2-1	3.00E+11	0.0	29400.0	
Reverse Arhenius coefficients:	7.44E+11	-0.5	13940.0	
2014. SC4H9O2<=>C4H8OOH2-3	2.00E+11	0.0	26850.0	
Reverse Arhenius coefficients:	3.99E+10	-0.2	13930.0	
2015. SC4H9O2<=>C4H8OOH2-4	3.75E+10	0.0	24400.0	
Reverse Arhenius coefficients:	9.30E+10	-0.5	8944.0	
2016. PC4H9O2<=>C4H8-1-HO2	5.04E+38	-8.1	40490.0	
Reverse Arhenius coefficients:	1.60E+30	-6.3	20350.0	
2017. SC4H9O2<=>C4H8-1-HO2	5.07E+42	-9.4	41490.0	
Reverse Arhenius coefficients:	2.60E+33	-7.3	16610.0	
2018. SC4H9O2<=>C4H8-2-HO2	5.04E+38	-8.1	40490.0	
Reverse Arhenius coefficients:	1.62E+29	-5.8	18300.0	
2019. C4H8OOH1-2<=>C4H8-1-HO2	8.83E+16	-1.5	16260.0	
Reverse Arhenius coefficients:	1.00E+11	0.0	11000.0	
2020. C4H8OOH2-1<=>C4H8-1-HO2	4.85E+20	-2.6	21180.0	
Reverse Arhenius coefficients:	1.00E+11	0.0	11750.0	
2021. C4H8OOH2-3<=>C4H8-2-HO2	6.22E+19	-2.5	21020.0	
Reverse Arhenius coefficients:	1.00E+11	0.0	11750.0	
2022. C4H8OOH1-2<=>C4H8O1-2-OH	6.00E+11	0.0	22000.0	
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0	
2023. C4H8OOH1-3<=>C4H8O1-3-OH	7.50E+10	0.0	15250.0	
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0	
2024. C4H8OOH1-4<=>C4H8O1-4-OH	9.38E+09	0.0	6000.0	
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0	
2025. C4H8OOH2-1<=>C4H8O1-2-OH	6.00E+11	0.0	22000.0	
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0	
2026. C4H8OOH2-3<=>C4H8O2-3-OH	6.00E+11	0.0	22000.0	
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0	
2027. C4H8OOH2-4<=>C4H8O1-3-OH	7.50E+10	0.0	15250.0	
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0	
2028. C4H8OOH1-4<=>NC3H7CHO+OH	9.00E+14	0.0	1500.0	
Reverse Arhenius coefficients:	1.73E+08	1.9	33470.0	
2029. C4H8OOH2-2<=>C2H5COCH3+OH	9.00E+14	0.0	1500.0	
Reverse Arhenius coefficients:	1.99E+10	1.3	35510.0	
2030. C4H8OOH1-3<=>OH-CH2O+C3H6	6.64E+13	-0.2	29900.0	
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0	
2031. C4H8OOH2-4<=>OH-CH3CHO+C2H4	1.94E+18	-1.6	26790.0	
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0	
2032. C4H8OOH1-202<=>C4H8OOH1-2+O2	2.59E+24	-2.7	39860.0	
Reverse Arhenius coefficients:	7.54E+12	0.0	0.0	
2033. C4H8OOH1-302<=>C4H8OOH1-3+O2	5.60E+22	-2.2	37960.0	
Reverse Arhenius coefficients:	7.54E+12	0.0	0.0	
2034. C4H8OOH1-402<=>C4H8OOH1-4+O2	2.57E+20	-1.6	35680.0	
Reverse Arhenius coefficients:	4.52E+12	0.0	0.0	
2035. C4H8OOH2-102<=>C4H8OOH2-1+O2	2.82E+20	-1.6	35700.0	
Reverse Arhenius coefficients:	4.52E+12	0.0	0.0	
2036. C4H8OOH2-302<=>C4H8OOH2-3+O2	4.52E+22	-2.2	37880.0	
Reverse Arhenius coefficients:	7.54E+12	0.0	0.0	
2037. C4H8OOH2-402<=>C4H8OOH2-4+O2	2.82E+20	-1.6	35700.0	
Reverse Arhenius coefficients:	4.52E+12	0.0	0.0	
2038. C4H8OOH1-202<=>NC4KET12+OH	2.00E+11	0.0	26400.0	
Reverse Arhenius coefficients:	3.20E+04	1.3	48930.0	
2039. C4H8OOH1-302<=>NC4KET13+OH	2.50E+10	0.0	21400.0	
Reverse Arhenius coefficients:	1.44E+03	1.5	44740.0	
2040. C4H8OOH1-402<=>NC4KET14+OH	3.12E+09	0.0	19350.0	
Reverse Arhenius coefficients:	1.73E+02	1.5	42690.0	
2041. C4H8OOH2-102<=>NC4KET21+OH	1.00E+11	0.0	23850.0	
Reverse Arhenius coefficients:	3.63E+02	1.8	50050.0	
2042. C4H8OOH2-302<=>NC4KET23+OH	1.00E+11	0.0	23850.0	
Reverse Arhenius coefficients:	1.74E+03	1.7	49130.0	
2043. C4H8OOH2-402<=>NC4KET24+OH	1.25E+10	0.0	17850.0	
Reverse Arhenius coefficients:	1.02E+02	1.8	43920.0	
2044. NC4KET12<=>C2H5CHO-HCO+OH	1.05E+16	0.0	41600.0	
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0	
2045. NC4KET13<=>CH3CHO-CH2CHO-OH	1.05E+16	0.0	41600.0	
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0	
2046. NC4KET14<=>CH2CH2CHO-CH2O+OH	1.50E+16	0.0	42000.0	
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0	
2047. NC4KET21<=>C2H5CO+OH	1.50E+16	0.0	42000.0	
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0	
2048. NC4KET23<=>CH3CHO+CH3CO+OH	1.05E+16	0.0	41600.0	
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0	
2049. NC4KET24<=>CH2O+CH3COCH2+OH	1.50E+16	0.0	42000.0	
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0	
2050. C2H5COCH3-OH<=>C2H2CH2COCH3-H2O	7.55E+09	1.0	1586.0	
Reverse Arhenius coefficients:	1.53E+09	1.0	21200.0	
2051. C2H5COCH3-OH<=>CH3CHCOCH3-H2O	8.45E+11	0.0	-228.0	
Reverse Arhenius coefficients:	1.59E+13	-0.2	28260.0	
2052. C2H5COCH3-OH<=>C2H5COCH2+H2O	5.10E+11	0.0	1192.0	
Reverse Arhenius coefficients:	6.63E+13	-0.7	27670.0	
2053. C2H5COCH3-HO2<=>C2H2CH2COCH3+H2O2	2.38E+04	2.5	16490.0	
Reverse Arhenius coefficients:	2.86E+04	2.2	4459.0	
2054. C2H5COCH3-HO2<=>CH3CHCOCH3+H2O2	2.00E+11	0.0	8698.0	
Reverse Arhenius coefficients:	2.23E+13	-0.6	6080.0	
2055. C2H5COCH3-HO2<=>C2H5COCH2+H2O2	2.38E+04	2.5	14690.0	
Reverse Arhenius coefficients:	1.84E+07	1.5	9702.0	
2056. C2H5COCH3-O<=>CH2CH2COCH3+OH	2.25E+13	0.0	7700.0	
Reverse Arhenius coefficients:	4.62E+11	0.0	9882.0	
2057. C2H5COCH3-O<=>CH3CHCOCH3+OH	3.07E+13	0.0	3400.0	
Reverse Arhenius coefficients:	5.85E+13	-0.2	15000.0	
2058. C2H5COCH3-O<=>C2H5COCH2+OH	5.00E+12	0.0	5962.0	
Reverse Arhenius coefficients:	6.59E+13	-0.7	15190.0	
2059. C2H5COCH3-H<=>CH2CH2COCH3+H2	9.16E+06	2.0	7700.0	
Reverse Arhenius coefficients:	4.28E+05	2.0	11980.0	
2060. C2H5COCH3-H<=>CH3CHCOCH3+H2	4.46E+06	2.0	3200.0	
Reverse Arhenius coefficients:	1.93E+07	1.8	16890.0	
2061. C2H5COCH3+H<=>C2H5COCH2+H2	9.30E+12	0.0	6357.0	
Reverse Arhenius coefficients:	2.79E+14	-0.7	17680.0	
2062. C2H5COCH3-O2<=>CH2CH2COCH3+H2O2	2.05E+13	0.0	51310.0	
Reverse Arhenius coefficients:	1.74E+10	0.3	-1895.0	
2063. C2H5COCH3-O2<=>CH3CHCOCH3+H2O2	1.55E+13	0.0	41970.0	
Reverse Arhenius coefficients:	1.22E+12	0.1	-1822.0	
2064. C2H5COCH3-O2<=>C2H5COCH2+H2O2	2.05E+13	0.0	49150.0	
Reverse Arhenius coefficients:	1.12E+13	-0.4	2988.0	
2065. C2H5COCH3+CH3<=>CH2CH2COCH3+CH4	3.19E+01	3.2	7172.0	
Reverse Arhenius coefficients:	3.89E+01	3.2	11930.0	
2066. C2H5COCH3+CH3<=>CH3CHCOCH3+CH4	1.74E+00	3.5	3680.0	
Reverse Arhenius coefficients:	1.97E+02	3.2	17850.0	
2067. C2H5COCH3+CH3<=>C2H5COCH2+CH4	1.62E+11	0.0	9630.0	
Reverse Arhenius coefficients:	1.27E+14	-0.7	21430.0	
2068. C2H5COCH3+CH3O<=>CH2CH2COCH3+CH3OH	2.17E+11	0.0		
Reverse Arhenius coefficients:	6460.0			
Reverse Arhenius coefficients:	4.89E+09	0.0	9007.0	
2069. C2H5COCH3+CH3O<=>CH3CHCOCH3+CH3OH	1.45E+11	0.0		
2070. C2H5COCH3+CH3O<=>C2H5COCH2+CH3OH	2.17E+11	0.0		
Reverse Arhenius coefficients:	4660.0			
Reverse Arhenius coefficients:	3.14E+12	-0.7	14250.0	
2071. C2H5COCH3+CH3O<=>CH2CH2COCH3+CH3O2H	3.01E+12	0.0		
19380.0				
Reverse Arhenius coefficients:	7.52E+12	-0.5	4329.0	
2072. C2H5COCH3+CH3O<=>CH3CHCOCH3+CH3O2H	2.00E+12	0.0		
15250.0				
Reverse Arhenius coefficients:	4.64E+14	-0.7	9612.0	
2073. C2H5COCH3+CH3O<=>C2H5COCH2+CH3O2H	3.01E+12	0.0		
17580.0				
Reverse Arhenius coefficients:	4.84E+15	-1.2	9572.0	
2074. C2H5COCH3+CH3<=>CH2CH2COCH3+C2H4	5.00E+11	0.0		
10400.0				
Reverse Arhenius coefficients:	3.44E+08	0.8	14030.0	
2075. C2H5COCH3+CH3<=>CH3CHCOCH3+C2H4	3.00E+11	0.0	3400.0	
Reverse Arhenius coefficients:	1.91E+10	0.6	16440.0	
2076. C2H5COCH3+CH3<=>C2H5COCH2+C2H4	6.15E+10	0.0	4278.0	
Reverse Arhenius coefficients:	2.72E+10	0.1	14950.0	
2077. C2H5COCH3+CH5<=>CH2CH2COCH3+C2H6	5.00E+10	0.0		
13400.0				
Reverse Arhenius coefficients:	9.55E+12	-0.6	13990.0	
2078. C2H5COCH3+CH5<=>CH3CHCOCH3+C2H6	3.00E+10	0.0	8600.0	
Reverse Arhenius coefficients:	5.32E+14	-0.8	18600.0	
2079. C2H5COCH3+CH5<=>C2H5COCH2+C2H6	5.00E+10	0.0	11600.0	
Reverse Arhenius coefficients:	6.14E+15	-1.3	19230.0	
2080. CH3CHOCOCH3<=>CH3CHCOCH3+O2	1.37E+17	-1.7	28460.0	
Reverse Arhenius coefficients:	1.00E+11	0.0	0.0	
2081. CH3CHOCOCH3<=>CH2CHOOHCOC3	8.90E+12	0.0	29700.0	
Reverse Arhenius coefficients:	4.70E+13	-0.5	16960.0	
2082. CH2CHOOHCOC3<=>C2H3COCH3+H2O2	2.03E+19	-2.4	14130.0	
Reverse Arhenius coefficients:	7.00E+10	0.0	7800.0	
2083. CH2CH2CHO<=>C2H4+HCO	3.13E+13	-0.5	24590.0	
Reverse Arhenius coefficients:	1.50E+11	0.0	8300.0	
2084. CH2CH2COCH3<=>C2H4+CH3CO	1.00E+14	0.0	18000.0	
Reverse Arhenius coefficients:	1.00E+11	0.0	0.0	
2085. C2H5COCH2<=>C2H2CO+C2H5	1.00E+14	0.0	35000.0	
Reverse Arhenius coefficients:	1.00E+11	0.0	0.0	
2086. CH3CHCOCH3<=>C2H3COCH3+H	3.42E+16	-0.8	41770.0	
Reverse Arhenius coefficients:	5.00E+12	0.0	1200.0	
2087. CH3CHCOCH3<=>CH3CHCO+CH3	1.41E+15	-0.4	38340.0	
Reverse Arhenius coefficients:	1.23E+11	0.0	7800.0	
2088. NC3H7CHO+O2<=>NC3H7CO+H2O	1.20E+05	2.5	37560.0	
Reverse Arhenius coefficients:	1.00E+07	0.5	4000.0	
2089. NC3H7CHO+OH<=>NC3H7CO+H2O	2.00E+06	1.8	-13000.0	
Reverse Arhenius coefficients:	1.55E+04	2.3	28050.0	
2090. NC3H7CHO+H<=>NC3H7CO+H2	4.14E+09	1.1	2320.0	
Reverse Arhenius coefficients:	3.03E+06	1.7	16780.0	
2091. NC3H7CHO+O<=>NC3H7CO+OH	5.94E+12	0.0	1868.0	
Reverse Arhenius coefficients:	2.26E+09	0.6	14920.0	
2092. NC3H7CHO+H2O<=>NC3H7CO+H2O2	4.09E+04	2.5	10200.0	
Reverse Arhenius coefficients:	1.73E+04	2.4	8662.0	
2093. NC3H7CHO+CH3<=>NC3H7CO+H4	2.89E-03	4.6	3210.0	
Reverse Arhenius coefficients:	1.93E-03	4.8	19210.0	
2094. NC3H7CHO+CH3O<=>NC3H7CO+CH3OH	1.00E+12	0.0	3300.0	
Reverse Arhenius coefficients:	1.57E+10	0.4	17990.0	
2095. NC3H7CHO+CH3O2<=>NC3H7CO+CH3O2H	4.09E+04	2.5	10200.0	
Reverse Arhenius coefficients:	3.37E+05	2.0</		

Reverse Arrhenius coefficients:	1.07E+13	-0.3	17890.0		Reverse Arrhenius coefficients:	2.00E+10	0.0	15000.0	
2117. SC3HSCHO+CH3<=>S-C3H5CO+CH4	3.98E+12	0.0	8700.0		2172. TC4H9O2+C3H6<=>TC4H9O2H+C3H5-A	3.24E+11	0.0	14900.0	
Reverse Arrhenius coefficients:	4.31E+13	0.0	31460.0		Reverse Arrhenius coefficients:	2.00E+10	0.0	15000.0	
2118. SC3HSCHO+O<=>S-C3H5CO+OH	7.18E+12	0.0	1389.0		2173. IC4H9O2+I-C4H8<=>IC4H9O2H+I-C4H7	1.40E+12	0.0	14900.0	
Reverse Arrhenius coefficients:	1.31E+12	0.0	21570.0		Reverse Arrhenius coefficients:	3.16E+11	0.0	13000.0	
2119. SC3HSCHO+O2<=>S-C3H5CO+HO2	4.00E+13	0.0	37600.0		2174. TC4H9O2+I-C4H8<=>TC4H9O2H+I-C4H7	1.40E+12	0.0	14900.0	
Reverse Arrhenius coefficients:	3.01E+11	0.3	23940.0		2175. PC4H9O2+I-C4H8<=>PC4H9O2H+I-C4H7	1.40E+12	0.0	14900.0	
2120. SC3HSCHO+H<=>S-C3H5CO+H2	2.60E+12	0.0	2600.0		Reverse Arrhenius coefficients:	3.16E+11	0.0	13000.0	
Reverse Arrhenius coefficients:	1.08E+12	0.0	24880.0		2176. SC4H9O2+I-C4H8<=>SC4H9O2H+I-C4H7	1.40E+12	0.0	14900.0	
2121. C2H3COCH3+OH<=>CH3CHO+CH3CO	1.00E+11	0.0	0.0		Reverse Arrhenius coefficients:	3.16E+11	0.0	13000.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		2177. IC3H7O2+I-C4H8<=>IC3H7O2H+I-C4H7	1.40E+12	0.0	14900.0	
2122. C2H3COCH3+OH<=>CH2CHO+C2H3+H2O	5.10E+11	0.0	1192.0		Reverse Arrhenius coefficients:	3.16E+11	0.0	13000.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		2178. NC3H7O2+I-C4H8<=>NC3H7O2H+I-C4H7	1.40E+12	0.0	14900.0	
2123. C2H3COCH3+HO2<=>CH2CHO+CH3CO+OH	6.03E+09	0.0	7949.0		Reverse Arrhenius coefficients:	3.16E+11	0.0	13000.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		2179. IC4H9O2+I-C4H8<=>IC4H9O2H+I-C4H7-3	1.40E+12	0.0	14900.0	
2124. C2H3COCH3+HO2<=>CH2CO+C2H3+H2O2	8.50E+12	0.0	20460.0		Reverse Arrhenius coefficients:	3.16E+11	0.0	13000.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		2180. TC4H9O2+I-C4H8<=>TC4H9O2H+C4H7-3	1.40E+12	0.0	14900.0	
2125. C2H3COCH3+CH3O2<=>CH2CHO+CH3CO+CH3O	3.97E+11	0.0	17050.0		Reverse Arrhenius coefficients:	3.16E+11	0.0	13000.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		2181. IC4H9O2+I-C4H8<=>IC4H9O2H+C4H7-3	1.40E+12	0.0	14900.0	
2126. C2H3COCH3+CH3O2<=>CH2CO+C2H3+CH3O2H	3.01E+12	0.0	17580.0		Reverse Arrhenius coefficients:	3.16E+11	0.0	13000.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		2182. TC4H9O2+I-C4H8<=>TC4H9O2H+C4H7-3	1.40E+12	0.0	14900.0	
2127. I-C4H10-(M)<=>CH3-I-C3H7(+M)	4.83E+16	0.0	79900.0		Reverse Arrhenius coefficients:	3.16E+11	0.0	13000.0	
Low pressure limit:	0.2410E+20	0.0000E+00	5.2576E+05		2183. CC4H8O+OH<=>CH2O+C3H5-A+H2O	5.00E+12	0.0	0.0	
TROE centering:	0.2500E+00	0.7500E+03	0.1000E+09	0.10000E+11	Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2128. I-C4H10+CH3O2<=>I-C4H9+CH3O2H	2.08E+00	4.0	18280.0		2184. CC4H8O+H<=>CH2O+C3H5-A+H2	3.51E+07	2.0	5000.0	
Reverse Arrhenius coefficients:	2.13E+00	3.5	3026.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2129. I-C4H10+CH2O5<=>I-C4H9+C2H5O2H	2.55E+13	0.0	20460.0		2185. CC4H8O+H<=>CH2O+C3H5-A+OH	1.12E+14	0.0	5200.0	
Reverse Arrhenius coefficients:	2.62E+13	-0.5	5208.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2130. I-C4H10+CH3C03<=>I-C4H9+CH3C03H	2.55E+13	0.0	20460.0		2186. CC4H8O+HO<=>CH2O+C3H5-A+H2O2	1.00E+13	0.0	15000.0	
Reverse Arrhenius coefficients:	2.15E+12	0.0	9570.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2131. I-C4H10+NC3H7O2<=>I-C4H9+NC3H7O2H	2.55E+13	0.0	20460.0		2187. CC4H8O+CH3O2<=>CH2O+C3H5-A+CH3O2H	1.00E+13	0.0	19000.0	
Reverse Arrhenius coefficients:	2.68E+13	-0.5	5000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2132. I-C4H10+IC3H7O2<=>I-C4H9+IC3H7O2H	2.55E+13	0.0	20460.0		2188. CC4H8O+CH3<=>CH2O+C3H5-A+CH4	2.00E+11	0.0	10000.0	
Reverse Arrhenius coefficients:	2.69E+13	-0.5	5000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2133. I-C4H10+IC4H9O2<=>I-C4H9+IC4H9O2H	2.55E+13	0.0	20460.0		2189. C2H4+TC4H9O2<=>C2H3+TC4H9O2H	7.00E+11	0.0	17110.0	
Reverse Arrhenius coefficients:	2.68E+13	-0.5	5010.0		Reverse Arrhenius coefficients:	1.00E+11	0.0	10000.0	
2134. I-C4H10+TC4H9O2<=>I-C4H9+TC4H9O2H	2.55E+13	0.0	20460.0		2190. TC4H9O2+CH4<=>TC4H9O2H+C3H3	1.13E+13	0.0	20460.0	
Reverse Arrhenius coefficients:	2.68E+13	-0.5	5010.0		Reverse Arrhenius coefficients:	7.50E+08	0.0	1280.0	
2135. I-C4H10+O2CHO<=>I-C4H9+HO2CHO	2.52E+13	0.0	20440.0		2191. H2+TC4H9O<=>H+TC4H9O2H	3.01E+13	0.0	26030.0	
Reverse Arrhenius coefficients:	1.01E+00	3.1	2375.0		Reverse Arrhenius coefficients:	4.80E+13	0.0	7950.0	
2136. I-C4H10+O2CHO<=>T-C4H9+HO2CHO	2.80E+12	0.0	16010.0		2192. TC4H9O2+C2H6<=>TC4H9O2H+C2H5	1.70E+13	0.0	20460.0	
Reverse Arrhenius coefficients:	1.89E+01	2.7	4678.0		Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0	
2137. I-C4H10+SC4H9O2<=>I-C4H9+SC4H9O2H	2.25E+13	0.0	20460.0		2193. TC4H9O2+C3H8<=>TC4H9O2H+I-C3H7	2.00E+12	0.0	17000.0	
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0		Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0	
2138. I-C4H10+SC4H9O2<=>T-C4H9+SC4H9O2H	2.80E+12	0.0	16000.0		2194. TC4H9O2+C3H8<=>TC4H9O2H+N-C3H7	1.70E+13	0.0	20460.0	
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0		Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0	
2139. I-C4H10+PC4H9O2<=>I-C4H9+PC4H9O2H	2.25E+13	0.0	20460.0		2195. TC4H9O2+CH3O<=>TC4H9O2H+CH2OH	6.30E+12	0.0	19360.0	
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0		Reverse Arrhenius coefficients:	1.00E+09	0.0	10000.0	
2140. I-C4H10+PC4H9O2<=>T-C4H9+PC4H9O2H	2.80E+12	0.0	16000.0		2196. TC4H9O2+C2H5OH<=>TC4H9O2H+PC2H4OH	6.30E+12	0.0	19360.0	
Reverse Arrhenius coefficients:	5.00E+11	0.0	6500.0		19360.0				
2141. I-C4H10+CH3O2<=>T-C4H9+CH3O2H	1.37E+02	3.1	13190.0		Reverse Arrhenius coefficients:	3.06E+12	0.0	22100.0	
Reverse Arrhenius coefficients:	2.77E+00	3.2	2228.0		2197. TC4H9O2+C2H5OH<=>TC4H9O2H+SC2H4OH	4.20E+12	0.0	15000.0	
2142. I-C4H10+C2H5O2<=>T-C4H9+C2H5O2H	2.80E+12	0.0	16000.0		Reverse Arrhenius coefficients:	2.04E+12	0.0	17740.0	
Reverse Arrhenius coefficients:	1.00E+11	0.0	10000.0		2198. IC4H9O2+CH3CHO<=>IC4H9O2H+CH3CO	2.80E+12	0.0	13600.0	
2143. I-C4H10+CH3C03<=>T-C4H9+CH3C03H	2.80E+12	0.0	16000.0		Reverse Arrhenius coefficients:	1.00E+12	0.0	10000.0	
Reverse Arrhenius coefficients:	1.00E+11	0.0	10000.0		2199. TC4H9O2+CH3CHO<=>TC4H9O2H+CH3CO	2.80E+12	0.0	13600.0	
2144. I-C4H10+NC3H7O2<=>T-C4H9+NC3H7O2H	2.80E+12	0.0	16000.0		Reverse Arrhenius coefficients:	1.00E+12	0.0	10000.0	
Reverse Arrhenius coefficients:	1.00E+11	0.0	10000.0		2200. IC4H9O2+C2H3CHO<=>IC4H9O2H+C2H3CO	2.80E+12	0.0	13600.0	
2145. I-C4H10+IC3H7O2<=>T-C4H9+IC3H7O2H	2.80E+12	0.0	16000.0		Reverse Arrhenius coefficients:	1.00E+12	0.0	10000.0	
Reverse Arrhenius coefficients:	1.00E+11	0.0	10000.0		2201. TC4H9O2+C2H3CHO<=>TC4H9O2H+C2H3CO	2.80E+12	0.0	13600.0	
2146. I-C4H10+IC4H9O2<=>T-C4H9+IC4H9O2H	2.80E+12	0.0	16000.0		Reverse Arrhenius coefficients:	1.00E+12	0.0	10000.0	
Reverse Arrhenius coefficients:	1.00E+11	0.0	10000.0		2202. IC4H9O2+C2H5CHO<=>IC4H9O2H+C2H5CO	2.80E+12	0.0	13600.0	
2147. I-C4H10+TC4H9O2<=>T-C4H9+TC4H9O2H	2.80E+12	0.0	16000.0		Reverse Arrhenius coefficients:	1.00E+12	0.0	10000.0	
Reverse Arrhenius coefficients:	1.00E+11	0.0	10000.0		2203. TC4H9O2+C2H5CHO<=>TC4H9O2H+C2H5CO	2.80E+12	0.0	13600.0	
2148. I-C4H10+I-C4H9<=>T-C4H9+I-C4H10	2.50E+10	0.0	7900.0		Reverse Arrhenius coefficients:	1.00E+12	0.0	10000.0	
Reverse Arrhenius coefficients:	2.25E+11	0.0	12300.0		2204. IC4H9O2+HO2<=>IC4H9O2H+O2	1.75E+10	-0.0	-3275.0	
2149. I-C4H9+HO2<=>IC4H9+OH	7.00E+12	0.0	-1000.0		Reverse Arrhenius coefficients:	3.84E+13	-0.8	33620.0	
Reverse Arrhenius coefficients:	3.71E+15	-0.7	26540.0		2205. TC4H9O2+HO2<=>TC4H9O2H+O2	1.75E+10	0.0	-3275.0	
2150. T-C4H9+HO2<=>TC4H9+OH	7.00E+12	0.0	-1000.0		Reverse Arrhenius coefficients:	3.85E+13	-0.8	33620.0	
Reverse Arrhenius coefficients:	4.08E+18	-1.3	28650.0		2206. IC4H9O2+H2O2<=>IC4H9O2H+HO2	2.40E+12	0.0	10000.0	
2151. CH3O2+I-C4H9<=>CH3O-I-C4H9O	7.00E+12	0.0	-1000.0		Reverse Arrhenius coefficients:	2.40E+12	0.0	10000.0	
Reverse Arrhenius coefficients:	2.32E+14	-0.4	30780.0		2207. TC4H9O2+H2O2<=>TC4H9O2H+HO2	2.40E+12	0.0	10000.0	
2152. CH3O2+T-C4H9<=>CH3O+TC4H9O	7.00E+12	0.0	-1000.0		Reverse Arrhenius coefficients:	2.40E+12	0.0	10000.0	
Reverse Arrhenius coefficients:	2.55E+17	-1.0	32890.0		2208. IC4H9O2+CH2O<=>IC4H9O2H+HCO	1.30E+11	0.0	9000.0	
2153. NC3H7O2+I-C4H9<=>NC3H7O+IC4H9O	7.00E+12	0.0	-1000.0		Reverse Arrhenius coefficients:	2.50E+10	0.0	10100.0	
Reverse Arrhenius coefficients:	4.54E+14	-0.5	29220.0		2209. TC4H9O2+CH2O<=>TC4H9O+CH3O-O2	1.30E+11	0.0	9000.0	
2154. NC3H7O2+T-C4H9<=>NC3H7O+TC4H9O	7.00E+12	0.0	-1000.0		Reverse Arrhenius coefficients:	2.50E+10	0.0	10100.0	
Reverse Arrhenius coefficients:	5.00E+17	-1.2	31330.0		2210. IC4H9O2+CH3O2<=>IC4H9O+CH3O-O2	1.40E+11	-1.6	1860.0	
2155. NC3H7O2+I-C4H7<=>NC3H7O+IC4H7O	7.00E+12	0.0	-1000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
Reverse Arrhenius coefficients:	4.18E+11	0.2	13500.0		2211. TC4H9O2+CH3O2<=>TC4H9O+CH3O+O2	1.40E+16	-1.6	1860.0	
2156. SC4H9O2+I-C4H9<=>SC4H9O+IC4H9O	7.00E+12	0.0	-1000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
Reverse Arrhenius coefficients:	1.01E+15	-0.2	28410.0		2212. IC4H9O2+CH2S<=>IC4H9O+CH2S+O2	1.40E+16	-1.6	1860.0	
2157. SC4H9O2+T-C4H9<=>SC4H9O+TC4H9O	7.00E+12	0.0	-1000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
Reverse Arrhenius coefficients:	1.11E+18	-1.1	30520.0		2213. TC4H9O2+C2H5O2<=>TC4H9O+C2H5O+O2	1.40E+16	-1.6	1860.0	
2158. PC4H9O2+I-C4H9<=>PC4H9O+IC4H9O	7.00E+12	0.0	-1000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
Reverse Arrhenius coefficients:	5.31E+14	-0.6	28930.0		2214. IC4H9O2+CH3CO3<=>IC4H9O+CH3CO2+O2	1.40E+16	-1.6	1860.0	
2159. PC4H9O2+T-C4H9<=>PC4H9O+TC4H9O	7.00E+12	0.0	-1000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
Reverse Arrhenius coefficients:	5.84E+17	-1.2	31040.0		2215. TC4H9O2+CH3CO3<=>TC4H9O+CH3CO2+O2	1.40			

2224. TC4H9O2+NC3H7O2=>TC4H9O+NC3H7O+O2	1.40E+16	-1.6
1860.0 Reverse Arrhenius coefficients:	0.00E+00	0.0
2225. IC4H9O2+IC3H7O2=>IC4H9O+IC3H7O+O2	1.40E+16	-1.6
1860.0 Reverse Arrhenius coefficients:	0.00E+00	0.0
2226. TC4H9O2+IC3H7O2=>TC4H9O+IC3H7O+O2	1.40E+16	-1.6
1860.0 Reverse Arrhenius coefficients:	0.00E+00	0.0
2227. IC4H9O2+HO2=>IC4H9O+OH+O2	1.40E+16	-1.6
1860.0 Reverse Arrhenius coefficients:	0.00E+00	0.0
2228. TC4H9O2+HO2=>TC4H9O+OH+O2	1.40E+16	-1.6
1860.0 Reverse Arrhenius coefficients:	0.00E+00	0.0
2229. IC4H9O2+CH3=>IC4H9O+CH3O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	5.72E+12	0.0
2230. IC4H9O2+C2H5=>IC4H9O+C2H5O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	8.13E+14	-0.6
30430.0 2231. IC4H9O2+I-C3H7=>IC4H9O+IC3H7O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	1.39E+15	-0.4
31100.0 2232. IC4H9O2+N-C3H7=>IC4H9O+NC3H7O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	8.21E+14	-0.6
29100.0 2233. IC4H9O2-P-C4H9=>IC4H9O+PC4H9O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	1.14E+15	-0.6
28780.0 2234. IC4H9O2-S-C4H9=>IC4H9O+SC4H9O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	1.97E+17	-1.1
30490.0 2235. IC4H9O2+I-C4H9=>IC4H9O+IC4H9O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	4.90E+14	-0.5
30320.0 2236. IC4H9O2-T-C4H9=>IC4H9O+TC4H9O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	5.39E+17	-1.2
32430.0 2237. IC4H9O2-C3H5-A=>IC4H9O+C3H5O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	2.12E+11	0.2
15440.0 2238. IC4H9O2-C4H71-3=>IC4H9O+C4H7O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	1.10E+14	-0.7
17490.0 2239. IC4H9O2-I-C4H7=>IC4H9O+IC4H7O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	4.51E+11	0.2
14600.0 2240. TC4H9O2+CH3=>TC4H9O+CH3O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	7.82E+11	0.0
28340.0 2241. TC4H9O2+C2H5=>TC4H9O+C2H5O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	1.11E+14	-0.4
30750.0 2242. TC4H9O2-L-C3H7=>TC4H9O+IC3H7O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	1.90E+14	-0.2
31240.0 2243. TC4H9O2-N-C3H7=>TC4H9O+NC3H7O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	1.12E+14	-0.3
29420.0 2244. TC4H9O2-P-C4H9=>TC4H9O+PC4H9O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	1.56E+14	-0.4
29100.0 2245. TC4H9O2-S-C4H9=>TC4H9O+SC4H9O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	2.69E+16	-0.9
30810.0 2246. TC4H9O2-L-C4H9=>TC4H9O+IC4H9O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	6.70E+13	-0.3
30640.0 2247. TC4H9O2-T-C4H9=>TC4H9O+TC4H9O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	7.37E+16	-1.0
32750.0 2248. TC4H9O2+C3H5-A=>TC4H9O+C3H5O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	2.90E+10	0.4
15760.0 2249. TC4H9O2-C4H71-3=>TC4H9O+C4H7O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	1.50E+13	-0.5
17810.0 2250. TC4H9O2-I-C4H7=>TC4H9O+IC4H7O	7.00E+12	0.0
-1000.0 Reverse Arrhenius coefficients:	6.17E+10	0.4
14920.0 2251. IC4H9O2+C2H4=>IC4H9O2H+C2H3	2.00E+11	0.0
6000.0 Reverse Arrhenius coefficients:	2.00E+10	0.0
8000.0 2252. IC4H9O2-CH4=>IC4H9O2H-CH3	1.13E+13	0.0
20460.0 Reverse Arrhenius coefficients:	7.50E+08	0.0
1280.0 2253. H2+IC4H9O2-C-H=IC4H9O2H	3.01E+13	0.0
26030.0 Reverse Arrhenius coefficients:	4.80E+13	0.0
79500.0 2254. IC4H9O2-C2H6=>IC4H9O2H+C2H5	1.70E+13	0.0
20460.0 Reverse Arrhenius coefficients:	5.00E+11	0.0
6500.0 2255. IC4H9O2-C3H8=>IC4H9O2H+I-C3H7	2.00E+12	0.0
17000.0 Reverse Arrhenius coefficients:	5.00E+11	0.0
6500.0 2256. IC4H9O2+C3H8=>IC4H9O2H-N-C3H7	1.70E+13	0.0
20460.0 Reverse Arrhenius coefficients:	5.00E+11	0.0
6500.0 2257. IC4H9O2+CH3OH=>IC4H9O2H+CH2OH	6.30E+12	0.0
19360.0 Reverse Arrhenius coefficients:	1.00E+09	0.0
10000.0 2258. IC4H9O2+C2H5OH=>IC4H9O2H+PC2H4OH	6.30E+12	0.0
19360.0 Reverse Arrhenius coefficients:	3.06E+12	0.0
22100.0 2259. IC4H9O2+C2H5OH=>IC4H9O2H+SC2H4OH	4.20E+12	0.0
15000.0 Reverse Arrhenius coefficients:	2.04E+12	0.0
17740.0 2260. IC4H9O2H=>IC4H9O+OH	1.50E+16	0.0
42500.0 Reverse Arrhenius coefficients:	1.23E+08	1.7
29420.0 2261. TC4H9O2H=>TC4H9O+OH	5.95E+15	0.0
42540.0 Reverse Arrhenius coefficients:	6.68E+06	1.9
2582.0 2262. IC4H9O+H02=>IC3H7CHO+H02	1.00E+12	0.0
0.0 Reverse Arrhenius coefficients:	1.38E+13	-0.2
72130.0 2263. IC4H9O+OH=>IC3H7CHO+H2O	1.81E+13	0.0
0.0 Reverse Arrhenius coefficients:	4.21E+13	0.1
103600.0 2264. IC4H9O+CH3=>IC3H7CHO+CH4	2.40E+13	0.0
0.0 Reverse Arrhenius coefficients:	3.37E+14	0.1
88920.0 2265. IC4H9O+O=>IC3H7CHO+OH	6.00E+12	0.0
0.0 Reverse Arrhenius coefficients:	1.42E+12	0.1
86350.0 2266. IC4H9O+H=>IC3H7CHO+H2	1.99E+13	0.0
0.0 Reverse Arrhenius coefficients:	1.07E+13	0.1
88440.0 2267. IC4H9O+O2=>IC3H7CHO+H2O	4.00E+14	0.0
21500.0 Reverse Arrhenius coefficients:	1.14E+10	1.1
2500.0 2268. IC4H9O+<=CH2O+I-C3H7	2.00E+14	0.0
17500.0 Reverse Arrhenius coefficients:	1.88E+02	2.8
45910.0 2269. TC4H9O+<=CH3COC3H->CH3	9.56E+22	-2.5
18650.0 Reverse Arrhenius coefficients:	1.50E+11	0.0
11900.0 2270. IC4H9O+O2=>IC3H7CHO+H02	1.93E+11	0.0
1660.0 Reverse Arrhenius coefficients:	7.03E+08	0.6
33200.0 2271. TC4H9O+O2=>IC4H8O+H02	8.10E+11	0.0
4700.0 Reverse Arrhenius coefficients:	1.00E+11	0.0
32000.0 2272. IC4H8O=>IC3H7CHO	4.18E+13	0.0
52720.0 Reverse Arrhenius coefficients:	1.39E+10	0.6
72050.0 2273. IC4H8O+OH=>IC3H6CHO+H02	1.25E+12	0.0
0.0 Reverse Arrhenius coefficients:	9.61E+05	1.1
36560.0 2274. IC4H8O+H=>IC3H6CHO+H2	1.25E+12	0.0
0.0 Reverse Arrhenius coefficients:	9.06E+04	1.2
21670.0 2275. IC4H8O+H02=>IC3H6CHO+H02	2.50E+12	0.0
15000.0 Reverse Arrhenius coefficients:	1.05E+08	0.5
20660.0 2276. IC4H8O+CH3O2=>IC3H6CHO+CH3O2H	2.50E+12	0.0
19000.0 Reverse Arrhenius coefficients:	2.04E+09	0.0
23070.0 2277. IC4H8O+CH3=>IC3H6CHO+CH4	5.00E+10	0.0
10000.0 Reverse Arrhenius coefficients:	3.31E+06	0.7
33210.0 2278. IC4H8O+O=>IC3H6CHO+OH	1.25E+12	0.0
0.0 Reverse Arrhenius coefficients:	4.70E+04	1.2
20250.0 2279. IC3H7CHO=>I-C3H7+HCO	1.13E+17	0.0
79760.0 Reverse Arrhenius coefficients:	1.81E+13	0.0
0.0 2280. IC3H7CHO-CH3O2=>IC3H6CHO+CH3O2H	4.76E+04	2.5
16490.0 Reverse Arrhenius coefficients:	3.00E+10	0.0
16490.0 Reverse Arrhenius coefficients:	2.38E+05	2.0
3742.0 2281. IC3H7CO=>I-C3H7+CO	2.87E+20	-2.2
14970.0 Reverse Arrhenius coefficients:	1.50E+11	0.0
4810.0 2282. IC3H6CHO=>C3H6+HCO	1.03E+15	-0.6
23170.0 Reverse Arrhenius coefficients:	1.00E+11	0.0
7800.0 2283. IC3H6CHO=>C2H3CHO+CH3	2.42E+13	-0.3
22470.0 Reverse Arrhenius coefficients:	1.00E+11	0.0
7800.0 2284. IC4H8O=>I-C4H8+OH	1.00E+11	0.0
28050.0 Reverse Arrhenius coefficients:	9.93E+11	0.0
960.0 2285. IO2C4H8O=>IC4H8O+H02	1.92E+21	-2.3
35790.0 Reverse Arrhenius coefficients:	1.20E+11	0.0
1100.0 2286. IO2C4H8O=>C3HCOCH3+CH2O+OH	1.25E+10	0.0
18900.0 Reverse Arrhenius coefficients:	0.00E+00	0.0
0.0 2287. IC4H9O2=>IC4H8O2H-1	7.50E+10	0.0
24400.0 Reverse Arrhenius coefficients:	1.82E+11	-0.5
8946.0 2288. TC4H9O2=>TC4H8O2H-1	9.00E+11	0.0
34500.0 Reverse Arrhenius coefficients:	2.03E+09	0.1
16940.0 2289. IC4H9O2=>IC4H8O2H-T	1.00E+11	0.0
29200.0 Reverse Arrhenius coefficients:	5.08E+06	0.8
15880.0 2290. IC4H9O2=>I-C4H8+HO2	2.27E+35	-7.2
39490.0 Reverse Arrhenius coefficients:	3.00E+26	-5.3
21240.0 2291. TC4H9O2=>I-C4H8+H02	7.61E+42	-9.4
41490.0 Reverse Arrhenius coefficients:	6.34E+31	-7.2
17160.0 2292. IC4H8O0H=>IC4H8O2H-I-O2	1.44E+20	-1.6
35690.0 Reverse Arrhenius coefficients:	2.26E+12	0.0
0.0 2293. TC4H8O0H=>TC4H8O2H-I+O2	5.17E+22	-2.3
37800.0 Reverse Arrhenius coefficients:	2.26E+12	0.0
0.0 2294. IC4H8O0H=>TC4H8O2H-T+O2	2.27E+27	-3.2
39640.0 Reverse Arrhenius coefficients:	1.41E+13	0.0
0.0 2295. IC4H8O0H=>IC4KETIT+OH	4.00E+11	0.0
31500.0 Reverse Arrhenius coefficients:	1.91E+05	1.2
53830.0 2296. TC4H8O0H=>TC4H7Q2-I	7.50E+10	0.0
24400.0 Reverse Arrhenius coefficients:	6.36E+08	0.1
11720.0 2297. TC4H7Q2-I=>IC4H7OOH+HO2	1.94E+20	-2.2
22590.0 Reverse Arrhenius coefficients:	1.00E+11	0.0
106000.0 2298. IC4H8O0H=>IC4H7Q2-I	7.65E+19	-1.7
38310.0 Reverse Arrhenius coefficients:	8.50E+10	0.0
10600.0 2299. IIC4H7Q2-T=>IC4H7OOH+HO2	4.08E+17	-1.6
18390.0 Reverse Arrhenius coefficients:	1.00E+11	0.0
7800.0 2300. IC4H8O0H=>I-C4H8+H02	1.00E+11	0.0
1500.0 Reverse Arrhenius coefficients:	9.00E+14	0.0
1500.0 2301. IC4H7Q2-H=>IC3H5OOH+CH2O2H	8.50E+10	0.0
10600.0 Reverse Arrhenius coefficients:	4.08E+17	-1.6
18390.0 Reverse Arrhenius coefficients:	1.00E+11	0.0
7800.0 2302. IIC4H7Q2-H=>IC4H7OOH+HO2	1.44E+20	-1.6
38310.0 Reverse Arrhenius coefficients:	1.00E+11	0.0
7800.0 2303. CH2O2H=>CH2O+OH	1.00E+11	0.0
1500.0 Reverse Arrhenius coefficients:	9.00E+14	0.0
1500.0 2304. IC4KETIT=>CH2O+CH2C5O+OH	1.50E+16	0.0
42000.0 Reverse Arrhenius coefficients:	0.00E+00	0.0
0.0 2305. IC4KETIT=>C3HCOCH3+HCO+OH	9.50E+15	0.0
42540.0 Reverse Arrhenius coefficients:	0.00E+00	0.0
0.0 2306. TC4H8O2H-L=>I-C4H8+H02	1.07E+20	-2.1
19390.0 Reverse Arrhenius coefficients:	3.97E+11	0.0
12620.0 2307. IC4H8O2H-T=>I-C4H8+H02	1.53E+16	-1.1
17560.0 Reverse Arrhenius coefficients:	3.97E+11	0.0
12620.0 2308. IC4H8O2H-I=>IC4H8+OH+OH	2.00E+11	0.0
19500.0 Reverse Arrhenius coefficients:	0.00E+00	0.0
0.0 2309. IC4H8O2H-T=>IC4H8+OH+OH	1.38E+12	0.0
14800.0 Reverse Arrhenius coefficients:	0.00E+00	0.0
0.0 2310. TC4H8O2H-I=>IC4H8+OH+OH	4.00E+12	0.0
17000.0 Reverse Arrhenius coefficients:	0.00E+00	0.0
0.0 2311. IC4H8O2H-I=>O+CH2+C3H6	8.45E+15	-0.7
29170.0 Reverse Arrhenius coefficients:	0.00E+00	0.0
0.0 2312. I-C4H8=>C3H5-T+CH3	1.92E+66	-14.2
128100.0 Reverse Arrhenius coefficients:	1.56E+56	-12.3
26100.0 2313. I-C4H8+O=>IC3H6CO+H+H	1.66E+07	1.8
76.0 Reverse Arrhenius coefficients:	0.00E+00	0.0
0.0 2314. I-C4H8+O2CHO=>IC4H7+HO2CHO	1.93E+04	2.6
13910.0 Reverse Arrhenius coefficients:	6.51E-07	4.9
3468.0 2315. I-C4H8+O2CHO=>I-C4H7+H02	5.85E+12	0.3
383.0 Reverse Arrhenius coefficients:	7.94E+11	0.0
20500.0 2316. I-C4H8+CH3S=>I-C4H7+C3H6	4.40E+20	-1.3
60610.0 Reverse Arrhenius coefficients:	3.37E+13	-0.6
73010.0 2317. I-C4H8+C3H5-S=>I-C4H7+C3H6	7.94E+11	0.0
20500.0 Reverse Arrhenius coefficients:	5.59E+20	-1.3
82170.0 2318. I-C4H8+C3H5-S=>I-C4H7+C3H6	7.94E+11	0.0
20500.0 Reverse Arrhenius coefficients:	5.59E+20	-1.3
80170.0 2319. I-C4H8+H02=>IC4H8+OH+OH	1.29E+12	0.0
13340.0 Reverse Arrhenius coefficients:	1.00E+12	0.0
7500.0 2320. I-C4H7+O2=>C3H5+CH3+OH	2.84E+16	-0.5
66730.0 Reverse Arrhenius coefficients:	2.47E+13	-0.5
23020.0 2321. I-C4H7+O2=>C3H5COCH2+CH2O	3.37E+13	-0.6
73010.0 Reverse Arrhenius coefficients:	7.00E+12	0.0
10000.0 2322. I-C4H7+O2=>C3H4+A+CH2O+OH	1.70E+12	-0.4
88250.0 Reverse Arrhenius coefficients:	5.10E+12	0.0
21450.0 2323. I-C4H7+O2=>C3H4+A+CH2O+OH	2.14E+11	0.3
15060.0 Reverse Arrhenius coefficients:	3.42E+12	0.1
10820.0 2324. I-C4H7+H02=>C3H4+T+CH2O	7.00E+12	-0.0
100		

Reverse Arrhenius coefficients:	6.31E+10	-0.1	38980.0		Reverse Arrhenius coefficients:	1.61E+40	-8.6	20330.0	
2338. IC4H7O+H02<=>IC3H5CHO+H2O2	3.00E+11	0.0	0.0		2395. CH2CCH2OH<=>C3H4-A+OH	6.70E+16	-1.1	42580.0	
Reverse Arrhenius coefficients:	8.93E+14	-0.8	78500.0		Reverse Arrhenius coefficients:	8.50E+12	0.0	2000.0	
2339. IC4H7O+CH3<=>IC3H5CHO+CH4	2.40E+13	0.0	0.0		2396. NC5H12<=>C5H11-1+H	1.38E+17	-0.4	101200.0	
Reverse Arrhenius coefficients:	7.26E+16	-0.5	95290.0		Reverse Arrhenius coefficients:	3.61E+13	0.0	0.0	
2340. IC4H7O+O<=>IC3H5CHO+OH	6.00E+12	0.0	0.0		2397. NC5H12<=>C5H11-2+H	3.32E+18	-0.8	98800.0	
Reverse Arrhenius coefficients:	3.05E+14	-0.5	92720.0		Reverse Arrhenius coefficients:	3.61E+13	0.0	0.0	
2341. IC4H7O+OH<=>IC3H5CHO+H2O	1.81E+13	0.0	0.0		2398. NC5H12<=>C5H11-3+H	1.60E+18	-0.8	98790.0	
Reverse Arrhenius coefficients:	9.08E+15	-0.5	110000.0		Reverse Arrhenius coefficients:	3.61E+13	0.0	0.0	
2342. IC4H7O+H<=>IC3H5CHO+H2	1.99E+13	0.0	0.0		2399. NC5H12<=>CH3-P+C4H9	6.10E+22	-1.9	89430.0	
Reverse Arrhenius coefficients:	2.30E+15	-0.5	94810.0		Reverse Arrhenius coefficients:	4.00E+12	0.0	-596.0	
2343. IC3H5CHO+OH<=>IC3H5CO+H2O	2.69E+10	0.8	-340.0		2400. NC5H12<=>N-C3H7+C2H5	3.08E+24	-2.3	88440.0	
Reverse Arrhenius coefficients:	4.40E+10	0.8	36080.0		Reverse Arrhenius coefficients:	4.00E+12	0.0	-596.0	
2344. IC3H5CHO+HO2<=>IC3H5CO+H2O	1.00E+12	0.0	11920.0		2401. NC5H12-H<=>C5H11-1+H2	1.88E+05	2.8	6280.0	
Reverse Arrhenius coefficients:	9.71E+12	-0.3	16880.0		Reverse Arrhenius coefficients:	1.97E+01	3.4	8610.0	
2345. IC3H5CO+CH3<=>IC3H5CO+CH4	3.98E+12	0.0	8700.0		2402. NC5H12-H<=>C5H11-2+H2	2.60E+06	2.4	4471.0	
Reverse Arrhenius coefficients:	3.93E+13	0.0	30450.0		Reverse Arrhenius coefficients:	1.13E+01	3.4	9236.0	
2346. IC3H5CO-O<=>IC3H5CO+OH	7.18E+12	0.0	1389.0		2403. NC5H12-H<=>C5H11-3+H2	1.30E+06	2.4	4471.0	
Reverse Arrhenius coefficients:	1.19E+12	0.0	20560.0		Reverse Arrhenius coefficients:	1.17E+01	3.4	9244.0	
2347. IC3H5CO-O2<=>IC3H5CO+H2O	2.00E-13	0.0	40700.0		2404. NC5H12-OH<=>C5H11-1+H2O	1.05E+10	1.0	1590.0	
Reverse Arrhenius coefficients:	1.82E+11	0.3	5337.0		Reverse Arrhenius coefficients:	1.17E+07	1.5	18810.0	
2348. IC3H5CO+H<=>IC3H5CO+H2	2.60E+12	0.0	2600.0		2405. NC5H12-OH<=>C5H11-2+H2O	9.34E+07	1.6	-35.0	
Reverse Arrhenius coefficients:	9.82E+11	0.0	23870.0		Reverse Arrhenius coefficients:	4.30E+03	2.5	19620.0	
2349. IC3H5CO<=>C3H5-T+CO	1.28E+20	-1.9	34460.0		2406. NC5H12-OH<=>C5H11-3+H2O	4.67E+07	1.6	-35.0	
Reverse Arrhenius coefficients:	1.51E+11	0.0	4809.0		Reverse Arrhenius coefficients:	4.46E+03	2.5	19630.0	
2350. TC3H6CHO+H02<=>TC3H6OCHO+OH	9.64E+12	0.0	0.0		Reverse Arrhenius coefficients:	2.09E+06	2.4	4766.0	
Reverse Arrhenius coefficients:	2.02E+17	-1.2	21010.0		2408. NC5H12-O<=>C5H11-2+OH	1.14E+02	3.0	5684.0	
2351. TC3H6OCHO<=>C3HCOCH3+HCO	3.98E+13	0.0	9700.0		Reverse Arrhenius coefficients:	1.19E+06	2.4	2846.0	
Reverse Arrhenius coefficients:	2.17E+08	0.8	14240.0		2409. NC5H12+Q<=>C5H11-3+OH	2.68E+00	3.5	6199.0	
2352. TC3H6CHO<=>IC3H5CHO+H	1.32E+14	0.0	39340.0		Reverse Arrhenius coefficients:	5.95E+05	2.4	2846.0	
Reverse Arrhenius coefficients:	1.30E+13	0.0	1200.0		2410. NC5H12+CH3<=>C5H11-1+CH4	2.78E+00	3.5	6207.0	
2353. TC3H6CHO<=>IC3H6CO+H	4.09E+14	-0.1	42410.0		Reverse Arrhenius coefficients:	8.65E-02	3.8	11020.0	
Reverse Arrhenius coefficients:	1.30E+13	0.0	4800.0		2411. NC5H12+CH3<=>C5H11-2+CH4	1.68E+05	2.1	7574.0	
2354. IC4H7OOH<=>IC4H7-OH	6.40E+15	0.0	45550.0		Reverse Arrhenius coefficients:	6.65E+02	2.7	13880.0	
Reverse Arrhenius coefficients:	1.00E+11	0.0	0.0		2412. NC5H12+CH3<=>C5H11-3+CH4	8.40E+04	2.1	7574.0	
2355. IC4H7OH<=>IC4H7-OH	5.97E+16	-0.6	105900.0		Reverse Arrhenius coefficients:	6.90E+02	2.7	13890.0	
Reverse Arrhenius coefficients:	4.00E+13	0.0	0.0		2413. NC5H12+H02<=>C5H11-1+H2O2	4.08E+01	3.6	17160.0	
2356. IC4H8OH<=>IC4H7OH+H	1.71E+12	0.3	38850.0		Reverse Arrhenius coefficients:	2.48E+00	3.5	3490.0	
Reverse Arrhenius coefficients:	1.00E+13	0.0	1200.0		2414. NC5H12+H02<=>C5H11-2+H2O2	1.26E+02	3.4	13720.0	
2357. IC4H7OH+H2<=>IC4H7OH+H	9.05E+06	2.0	17830.0		Reverse Arrhenius coefficients:	3.17E-01	3.7	2483.0	
Reverse Arrhenius coefficients:	7.16E+05	2.4	16310.0		2415. NC5H12+H02<=>C5H11-3+H2O2	6.32E+01	3.4	13720.0	
2358. IC4H7OH<=>IC4H7-OH	7.31E+16	-0.4	79700.0		Reverse Arrhenius coefficients:	3.29E-01	3.7	2491.0	
Reverse Arrhenius coefficients:	3.00E+13	0.0	0.0		2416. NC5H12+CH3O2<=>C5H11-1+CH3O2H	4.08E+01	3.6	17160.0	
2359. IC4H7OH+H2O<=>IC4H7OH+HCO	1.15E+11	0.0	1280.0		Reverse Arrhenius coefficients:	4.82E+01	3.1	1895.0	
Reverse Arrhenius coefficients:	3.02E+11	0.0	18160.0		2417. NC5H12+CH3O2<=>C5H11-2+CH3O2H	1.26E+02	3.4	13720.0	
2360. TC3H6CHO+H2O<=>IC3H7CHO+HCO	2.52E+08	1.9	18190.0		Reverse Arrhenius coefficients:	6.17E+00	3.3	888.0	
Reverse Arrhenius coefficients:	1.23E+07	2.0	17420.0		2418. NC5H12+CH3O2<=>C5H11-3+CH3O2H	6.32E+01	3.4	13720.0	
2361. TC3H6CHO+IC4H8-O<=>IC3H7CHO+I-C4H7	4.70E+02	3.3	19840.0		Reverse Arrhenius coefficients:	6.41E+00	3.3	896.0	
Reverse Arrhenius coefficients:	6.61E+00	3.4	8672.0		2419. NC5H12+C2H5<=>C5H11-1+C2H6	1.00E+11	0.0	13400.0	
2362. IC3H6CO+OH<=>IC3H7-CO2	1.73E+12	0.0	-1010.0		Reverse Arrhenius coefficients:	3.20E+11	0.0	12300.0	
Reverse Arrhenius coefficients:	2.58E+14	-0.4	55480.0		2420. NC5H12+C2H5<=>C5H11-2+C2H6	1.00E+11	0.0	10400.0	
2363. TC3H6OCHO<=>TC3H6CO+OH	9.99E+20	-1.5	87480.0		Reverse Arrhenius coefficients:	1.00E+11	0.0	12900.0	
Reverse Arrhenius coefficients:	5.00E+13	0.0	0.0		2421. NC5H12+C2H5<=>C5H11-3+C2H6	5.00E+10	0.0	10400.0	
2364. TC3H6OHCCHO<=>TC3H6OCHO+HCO	5.16E+23	-1.9	76850.0		Reverse Arrhenius coefficients:	1.00E+11	0.0	12900.0	
Reverse Arrhenius coefficients:	1.81E+13	0.0	0.0		2422. NC5H12+C2H3<=>C5H11-1+C2H4	1.00E+12	0.0	18000.0	
2365. TC3H6OH<=>CH3COCH3+H	5.00E+13	0.0	21860.0		Reverse Arrhenius coefficients:	2.60E+12	0.0	25400.0	
Reverse Arrhenius coefficients:	1.00E+12	0.0	0.0		2423. NC5H12+C2H3<=>C5H11-2+C2H4	8.00E+11	0.0	16800.0	
2366. TC3H6OH<=>C3H5OH+H	6.20E+15	-0.7	40340.0		Reverse Arrhenius coefficients:	2.00E+12	0.0	24200.0	
Reverse Arrhenius coefficients:	1.30E+13	0.0	1560.0		2424. NC5H12+C2H3<=>C5H11-3+C2H4	4.00E+11	0.0	16800.0	
2367. I-C3H5OH<=>C3H5-T+OH	7.37E+19	-0.9	109100.0		Reverse Arrhenius coefficients:	2.00E+12	0.0	24200.0	
Reverse Arrhenius coefficients:	5.00E+13	0.0	0.0		2425. NC5H12+C5H11-1<=>C5H11-2+NC5H12	1.00E+11	0.0	10400.0	
2368. TC3H6O2CHO<=>TC3H6CHO-O2	2.46E+25	-4.1	27080.0		Reverse Arrhenius coefficients:	1.00E+11	0.0	12900.0	
Reverse Arrhenius coefficients:	1.99E+17	-2.1	0.0		2426. NC5H12+C5H11-1<=>C5H11-3+NC5H12	5.00E+10	0.0	10400.0	
2369. TC3H6O2CHO<=>IC3H5O2HCHO	6.00E+11	0.0	29880.0		Reverse Arrhenius coefficients:	1.00E+11	0.0	12900.0	
Reverse Arrhenius coefficients:	3.01E+12	-0.5	17110.0		2427. NC5H12+C5H11-1<=>C5H11-2+NC5H12	5.00E+10	0.0	12300.0	
2370. TC3H6O2CHO<=>TC3H6O2HCHO	1.00E+11	0.0	25750.0		Reverse Arrhenius coefficients:	1.00E+11	0.0	12300.0	
Reverse Arrhenius coefficients:	1.63E+12	-0.5	25100.0		2428. NC5H12+O2CHO<=>C5H11-1+H2CHO	1.68E+13	0.0	20440.0	
2371. IC3H5O2HCHO<=>IC3H5CHO+H02	8.94E+20	-2.4	15030.0		Reverse Arrhenius coefficients:	1.37E+00	3.1	2295.0	
Reverse Arrhenius coefficients:	2.23E+11	0.0	10600.0		2429. NC5H12+O2CHO<=>C5H11-2+H2CHO	1.12E+13	0.0	17690.0	
2372. TC3H6O2HCHO<=>C3HCOCH3+CO+OH	4.24E+18	-1.4	4800.0		Reverse Arrhenius coefficients:	4.31E+03	2.1	4147.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		2430. NC5H12+O2CHO<=>C5H11-3+H2CHO	5.60E-12	0.0	17690.0	
2373. TC3H6CHO+H02<=>C3HCOCH3+H2O2	2.23E+13	0.0	0.0		Reverse Arrhenius coefficients:	4.32E+03	2.1	4149.0	
Reverse Arrhenius coefficients:	6.53E+13	-1.2	25610.0		2431. NC5H12+CH3O<=>C5H11-1+CH3OH	3.00E+11	0.0	7000.0	
2374. IC3H6CO+OH<=>TC3H6OH+CO	2.00E+12	0.0	-1010.0		Reverse Arrhenius coefficients:	1.20E+10	0.0	9200.0	
Reverse Arrhenius coefficients:	1.01E+09	0.9	31540.0		2432. NC5H12+CH3O<=>C5H11-2+CH3OH	2.20E+11	0.0	5000.0	
2375. TC3H6CHO+O2<=>IC3H5CHO+H02	2.72E-19	0.0	7240.0		Reverse Arrhenius coefficients:	9.00E+09	0.0	7200.0	
Reverse Arrhenius coefficients:	1.39E+11	-0.2	17310.0		2433. NC5H12+CH3O<=>C5H11-3+CH3OH	1.10E+11	0.0	5000.0	
2376. TC3H6CHO+O2<=>C3HCOCH3+CO+OH	3.62E+20	0.0	0.0		Reverse Arrhenius coefficients:	9.00E+09	0.0	7200.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		2434. NC5H12+O2<=>C5H11-1+H2O2	4.20E+13	0.0	52800.0	
2377. TC3H6CHO+CH3<=>IC3H5CHO+CH4	3.01E+12	-0.3	-131.0		Reverse Arrhenius coefficients:	2.31E+10	0.3	446.0	
Reverse Arrhenius coefficients:	2.21E+15	-0.8	67900.0		2435. NC5H12+O2<=>C5H11-2+H2O2	2.80E+13	0.0	50160.0	
2378. TC4H8CHO<=>IC3H5CHO+CH3	1.00E+13	0.0	26290.0		Reverse Arrhenius coefficients:	6.37E+08	0.7	231.0	
Reverse Arrhenius coefficients:	2.23E+11	0.0	10600.0		2436. NC5H12+O2<=>C5H11-3+H2O2	1.40E+13	0.0	50160.0	
2379. TC4H8CHO<=>I-C4H8+HCO	8.52E+12	0.0	20900.0		Reverse Arrhenius coefficients:	6.61E+08	0.7	239.0	
Reverse Arrhenius coefficients:	1.00E+11	0.0	6000.0		2437. C5H11-1<=>C2H4-N-C3H7	3.20E+12	0.5	29430.0	
2380. O2C4H8CHO<=>TC4H8CHO+O2	1.52E+19	-1.4	34510.0		Reverse Arrhenius coefficients:	8.80E+03	2.5	6130.0	
Reverse Arrhenius coefficients:	2.00E+12	0.0	0.0		2438. C5H11-1<=>H-C5H10-1	3.35E+11	0.6	35640.0	
2381. O2C4H8CHO<=>O2C4H8CO	2.16E+11	0.0	15360.0		Reverse Arrhenius coefficients:	2.50E+11	0.5	2620.0	
Reverse Arrhenius coefficients:	1.17E+13	-0.7	14880.0		2439. C5H11-1<=>C5H11-2	3.88E+09	0.4	19760.0	
2382. O2C4H8CHO<=>IC4H8O2H-T+CO	3.30E+22	-2.7	11760.0		Reverse Arrhenius coefficients:	1.60E+08	0.8	22200.0	
Reverse Arrhenius coefficients:	1.50E+11	0.0	4809.0		2440. C5H11-2<=>C3H6+C2H5	8.80E+03	2.5	6130.0	
2383. IC4H7O+I-C4H8<=>IC4H7OH+I-C4H7	2.70E+11	0.0	4000.0		Reverse Arrhenius coefficients:	2.35E+10	1.0		

Reverse Arrhenius coefficients:	1.42E+03	2.9	6915.0	Reverse Arrhenius coefficients:	1.00E+11	0.0	15000.0
2452. CSH10-1-OH<=>CSH91-3-H2O	2.76E+04	2.6	-1919.0	2509. C5H8I-3+OH<=>C2H3CHO+C2H5	1.00E+12	0.0	0.0
Reverse Arrhenius coefficients:	1.10E+05	2.8	33350.0	2510. C5H8I-3+OH<=>CH3CHO+C3H5-S	1.00E+12	0.0	0.0
2453. CSH10-1-OH<=>CSH91-4+H2O	4.67E+07	1.6	-35.0	Reverse Arrhenius coefficients:	1.00E+11	0.0	15000.0
Reverse Arrhenius coefficients:	4.32E+04	2.4	21890.0	2511. C5H9O2-4=<>SC3H5CHO+CH3	5.98E+15	-1.1	9941.0
2454. CSH10-1-OH<=>CSH91-5+H2O	5.27E+09	1.0	1586.0	Reverse Arrhenius coefficients:	1.00E+11	0.0	9600.0
Reverse Arrhenius coefficients:	7.52E+07	1.4	21000.0	2512. C5H9O2-4=<>CH3CHO+C3H5-S	1.07E+22	-2.7	29650.0
2455. CSH10-1-CH3<=>CSH91-3+CH4	3.69E+00	3.3	4002.0	Reverse Arrhenius coefficients:	1.00E+11	0.0	9600.0
2456. CSH10-1-CH3<=>CSH91-4+CH4	1.51E+00	3.5	5481.0	2513. C5H10-2<=>CH3+C4H7I-3	6.49E+19	-1.4	76320.0
Reverse Arrhenius coefficients:	8.43E-03	4.2	12730.0	Reverse Arrhenius coefficients:	8.00E+12	0.0	-596.0
2457. CSH10-1-CH3<=>CSH91-5+CH4	4.52E-01	3.6	7154.0	2514. C5H11-1+O2=<>C5H11-1+HO2	8.37E-01	3.6	11960.0
Reverse Arrhenius coefficients:	3.89E-02	4.1	11890.0	Reverse Arrhenius coefficients:	1.31E+00	3.4	27810.0
2458. CSH10-1-O2<=>CSH91-3+HO2	2.20E+12	0.0	37220.0	2515. C5H11-2+O2=<>C5H11-1+HO2	5.35E-01	3.7	9322.0
Reverse Arrhenius coefficients:	3.66E+10	0.5	-152.0	2516. C5H11-2+O2=<>C5H11-2+HO2	2.02E+01	3.1	22740.0
2459. CSH10-1-O2<=>CSH91-4+HO2	2.00E+13	0.0	49640.0	Reverse Arrhenius coefficients:	1.07E+00	3.7	9322.0
Reverse Arrhenius coefficients:	7.76E+07	1.1	-1072.0	2517. C5H11-3+O2=<>C5H11-2+HO2	1.41E+00	3.7	25590.0
2460. CSH10-1-O2<=>CSH91-5+HO2	3.00E+13	0.0	52920.0	Reverse Arrhenius coefficients:	2.14E+00	3.7	9322.0
Reverse Arrhenius coefficients:	1.80E+09	0.8	-932.0	2518. C5H11-1+HO2<=>C5H11-1+OH	1.35E+00	3.7	25580.0
2461. CSH10-1-HO2<=>CSH91-3+H2O2	4.82E+03	2.5	10530.0	Reverse Arrhenius coefficients:	9.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	1.14E+05	2.4	14330.0	2519. C5H11-2+HO2<=>C5H11-2+OH	1.94E+15	-0.5	26210.0
2462. CSH10-1-HO2<=>CSH91-4+H2O2	9.64E+03	2.6	13910.0	Reverse Arrhenius coefficients:	9.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	5.29E+01	3.0	43720.0	2520. C5H11-3+HO2<=>C5H11-3+OH	3.14E+17	-1.1	28220.0
2463. CSH10-1-HO2<=>CSH91-5+H2O2	2.38E+04	2.5	16490.0	Reverse Arrhenius coefficients:	9.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	2.02E+03	2.6	44460.0	2521. C5H11-3+CH3O2<=>C5H11-1+CH3O	3.02E+17	-1.1	28210.0
2464. CSH10-1-CH3O2<=>CSH91-3+CH3O2H	4.82E-03	2.5	10530.0	Reverse Arrhenius coefficients:	9.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	2.37E+05	2.2	11310.0	2522. C5H11-3+CH3O2<=>C5H11-2+CH3O	1.22E+14	-0.2	30450.0
2465. CSH10-1-CH3O2<=>CSH91-4+CH3O2H	9.64E-03	2.6	13910.0	Reverse Arrhenius coefficients:	9.00E+12	0.0	-1000.0
Reverse Arrhenius coefficients:	1.10E+02	2.9	1352.0	2523. C5H11-3+CH3O2<=>C5H11-3+CH3O	1.97E+16	-0.8	32460.0
2466. CSH10-1-CH3O2<=>CSH91-5+CH3O2H	2.38E-04	2.5	16490.0	Reverse Arrhenius coefficients:	1.89E+16	-0.8	32450.0
Reverse Arrhenius coefficients:	4.20E+03	2.5	14260.0	2524. C5H11O2-1+NC5H12<=>C5H11O2H-1+CSH1-1	1.21E+13	0.0	20430.0
2467. CSH10-1-CH3O<=>CSH91-3+CH3OH	4.00E+01	2.9	8609.0	Reverse Arrhenius coefficients:	1.44E+10	0.0	15000.0
Reverse Arrhenius coefficients:	1.77E+01	3.1	26990.0	2525. C5H11O2-2+NC5H12<=>C5H11O2H-2+CSH1-1	1.21E+13	0.0	20430.0
2468. CSH10-1-CH3O<=>CSH91-4+CH3OH	1.45E+11	0.0	4571.0	Reverse Arrhenius coefficients:	1.44E+10	0.0	15000.0
Reverse Arrhenius coefficients:	1.49E+07	0.8	9611.0	2526. C5H11O2-3+NC5H12<=>C5H11O2H-3+CSH1-2	1.44E+10	0.0	20430.0
2469. CSH10-1-CH3O<=>CSH91-5+CH3OH	2.17E+11	0.0	6458.0	Reverse Arrhenius coefficients:	1.44E+10	0.0	15000.0
Reverse Arrhenius coefficients:	3.45E+08	0.5	8988.0	2527. C5H11O2-2+NC5H12<=>C5H11O2H-2+CSH1-2	1.44E+10	0.0	17700.0
2470. CSH10-2-H<=>CSH91-3+H2	1.73E+03	2.5	2492.0	Reverse Arrhenius coefficients:	1.44E+10	0.0	17700.0
Reverse Arrhenius coefficients:	4.56E+06	2.1	19750.0	2528. C5H11O2-2+NC5H12<=>C5H11O2H-2+CSH1-2	1.44E+10	0.0	17700.0
2471. CSH10-2-H<=>CSH92-4+H2	3.38E+05	2.4	207.0	Reverse Arrhenius coefficients:	1.44E+10	0.0	15000.0
Reverse Arrhenius coefficients:	4.36E+06	2.1	20330.0	2529. C5H11O2-3+NC5H12<=>C5H11O2H-3+CSH1-2	1.44E+10	0.0	17700.0
2472. CSH10-2-H<=>CSH92-5+H2	6.65E-05	2.5	756.0	Reverse Arrhenius coefficients:	1.44E+10	0.0	15000.0
Reverse Arrhenius coefficients:	3.08E-04	2.5	11050.0	2530. C5H11O2-1+NC5H12<=>C5H11O2H-1+CSH1-3	4.05E+12	0.0	17700.0
2473. CSH10-2-O<=>CSH91-3+OH	4.41E+05	2.4	3150.0	Reverse Arrhenius coefficients:	1.44E+10	0.0	15000.0
Reverse Arrhenius coefficients:	5.11E+06	2.0	18310.0	2531. C5H11O2-2+NC5H12<=>C5H11O2H-2+CSH1-3	4.05E+12	0.0	17700.0
2474. CSH10-2-O<=>CSH92-4+OH	9.90E-05	2.4	1210.0	Reverse Arrhenius coefficients:	1.44E+10	0.0	15000.0
Reverse Arrhenius coefficients:	5.62E+06	2.2	19240.0	2532. C5H11O2-3+NC5H12<=>C5H11O2H-3+CSH1-3	4.05E+12	0.0	17700.0
2475. CSH10-2-O<=>CSH92-5+OH	9.80E-05	2.4	4750.0	Reverse Arrhenius coefficients:	1.44E+10	0.0	15000.0
Reverse Arrhenius coefficients:	2.00E+04	2.4	6931.0	2533. C5H11-1+CSH1-1+O2<=>C5H11O-1+CSH1-1	9.00E+12	0.0	-1000.0
2476. CSH10-2-OH<=>CSH91-3+H2O	3.12E-06	2.0	-298.0	Reverse Arrhenius coefficients:	5.94E+13	-0.1	29910.0
Reverse Arrhenius coefficients:	3.56E+08	1.6	32110.0	2534. C5H11-1+CSH1-1O2-2<=>C5H11O-1+CSH1-2	9.00E+12	0.0	-1000.0
2477. CSH10-2-OH<=>CSH92-4+H2O	2.76E-04	2.6	-1919.0	Reverse Arrhenius coefficients:	5.28E+13	-0.1	29600.0
Reverse Arrhenius coefficients:	1.55E+06	2.4	33660.0	2535. C5H11-1+CSH1-1O2-3<=>C5H11O-1+CSH1-3	9.00E+12	0.0	-1000.0
2478. CSH10-2-OH<=>CSH92-5+H2O	5.27E-09	1.0	1586.0	Reverse Arrhenius coefficients:	1.05E+14	-0.1	29600.0
Reverse Arrhenius coefficients:	1.06E+09	1.0	21020.0	2536. C5H11-2+CSH1O2-1<=>C5H11O-2+CSH1O-1	9.00E+12	0.0	-1000.0
2479. CSH10-2-CH3<=>CSH91-3+CH4	2.21E-06	3.5	5675.0	Reverse Arrhenius coefficients:	9.60E-15	-0.8	31920.0
Reverse Arrhenius coefficients:	1.52E+03	3.1	23410.0	2537. C5H11-2+CSH1O2-2<=>C5H11O-2+CSH1O-2	9.00E+12	0.0	-1000.0
2480. CSH10-2-CH3<=>CSH92-4+CH4	3.69E-06	3.3	4002.0	Reverse Arrhenius coefficients:	8.54E-15	-0.8	31620.0
Reverse Arrhenius coefficients:	1.24E+03	3.0	24610.0	2538. C5H11-2+CSH1O2-3<=>C5H11O-2+CSH1O-3	9.00E+12	0.0	-1000.0
2481. CSH10-2-CH3<=>CSH92-5+CH4	4.52E-01	3.6	7154.0	Reverse Arrhenius coefficients:	1.70E+16	-0.8	31620.0
Reverse Arrhenius coefficients:	5.48E-01	3.6	11910.0	2539. C5H11-2+CSH1O2-1<=>C5H11O-3+CSH1O-1	9.00E+12	0.0	-1000.0
2482. CSH10-2-O2<=>CSH91-3+H2O2	3.30E-12	0.0	39900.0	Reverse Arrhenius coefficients:	9.22E-15	-0.8	31920.0
Reverse Arrhenius coefficients:	1.58E-12	-0.1	-326.0	2540. C5H11-3+CSH1O2-2<=>C5H11O-3+CSH1O-2	9.00E+12	0.0	-1000.0
2483. CSH10-2-O2<=>CSH92-4+H2O2	2.20E-12	0.0	37220.0	Reverse Arrhenius coefficients:	8.21E+15	-0.8	31610.0
Reverse Arrhenius coefficients:	5.16E+11	0.1	-136.0	2541. C5H11-3+CSH1O2-3<=>C5H11O-3+CSH1O-3	9.00E+12	0.0	-1000.0
2484. CSH10-2-O2<=>CSH92-5+H2O2	3.00E-13	0.0	52290.0	Reverse Arrhenius coefficients:	1.64E-16	-0.8	31610.0
Reverse Arrhenius coefficients:	2.53E+10	0.3	-916.0	2542. C5H11O2-1+CSH11O2-2<=>O2+C5H11O-1+CSH1O-2	1.40E+16	-1.6	1860.0
2485. CSH10-2-HO2<=>CSH91-3+H2O2	9.64E+03	2.6	13910.0	Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	6.53E+06	1.8	14860.0	2543. C5H11O2-1+CSH11O2-3<=>O2+C5H11O-1+CSH11O-3	1.40E+16	-1.6	1860.0
2486. CSH10-2-HO2<=>CSH92-4+H2O2	4.82E+03	2.5	10530.0	Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	1.60E+06	2.0	14350.0	2544. C5H11O2-1+CH3O2<=>O2+C5H11O-1+CH3O	1.40E+16	-1.6	1860.0
2487. CSH10-2-HO2<=>CSH92-5+H2O2	2.38E+04	2.5	16490.0	Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	2.84E+04	2.2	4462.0	2545. C5H11O2-1+CSH11O2-1<=>O2+C5H11O-1+CSH11O-1	1.40E+16	-1.6	1860.0
2488. CSH10-2-CH3O2<=>CSH91-3+CH3O2H	9.64E-03	2.6	13910.0	Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	1.36E+07	1.7	11840.0	2546. H2O2+C5H11O2-1<=>H2+C5H11O2H-1	2.40E+12	0.0	10000.0
2489. CSH10-2-CH3O2<=>CSH92-4+CH3O2H	4.82E-03	2.5	10530.0	Reverse Arrhenius coefficients:	2.40E+12	0.0	10000.0
Reverse Arrhenius coefficients:	3.33E+06	1.8	11330.0	2547. C5H11O2-1+H2O2<=>C5H11O2H-1+O2	1.75E+10	0.0	-3275.0
2490. CSH10-2-CH3O2<=>CSH92-5+CH3O2H	2.38E-04	2.5	16490.0	Reverse Arrhenius coefficients:	3.75E-13	-0.8	33620.0
Reverse Arrhenius coefficients:	5.91E+04	2.0	1442.0	2548. C5H11O2-2+CH3O2<=>O2+C5H11O-2+CH3O	1.40E+16	-1.6	1860.0
2491. CSH10-2-CH3O<=>CSH91-3-CH3OH	9.00E+01	3.0	11990.0	Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	1.44E+03	2.5	27510.0	2549. C5H11O2-3+CSH102-3<=>C5H11O-3+CSH10-3	1.40E+16	-1.6	1860.0
2492. CSH10-2-CH3O<=>CSH92-4-CH3OH	4.00E+01	2.9	8609.0	Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	2.49E+02	2.7	27010.0	2550. C5H11O2-3+CSH102-3<=>C5H11O-3+CSH10-3	1.40E+16	-1.6	1860.0
2493. CSH10-2-CH3O<=>CSH92-5+CH3OH	2.17E+11	0.0	6458.0	Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	4.85E+09	0.0	-9004.0	2551. C5H11O2-3+CSH102-3<=>O2+C5H11O-3+CSH10-3	1.40E+16	-1.6	1860.0
2494. CSH91-3-H2O2<=>CSH901-3+OH	9.64E+12	0.0	0.0	Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	6.09E+15	-1.1	15720.0	2552. C5H11O2-3+CSH102-3<=>O2+C5H11O-3+CSH10-3	1.40E+16	-1.6	1860.0
2495. CSH91-3-CH3O2<=>CSH901-3+CH3O2H	9.64E-12	0.0	0.0	Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	5.95E+17	-1.6	20480.0	2553. C5H11O2-3+CSH102-3<=>O2+C5H11O-3+CSH10-3	1.40E+16	-1.6	1860.0
2496. CSH91-3-C2H5O2<=>CSH901-3+CH25O	9.64E+12	0.0	0.0	Reverse Arrhenius coefficients:	2.40E+12	0.0	10000.0
Reverse Arrhenius coefficients:	3.89E+14	-0.7	18330.0	2554. C5H11O2-3+CSH102-3<=>O2+C5H11O-3+CSH10-3	1.40E+16	-1.6	1860.0
2497. CSH92-4-H2O2<=>CSH902-4+OH	9.64E+12	0.0	0.0	Reverse Arrhenius coefficients:	2.40E+12	0.0	10000.0
Reverse Arrhenius coefficients:	6.86E+17	-1.8	20650.0	2555. C5H11O2-3+CSH102-3<=>O2+C5H11O-3+CSH10-3	1.40E+16	-1.6	1860.0
2498. CSH92-4-C2H5O2<=>CSH902-4+CH3O	4.96E+12	0.0	0.0	Reverse Arr			

Reverse Arrhenius coefficients:	8.50E+10	0.0	11900.0		2618. C5H10OOH1-3<=>OH+CH2O+C4H8-1	8.28E+13	-0.2	30090.0
2563. CSH1 102-1<=>C5H11-1+O2	2.34E+20	-1.6	35830.0	Reverse Arrhenius coefficients:	0.00E+00	0.0		Reverse Arrhenius coefficients:
Reverse Arrhenius coefficients:	4.52E+12	0.0		2619. C5H10OOH2-4<=>OH+CH3CHO+C3H6	8.31E+17	-1.4	27170.0	
2564. CSH1 102-2<=>C5H11-2+O2	7.09E+22	-2.3	38150.0	Reverse Arrhenius coefficients:	0.00E+00	0.0		Reverse Arrhenius coefficients:
Reverse Arrhenius coefficients:	7.54E+12	0.0		2620. C5H10OOH3-1<=>OH+CH2H5CHO+C2H4	3.10E+18	-1.7	26820.0	
2565. CSH1 102-3<=>C5H11-3+O2	3.41E+22	-2.3	38150.0	Reverse Arrhenius coefficients:	0.00E+00	0.0		Reverse Arrhenius coefficients:
Reverse Arrhenius coefficients:	7.54E+12	0.0		2621. C5H10OOH1-202<=>C5H10OOH1-2+O2	8.04E+22	-2.3	37970.0	
2566. CSH1 102-1<=>C5H10OOH1-2	2.00E+11	0.0	26850.0	Reverse Arrhenius coefficients:	7.54E+12	0.0		Reverse Arrhenius coefficients:
Reverse Arrhenius coefficients:	2.08E+10	-0.1	13850.0	2622. C5H10OOH1-302<=>C5H10OOH1-3+O2	8.04E+22	-2.3	37970.0	
2567. CSH1 102-1<=>C5H10OOH1-3	2.50E+10	0.0	20850.0	Reverse Arrhenius coefficients:	7.54E+12	0.0		Reverse Arrhenius coefficients:
Reverse Arrhenius coefficients:	2.60E+09	-0.1	7850.0	2623. C5H10OOH1-402<=>C5H10OOH1-4+O2	8.04E+22	-2.3	37970.0	
2568. CSH1 102-1<=>C5H10OOH1-4	3.12E+09	0.0	19050.0	Reverse Arrhenius coefficients:	7.54E+12	0.0		Reverse Arrhenius coefficients:
Reverse Arrhenius coefficients:	3.26E+08	-0.1	6050.0	2624. C5H10OOH1-502<=>C5H10OOH1-5+O2	2.78E+20	-1.6	35690.0	
2569. CSH1 102-1<=>C5H10OOH1-5	5.86E-08	0.0	25550.0	Reverse Arrhenius coefficients:	4.52E+12	0.0		Reverse Arrhenius coefficients:
Reverse Arrhenius coefficients:	1.38E-09	-0.5	10090.0	2625. C5H10OOH1-102<=>C5H10OOH1-1+O2	2.57E+20	-1.6	35650.0	
2570. CSH1 102-2<=>C5H10OOH2-1	3.00E+11	0.0	29400.0	Reverse Arrhenius coefficients:	4.52E+12	0.0		Reverse Arrhenius coefficients:
Reverse Arrhenius coefficients:	7.79E+11	-0.5	13960.0	2626. C5H10OOH2-302<=>C5H10OOH2-3+O2	7.25E+22	-2.3	37910.0	
2571. CSH1 102-2<=>C5H10OOH2-3	2.00E+11	0.0	26850.0	Reverse Arrhenius coefficients:	7.54E+12	0.0		Reverse Arrhenius coefficients:
Reverse Arrhenius coefficients:	2.70E+10	-0.1	13900.0	2627. C5H10OOH2-402<=>C5H10OOH2-4+O2	7.25E+22	-2.3	37910.0	
2572. CSH1 102-2<=>C5H10OOH2-4	2.50E+10	0.0	20850.0	Reverse Arrhenius coefficients:	7.54E+12	0.0		Reverse Arrhenius coefficients:
Reverse Arrhenius coefficients:	3.37E+09	-0.1	7900.0	2628. C5H10OOH2-502<=>C5H10OOH2-5+O2	2.57E+20	-1.6	35650.0	
2573. CSH1 102-2<=>C5H10OOH2-5	4.69E+09	0.0	22350.0	Reverse Arrhenius coefficients:	4.52E+12	0.0		Reverse Arrhenius coefficients:
Reverse Arrhenius coefficients:	1.22E+10	-0.5	6910.0	2629. C5H10OOH3-102<=>C5H10OOH3-1+O2	2.57E+20	-1.6	35650.0	
2574. CSH1 102-3<=>C5H10OOH3-1	7.50E+10	0.0	24400.0	Reverse Arrhenius coefficients:	4.52E+12	0.0		Reverse Arrhenius coefficients:
Reverse Arrhenius coefficients:	1.95E+11	-0.5	8960.0	2630. C5H10OOH3-202<=>C5H10OOH3-2+O2	7.25E+22	-2.3	37910.0	
2575. CSH1 102-3<=>C5H10OOH3-2	4.00E+11	0.0	26850.0	Reverse Arrhenius coefficients:	7.54E+12	0.0		Reverse Arrhenius coefficients:
Reverse Arrhenius coefficients:	2.56E+10	-0.1	13900.0	2631. C5H10OOH1-202<=>NC5KET12+OH	2.00E+11	0.0	26400.0	
2576. CSH1 102-1<=>C5H10-1+HO2	5.04E+38	-8.1	40490.0	Reverse Arrhenius coefficients:	2.78E+04	1.4	48950.0	
Reverse Arrhenius coefficients:	1.52E-31	-6.7	20510.0	2632. C5H10OOH1-302<=>NC5KET13+OH	2.50E+10	0.0	21400.0	
2577. CSH1 102-2<=>C5H10-1+HO2	5.07E-42	-9.4	41490.0	Reverse Arrhenius coefficients:	1.11E+03	1.5	44740.0	
Reverse Arrhenius coefficients:	2.04E-34	-7.7	16750.0	2633. C5H10OOH1-402<=>NC5KET14+OH	3.12E+09	0.0	19350.0	
2578. CSH1 102-2<=>C5H10-2+HO2	5.04E-38	-8.1	40490.0	Reverse Arrhenius coefficients:	1.39E+02	1.5	42690.0	
Reverse Arrhenius coefficients:	7.05E-28	-5.8	18600.0	2634. C5H10OOH1-502<=>NC5KET15+OH	3.91E+09	0.0	22550.0	
2579. CSH1 102-3<=>C5H10-2+HO2	1.01E-39	-8.1	40490.0	Reverse Arrhenius coefficients:	2.01E+01	1.5	45880.0	
Reverse Arrhenius coefficients:	1.41E-29	-5.8	18600.0	2635. C5H10OOH1-102<=>NC5KET21+OH	1.00E+11	0.0	23850.0	
2580. CSH100H1-2<=>C5H1001-2+OH	6.00E+11	0.0	22000.0	Reverse Arrhenius coefficients:	2.78E+02	1.9	50050.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2636. C5H100H1-302<=>NC5KET23+OH	1.00E+11	0.0	23850.0	
2581. CSH100H1-3<=>C5H1001-3+OH	7.50E+10	0.0	15250.0	Reverse Arrhenius coefficients:	1.35E+03	1.8	49200.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2637. C5H100H2-402<=>NC5KET24+OH	1.25E+10	0.0	17850.0	
2582. CSH100H1-4<=>C5H1001-4+OH	9.38E+09	0.0	6000.0	Reverse Arrhenius coefficients:	5.62E+01	1.9	43910.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2638. C5H100H2-502<=>NC5KET25+OH	1.56E+09	0.0	16050.0	
2583. CSH100H1-5<=>C5H1001-5+OH	1.17E+09	0.0	1800.0	Reverse Arrhenius coefficients:	9.72E+00	1.9	42120.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2639. C5H100H3-102<=>NC5KET31+OH	1.25E+10	0.0	17850.0	
2584. CSH100H2-1<=>C5H1001-2+OH	6.00E+11	0.0	22000.0	Reverse Arrhenius coefficients:	6.55E+01	1.9	44220.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2640. C5H100H3-202<=>NC5KET32+OH	1.00E+11	0.0	23850.0	
2585. CSH100H2-3<=>C5H1002-3+OH	6.00E+11	0.0	22000.0	Reverse Arrhenius coefficients:	9.88E+02	1.8	49390.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2641. NC5KET12<=>C3H7CHO-HCO+OH	1.05E+16	0.0	41600.0	
2586. CSH100H2-4<=>C5H1002-4+OH	7.50E+10	0.0	15250.0	Reverse Arrhenius coefficients:	0.00E+00	0.0		
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2642. NC5KET13<=>C2H5CHO-C2H2CHO+OH	1.05E+16	0.0	41600.0	
2587. CSH100H2-5<=>C5H1001-4+OH	9.38E+09	0.0	6000.0	Reverse Arrhenius coefficients:	0.00E+00	0.0		
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2643. NC5KET14<=>C3H3CHO-CH2CH2CHO+OH	1.05E+16	0.0	41600.0	
2588. CSH100H3-2<=>C5H1002-3+OH	6.00E+11	0.0	22000.0	Reverse Arrhenius coefficients:	0.00E+00	0.0		
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2644. NC5KET15<=>C2H2+C3H6CHO-1+OH	1.50E+16	0.0	42000.0	
2589. CSH100H3-3<=>C5H1001-3+OH	7.50E+10	0.0	15250.0	Reverse Arrhenius coefficients:	0.00E+00	0.0		
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2645. NC5KET21<=>C2H2+NC3H7CO+OH	1.50E+16	0.0	42000.0	
2590. CSH100H1-2+OH<=>C2H2CO+N-C3H7+H2O	2.50E+12	0.0	0.0	Reverse Arrhenius coefficients:	0.00E+00	0.0		
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2646. NC5KET23<=>C2H5CHO+CH3CO+OH	1.50E+16	0.0	42000.0	
2591. CSH100H1-3+OH<=>C2H4/C2H5CO-H2O	2.50E+12	0.0	0.0	Reverse Arrhenius coefficients:	0.00E+00	0.0		
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2647. NC5KET24<=>CH3CHO-CH2CH2CHO+OH	1.50E+16	0.0	42000.0	
2592. CSH100H1-4+OH<=>CH3COCH2+C2H4+H2O	2.50E+12	0.0	0.0	Reverse Arrhenius coefficients:	0.00E+00	0.0		
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2648. NC5KET25<=>CH2O+CH2CH2COCH3+OH	1.50E+16	0.0	42000.0	
2593. CSH100H1-5+OH<=>CH2CH2CHO+C2H4+H2O	2.50E+12	0.0	0.0	Reverse Arrhenius coefficients:	0.00E+00	0.0		
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2649. NC5KET31<=>C2H2+C2H5COCH2+OH	1.50E+16	0.0	42000.0	
2594. CSH100H2-3+OH<=>CH3CHO+C2H5+H2O	2.50E+12	0.0	0.0	Reverse Arrhenius coefficients:	0.00E+00	0.0		
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2650. NC5KET32<=>C3H3CHO-C2H5CO+OH	1.05E+16	0.0	41600.0	
2595. CSH100H2-4+OH<=>CH3CO+C3H6+H2O	2.50E+12	0.0	0.0	Reverse Arrhenius coefficients:	0.00E+00	0.0		
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2651. CSH100H-1<=>C5H10-1+OH	1.50E+13	0.0	25830.0	
2596. CSH100H1-2+OH<=>C2H3CHO+C2H5+H2O	2.50E+12	0.0	0.0	Reverse Arrhenius coefficients:	4.75E+12	-0.7	2820.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2652. C5H10H-2<=>C5H10-2+OH	1.50E+13	0.0	25830.0	
2597. CSH100H1-3+OH<=>C4H8-1+H2O	2.50E+12	0.0	0.0	Reverse Arrhenius coefficients:	4.75E+12	-0.7	2820.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2653. O2CSH100H-1<=>C5H10H-1+O2	1.06E+21	-1.8	37750.0	
2598. CSH100H1-4+OH<=>CH2CHO+C3H6+H2O	2.50E+12	0.0	0.0	Reverse Arrhenius coefficients:	2.00E+12	0.0		
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2654. O2CSH100H-1<=>NC3H7CHO+CH2O+OH	2.50E+10	0.0	18860.0	
2599. CSH100H1-5+OH<=>CH2O+C4H71-3+H2O	2.50E+12	0.0	0.0	Reverse Arrhenius coefficients:	0.00E+00	0.0		
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2655. O2CSH100H-2<=>C5H10H-2+O2	3.38E+21	-2.0	37870.0	
2600. CSH100H2-3+OH<=>C2H3COCH3-C3H3+H2O	2.50E+12	0.0	0.0	Reverse Arrhenius coefficients:	2.00E+12	0.0		
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2656. O2CSH100H-2<=>C2H5CHO+CH3CHO+OH	2.50E+10	0.0	18860.0	
2601. CSH100H2-4+OH<=>C3H3CHO+C3H5+S+H2O	2.50E+12	0.0	0.0	Reverse Arrhenius coefficients:	0.00E+00	0.0		
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2657. NC6H14<=>C5H11-1+CH3	1.61E+22	-1.6	89350.0	
2602. CSH100H1-2+H2O<=>CH2CO-N-C3H7+H2O2	5.00E+12	0.0	17700.0	Reverse Arrhenius coefficients:	4.00E+12	0.0	596.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2658. NC6H14<=>N-C3H7+H-C3H7+H2O	2.17E+24	-2.2	87840.0	
2603. CSH100H1-3+H2O<=>C2H4+C2H5CO+H2O2	5.00E+12	0.0	17700.0	Reverse Arrhenius coefficients:	4.00E+12	0.0	596.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2659. NC6H14<=>P-C4H9+C2H5	1.62E+24	-2.2	88580.0	
2604. CSH100H1-4+H2O2<=>CH3COCH2+C2H4+H2O2	5.00E+12	0.0	17700.0	Reverse Arrhenius coefficients:	4.00E+12	0.0	596.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2660. NC6H14<=>C6H13-1+H	1.36E+17	-0.4	101200.0	
2605. CSH100H1-5+H2O2<=>CH2CH2CHO+C2H4+H2O2	5.00E+12	0.0	17700.0	Reverse Arrhenius coefficients:	3.61E+13	0.0		
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2661. NC6H14<=>C6H13-2+H	3.61E+13	0.0		
2606. CSH100H2-3+OH<=>C2H3CHO+C2H5+H2O2	5.00E+12	0.0	17700.0	Reverse Arrhenius coefficients:	2.09E+18	-0.7	98710.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2662. NC6H14-3+H<=>C6H13-3+H2	3.61E+13	0.0		
2607. CSH100H2-4+OH<=>C3H3CHO+C2H4+H2O2	5.00E+12	0.0	17700.0	Reverse Arrhenius coefficients:	1.88E+05	2.8	6280.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2663. NC6H14-3+H<=>C6H13-1+H2	2.00E+01	3.4	8615.0	
2608. CSH100H2-5+OH<=>C2H3CHO+C2H4+H2O2	5.00E+12	0.0	17700.0	Reverse Arrhenius coefficients:	2.60E+06	2.4	4471.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2664. NC6H14-3+H<=>C6H13-2+H2	1.79E+01	3.4	9318.0	
2609. CSH100H1-3+H2O2<=>C4H8-1+H2O2	5.00E+12	0.0	17700.0	Reverse Arrhenius coefficients:	2.60E+06	2.4	4471.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2665. NC6H14-3+H<=>C6H13-3+H2	1.79E+01	3.4	9318.0	
2610. CSH100H1-4+H2O2<=>C2H2CHO+C3H6+H2O2	5.00E+12	0.0	17700.0	Reverse Arrhenius coefficients:	2.09E-06	2.4	4766.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2666. NC6H14-3+H<=>C6H13-2+H	1.17E-02	3.0	5689.0	
2611. CSH100H1-5+H2O2<=>C2H2O+C4H71-3+H2O2	5.00E+12	0.0	17700.0	Reverse Arrhenius coefficients:	1.19E-06	2.4	2846.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2667. NC6H14-3+H<=>C6H13-2+OH	4.31E+00	3.4	6281.0	
2612. CSH1002-3+H2O2<=>C2H3COCH3+C3H3+H2O2	5.00E+12	0.0	17700.0	Reverse Arrhenius coefficients:	1.19E-06	2.4	2846.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2668. NC6H14-3+H<=>C6H13-3+OH	4.31E+00	3.4	6281.0	
2613. CSH1002-4+H2O2<=>C3H3CHO+C3H5-S+H2O2	5.00E+12	0.0	17700.0	Reverse Arrhenius coefficients:	2.57E+07	1.8	954.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	2669. NC6H14-3+H<=>C6H13-2+H2O	2.91E+04	2.3	18180.0	
2614. CSH100H1-2<=>C5H10-1+HO2	3.45E+17	-1.6	17980.0	Reverse Arrhenius coefficients:	4.90E+06	2.0	-596.0	
Reverse Arrhenius coefficients:	1.00E+11	0.0	11000.0	2670. NC6H14-3+H<=>C6H13-2+H2O	3.60E+02	2.9	19140.0	
2615. CSH100H2-1<=>C5H10-1+HO2	6.46E+19	-2.2	21050.0	Reverse Arrhenius coefficients:	4.90E+06	2.0	-596.0	
Reverse Arrhenius coefficients:	1.00E+11	0.0	11750.0	2671. NC6H14-3+H<=>C6H13-3+H2O	3.60E+02	2.9		

2791. C6H12-3+CH3<=>C6H112-4+CH4	7.38E+00	3.3	4002.0
Reverse Arhenius coefficients:	9.18E+02	3.1	24690.0
2792. C6H12-3+HO2<=>C6H113-1+H2O2	4.76E+04	2.5	16490.0
Reverse Arhenius coefficients:	2.83E+04	2.2	4456.0
2793. C6H12-3+HO2<=>C6H112-4+H2O2	9.64E+03	2.5	10530.0
Reverse Arhenius coefficients:	1.18E+06	2.0	14430.0
2794. C6H12-3+CH3O2<=>C6H113-1+CH3O2H	4.76E+04	2.5	16490.0
Reverse Arhenius coefficients:	5.90E+04	2.0	1436.0
2795. C6H12-3+CH3O2<=>C6H112-4+CH3O2H	9.64E+03	2.5	10530.0
Reverse Arhenius coefficients:	2.46E+06	1.9	11410.0
2796. C6H12-3+CH3O2<=>C6H113-1+CH3OH	4.34E+11	0.0	6458.0
Reverse Arhenius coefficients:	4.84E+09	0.0	8998.0
2797. C6H12-3+CH3O2<=>C6H112-4+CH3OH	8.00E-01	2.9	8609.0
Reverse Arhenius coefficients:	1.84E+02	2.7	27090.0
2798. C6H111-3+HO2<=>C6H1101-3+OH	9.64E-12	0.0	0.0
Reverse Arhenius coefficients:	1.07E+16	-1.1	15800.0
2799. C6H111-3+CH3O2<=>C6H1101-3+CH3O	9.64E+12	0.0	0.0
Reverse Arhenius coefficients:	1.04E+18	-1.7	20570.0
2800. C6H111-3+CH5O2<=>C6H101-3+C2H5O	9.64E+12	0.0	0.0
Reverse Arhenius coefficients:	6.84E+14	-0.8	18410.0
2801. C6H111-<=>C6H111-3	1.11E-12	0.0	31700.0
Reverse Arhenius coefficients:	3.08E+14	-0.2	47550.0
2802. C6H112-4+HO2<=>C6H1102-4+OH	9.64E-12	0.0	0.0
Reverse Arhenius coefficients:	9.70E+15	-1.1	15790.0
2803. C6H112-4+CH3O2<=>C6H1102-4+CH3O	9.64E+12	0.0	0.0
Reverse Arhenius coefficients:	9.48E+17	-1.7	20560.0
2804. C6H112-4+CH2H5O2<=>C6H102-4+C2H5O	9.64E+12	0.0	0.0
Reverse Arhenius coefficients:	6.20E+14	-0.8	18400.0
2805. C6H1101-3<=>C2H3CHO+N-C3H7	1.43E-20	-2.0	11230.0
Reverse Arhenius coefficients:	1.00E+11	0.0	9600.0
2806. C6H1101-3<=>NC3H7CHO+C2H3	2.40E+18	-1.6	23410.0
Reverse Arhenius coefficients:	1.00E+11	0.0	9600.0
2807. C6H1102-4<=>SC3HSCHO+C2H5	5.45E+19	-1.9	10760.0
Reverse Arhenius coefficients:	1.00E+11	0.0	9600.0
2808. C6H1102-4<=>C2H5CHO+C3H5-S	2.35E-22	-2.6	29310.0
Reverse Arhenius coefficients:	1.00E+11	0.0	9600.0
2809. C6H1302-1<=>C6H13-1+O2	5.15E-20	-1.7	35790.0
Reverse Arhenius coefficients:	4.52E+12	0.0	0.0
2810. C6H1302-2<=>C6H13-2+O2	2.18E-23	-2.3	38040.0
Reverse Arhenius coefficients:	7.54E+12	0.0	0.0
2811. C6H1302-3<=>C6H13-3+O2	2.18E-23	-2.3	38040.0
Reverse Arhenius coefficients:	7.54E+12	0.0	0.0
2812. C6H13-1-C6H1302-1<=>C6H130-1+C6H130-1	7.00E+12	0.0	-1000.0
Reverse Arhenius coefficients:	9.78E+13	-0.2	29840.0
2813. C6H13-1-C6H1302-2<=>C6H130-1+C6H130-2	7.00E+12	0.0	-1000.0
Reverse Arhenius coefficients:	3.63E+13	-0.2	29500.0
2814. C6H13-1-C6H1302-3<=>C6H130-1+C6H130-3	7.00E+12	0.0	-1000.0
Reverse Arhenius coefficients:	3.63E+13	-0.2	29500.0
2815. C6H13-2-C6H1302-1<=>C6H130-2+C6H130-1	7.00E+12	0.0	-1000.0
Reverse Arhenius coefficients:	9.20E+15	-0.8	31760.0
2816. C6H13-2-C6H1302-2<=>C6H130-2+C6H130-2	7.00E+12	0.0	-1000.0
Reverse Arhenius coefficients:	3.41E+15	-0.8	31420.0
2817. C6H13-2-C6H1302-3<=>C6H130-2+C6H130-3	7.00E+12	0.0	-1000.0
Reverse Arhenius coefficients:	3.41E+15	-0.8	31420.0
2818. C6H13-3-C6H1302-1<=>C6H130-3+C6H130-1	7.00E+12	0.0	-1000.0
Reverse Arhenius coefficients:	9.20E+15	-0.8	31760.0
2819. C6H13-3-C6H1302-2<=>C6H130-3+C6H130-2	7.00E+12	0.0	-1000.0
Reverse Arhenius coefficients:	3.41E+15	-0.8	31420.0
2820. C6H13-3-C6H1302-3<=>C6H130-3+C6H130-3	7.00E+12	0.0	-1000.0
Reverse Arhenius coefficients:	3.41E+15	-0.8	31420.0
2821. C6H1302-1<=>C6H12-1+HO2	5.04E+38	-8.1	40490.0
Reverse Arhenius coefficients:	9.64E+29	-6.2	20470.0
2822. C6H1302-2<=>C6H12-1+HO2	5.07E+42	-9.4	41490.0
Reverse Arhenius coefficients:	5.89E+32	-7.2	16700.0
2823. C6H1302-2<=>C6H12-2+HO2	5.04E+38	-8.1	40490.0
Reverse Arhenius coefficients:	2.88E+28	-5.8	18570.0
2824. C6H1302-3<=>C6H12-3+HO2	1.01E+39	-8.1	40490.0
Reverse Arhenius coefficients:	1.57E+29	-5.8	18480.0
2825. C6H1302-1<=>C6H1200H1-2	2.00E+11	0.0	26850.0
Reverse Arhenius coefficients:	2.40E+10	-0.1	13860.0
2826. C6H1302-1<=>C6H1200H1-3	2.50E+10	0.0	20850.0
Reverse Arhenius coefficients:	3.00E+09	-0.1	7860.0
2827. C6H1302-1<=>C6H1200H1-4	3.12E+09	0.0	19050.0
Reverse Arhenius coefficients:	3.75E+08	-0.1	6060.0
2828. C6H1302-1<=>C6H1200H1-5	3.91E+08	0.0	22050.0
Reverse Arhenius coefficients:	4.69E+07	-0.1	9060.0
2829. C6H1302-2<=>C6H1200H2-1	3.00E+11	0.0	29400.0
Reverse Arhenius coefficients:	7.95E+11	-0.5	13950.0
2830. C6H1302-2<=>C6H1200H2-3	2.00E+11	0.0	26850.0
Reverse Arhenius coefficients:	2.58E+10	-0.1	13880.0
2831. C6H1302-2<=>C6H1200H2-4	2.50E+10	0.0	20850.0
Reverse Arhenius coefficients:	3.22E+09	-0.1	7880.0
2832. C6H1302-2<=>C6H1200H2-5	3.12E+09	0.0	19050.0
Reverse Arhenius coefficients:	4.03E+08	-0.1	6080.0
2833. C6H1302-2<=>C6H1200H2-6	5.86E+08	0.0	25550.0
Reverse Arhenius coefficients:	1.55E+09	-0.5	10100.0
2834. C6H1302-3<=>C6H1200H3-1	3.75E+10	0.0	24400.0
Reverse Arhenius coefficients:	9.94E+10	-0.5	8950.0
2835. C6H1302-3<=>C6H1200H3-2	2.00E+11	0.0	26850.0
Reverse Arhenius coefficients:	2.58E+10	-0.1	13880.0
2836. C6H1302-3<=>C6H1200H3-4	2.00E+11	0.0	26850.0
Reverse Arhenius coefficients:	2.58E+10	-0.1	13880.0
2837. C6H1302-3<=>C6H1200H3-5	2.50E+10	0.0	20850.0
Reverse Arhenius coefficients:	3.22E+09	-0.1	7880.0
2838. C6H1302-3<=>C6H1200H3-6	4.69E+09	0.0	22350.0
Reverse Arhenius coefficients:	1.24E+10	-0.5	6900.0
2839. C6H1302-1+HO2<=>C6H1302H-1+O2	1.75E+10	0.0	-3275.0
Reverse Arhenius coefficients:	3.54E+13	-0.8	33600.0
2840. C6H1302-2+HO2<=>C6H1302H-2+O2	1.75E+10	0.0	-3275.0
Reverse Arhenius coefficients:	4.45E+13	-0.8	33640.0
2841. C6H1302-3+HO2<=>C6H1302H-3+O2	1.75E+10	0.0	-3275.0
Reverse Arhenius coefficients:	4.45E+13	-0.8	33640.0
2842. C6H1302-1+H2O2<=>C6H1302H-1+HO2	2.40E+12	0.0	10000.0
Reverse Arhenius coefficients:	2.40E+12	0.0	10000.0
2843. C6H1302-2+H2O2<=>C6H1302H-2+HO2	2.40E+12	0.0	10000.0
Reverse Arhenius coefficients:	2.40E+12	0.0	10000.0
2844. C6H1302-3+H2O2<=>C6H1302H-3+HO2	2.40E+12	0.0	10000.0
Reverse Arhenius coefficients:	2.40E+12	0.0	10000.0
2845. C6H1302-1+CH3O2<=>C6H130-1+CH3O2	1.40E+16	-1.6	1860.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2846. C6H1302-2+CH3O2<=>C6H130-2+CH3O2	1.40E+16	-1.6	1860.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2847. C6H1302-3+CH3O2<=>C6H130-3+CH3O2	1.40E+16	-1.6	1860.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2848. C6H1302-1+C6H13O2-1<=>O2+C6H13O-1+C6H13O-1	1.40E+16	-1.6	1860.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2849. C6H1302-1+C6H13O2-2<=>O2+C6H13O-1+C6H13O-2	1.40E+16	-1.6	1860.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2850. C6H1302-1+C6H13O2-3<=>O2+C6H13O-1+C6H13O-3	1.40E+16	-1.6	1860.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2851. C6H1302-2+C6H13O2-2<=>O2+C6H13O-2+C6H13O-2	1.40E+16	-1.6	1860.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2852. C6H1302-2+C6H13O2-3<=>O2+C6H13O-2+C6H13O-3	1.40E+16	-1.6	1860.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2853. C6H1302-3+C6H13O2-3<=>O2+C6H13O-3+C6H13O-3	1.40E+16	-1.6	1860.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2854. C6H1302H-1<->C6H13O-1+OH	1.00E+16	0.0	39000.0
Reverse Arhenius coefficients:	2.02E+07	1.9	-6512.0
2855. C6H1302H-2<=>C6H13O-2+OH	1.00E+16	0.0	39000.0
Reverse Arhenius coefficients:	5.98E+06	2.0	-6892.0
2856. C6H1302H-3<=>C6H13O-3+OH	1.00E+16	0.0	39000.0
Reverse Arhenius coefficients:	5.98E+06	2.0	-6892.0
2857. C6H13O-1<=>C5H11-1+CH2O	5.23E+20	-2.1	24830.0
Reverse Arhenius coefficients:	1.00E+11	0.0	11900.0
2858. C6H13O-2<=>P-C4H9+CH3CHO	2.36E+22	-2.6	19620.0
Reverse Arhenius coefficients:	1.00E+11	0.0	11900.0
2859. C6H13O-3<=>C2H5CHO+N-C3H7	8.04E+17	-1.2	18170.0
Reverse Arhenius coefficients:	1.00E+11	0.0	11900.0
2860. C6H1200H-1<=>C6H12O1-2+OH	6.00E+11	0.0	22000.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2861. C6H1200H-1<=>C6H12O1-3+OH	7.50E+10	0.0	15250.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2862. C6H1200H-4<=>C6H12O1-4+OH	9.38E+09	0.0	7000.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2863. C6H1200H-5<=>C6H12O1-5+OH	1.17E+09	0.0	1800.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2864. C6H1200H-2<=>C6H12O1-2+OH	6.00E+11	0.0	22000.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2865. C6H1200H-3<=>C6H12O2-3+OH	6.00E+11	0.0	22000.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2866. C6H1200H-4<=>C6H12O2-4+OH	7.50E+10	0.0	15250.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2867. C6H1200H-5<=>C6H12O2-5+OH	9.38E+09	0.0	7000.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2868. C6H1200H-6<=>C6H12O2-6+OH	1.17E+09	0.0	1800.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2869. C6H1200H-3<=>C6H12O2-3+OH	6.00E+11	0.0	22000.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2870. C6H1200H-4<=>C6H12O3+OH	6.00E+11	0.0	22000.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2871. C6H1200H-1<=>C6H12O1-3+OH	7.50E+10	0.0	15250.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2872. C6H1200H-5<=>C6H12O2-4+OH	7.50E+10	0.0	15250.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2873. C6H1200H-6<=>C6H12O1-4+OH	9.38E+09	0.0	7000.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2874. C6H1200H-3<=>C6H12O1-3+OH	7.70E+13	-0.2	30090.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2875. C6H1200H-4<=>C6H12O1-4+CH2O+C5H10-1	2.93E+18	-1.7	24080.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2876. C6H1200H-5<=>C6H12O1-5+CH2O+C4H8-1	1.27E+18	-1.3	28880.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2877. C6H1200H-1<=>OH+CH3CHO+C2H4+C2H4	7.33E+18	-1.7	27420.0
Reverse Arhenius coefficients:	0.00E+00	0.0	0.0
2878. C6H1200H-2<=>C6H12O0H1-2+O2	8.87E+22	-2.3	37980.0
Reverse Arhenius coefficients:	7.54E+12	0.0	0.0
2879. C6H1200H-1<=>C6H12O0H1-3+O2	8.87E+22	-2.3	37980.0
Reverse Arhenius coefficients:	7.54E+12	0.0	0.0
2880. C6H1200H-4<=>C6H12O0H1-4+O2	8.87E+22	-2.3	37980.0
Reverse Arhenius coefficients:	7.54E+12	0.0	0.0
2881. C6H1200H-			

Reverse Arrhenius coefficients:	5.31E+01	1.9	44190.0	
2902. C6H12OOH3-2O2<=>NC6KET32+OH	1.00E+11	0.0	23850.0	
Reverse Arrhenius coefficients:	7.38E+02	1.8	49350.0	
2903. C6H12OOH3-4O2<=>NC6KET34+OH	1.00E+11	0.0	23850.0	
Reverse Arrhenius coefficients:	7.38E+02	1.8	49350.0	
2904. C6H12OOH3-5O2<=>NC6KET35+OH	1.25E+10	0.0	17850.0	
Reverse Arrhenius coefficients:	3.50E+01	2.0	44160.0	
2905. C6H12OOH3-6O2<=>NC6KET36+OH	1.56E+09	0.0	16050.0	
Reverse Arrhenius coefficients:	6.64E+00	1.9	42390.0	
2906. NC6KET12<=>NC4H9CHO+HCO+OH	1.00E+16	0.0	39000.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2907. NC6KET13<=>NC3H7CHO+CH2CHO+OH	1.00E+16	0.0	39000.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2908. NC6KET14<=>C2H3CHO+CH2CH2CHO+OH	1.00E+16	0.0		39000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2909. NC6KET15<=>C3H3CHO+C3H6CHO-1+OH	1.00E+16	0.0	39000.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2910. NC6KET21<=>CH2O+NC4H9CO-OH	1.00E+16	0.0	39000.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2911. NC6KET23<=>NC3H7CHO+CH3CO+OH	1.00E+16	0.0	39000.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2912. NC6KET24<=>C2H3CHO+CH3COCH2+OH	1.00E+16	0.0	39000.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2913. NC6KET25<=>C3H3CHO+CH2CH2COCH3+OH	1.00E+16	0.0		39000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2914. NC6KET26<=>CH2O+C3H6COCH3-1+OH	1.00E+16	0.0	39000.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2915. NC6KET31<=>CH2O+NC3H7COCH2+OH	1.00E+16	0.0	39000.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2916. NC6KET32<=>C3H3CHO+NC3H7CO+OH	1.00E+16	0.0	39000.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2917. NC6KET34<=>C2H3CHO+C2H5CO-OH	1.00E+16	0.0	39000.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2918. NC6KET35<=>C3H3CHO+C2H5COCH2+OH	1.00E+16	0.0	39000.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2919. NC6KET36<=>CH2O+C2H5COC2H4P+OH	1.00E+16	0.0	39000.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2920. C6H12O1-2+OH<=>C2H3CHO-N-C3H7+H2O	2.50E+12	0.0	0.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2921. C6H12O1-3+OH<=>C5H10-1+HCO-H2O	2.50E+12	0.0	0.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2922. C6H12O1-4+OH<=>C4H8-1+CH2CHO+H2O	2.50E+12	0.0	0.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2923. C6H12O1-5+OH<=>C3H6-CH2CH2CHO+H2O	2.50E+12	0.0	0.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2924. C6H12O2-3+OH<=>C2H3COCH3-C2H5+H2O	2.50E+12	0.0	0.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2925. C6H12O2-4+OH<=>C4H8-1+CH3CO+H2O	2.50E+12	0.0	0.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2926. C6H12O2-5+OH<=>C3H6-CH3COCH2+H2O	2.50E+12	0.0	0.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2927. C6H12O3-4+OH<=>C2H5COC2H3+CH3+H2O	2.50E+12	0.0	0.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2928. C6H12O1-2+OH<=>C2H2O+P-C4H9+H2O	2.50E+12	0.0	0.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2929. C6H12O1-3+OH<=>C2H4+NC3H7CO+H2O	2.50E+12	0.0	0.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2930. C6H12O1-4+OH<=>C2H4+CH2H5COCH2+H2O	2.50E+12	0.0	0.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2931. C6H12O1-5+OH<=>C2H4+CH2CH2COCH3+H2O	2.50E+12	0.0	0.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2932. C6H12O2-3+OH<=>C3H3CHO-N-C3H7-H2O	2.50E+12	0.0	0.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2933. C6H12O2-4+OH<=>C3H6-C2H5CO+H2O	2.50E+12	0.0	0.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2934. C6H12O2-5+OH<=>C3H3CHO+C4H7-1+H2O	2.50E+12	0.0	0.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2935. C6H12O3-4+OH<=>C2H5CHO+C3H5-S+H2O	2.50E+12	0.0	0.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2936. C6H12O1-2+H2O<=>C2H3CHO+N-C3H7+H2O	5.00E+12	0.0		17700.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2937. C6H12O1-3+H2O<=>C5H10-1+HCO+H2O	5.00E+12	0.0	0.0	17700.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2938. C6H12O1-4+H2O<=>C4H8-1+CH2CHO+H2O2	5.00E+12	0.0	0.0	17700.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2939. C6H12O1-5+H2O<=>C3H6+CH2CH2CHO+H2O2	5.00E+12	0.0	0.0	17700.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2940. C6H12O2-3+H2O<=>C2H3COCH3+C2H5+H2O2	5.00E+12	0.0	0.0	17700.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2941. C6H12O2-4+H2O<=>C4H8-1+CH3CO+H2O2	5.00E+12	0.0	0.0	17700.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2942. C6H12O2-5+H2O<=>C3H6+CH3COCH2+H2O2	5.00E+12	0.0	0.0	17700.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2943. C6H12O3-4+H2O<=>C2H5COC2H3+CH3+H2O2	5.00E+12	0.0	0.0	17700.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2944. C6H12O1-2+H2O<=>C2H4+C4H9+H2O2	5.00E+12	0.0	0.0	17700.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2945. C6H12O1-3+H2O<=>C2H4+NC3H7CO+H2O2	5.00E+12	0.0	0.0	17700.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2946. C6H12O1-4+H2O<=>C2H4+C2H5COCH2+H2O2	5.00E+12	0.0	0.0	17700.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2947. C6H12O1-5+H2O<=>C2H4+CH2CH2COCH3+H2O2	5.00E+12	0.0	0.0	17700.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2948. C6H12O2-3+H2O<=>C3H3CHO+N-C3H7+H2O2	5.00E+12	0.0	0.0	17700.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2949. C6H12O2-4+H2O<=>C2H4+C2H5CO+H2O2	5.00E+12	0.0	0.0	17700.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2950. C6H12O2-5+H2O<=>C3H3CHO-C4H7-1+H2O2	5.00E+12	0.0	0.0	17700.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2951. C6H12O3-4+H2O<=>C2H5CHO+C3H5-S+H2O2	5.00E+12	0.0	0.0	17700.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2952. C6H12-1+OH<=>C6H12OH-1	1.00E+13	0.0	0.0	
2953. C6H12OH-1+O2<=>O2C6H12OH-1	6.00E+12	0.0	0.0	
2954. O2C6H12OH-1<=>NC4H9CHO+CH2O+OH	1.00E+12	0.0	0.0	27800.0
Reverse Arrhenius coefficients:	1.00E+16	-1.0	0.0	29330.0
2955. C6H12OH-2<=>C6H12-2+OH	1.00E+12	0.0	-1042.0	
Reverse Arrhenius coefficients:	3.82E+21	-2.0	0.0	37830.0
2956. O2C6H12OH-2<=>C6H12OH-2+O2	2.00E+12	0.0	0.0	
Reverse Arrhenius coefficients:	2.00E+12	0.0	0.0	
2957. O2C6H12OH-2<=>NC3H7CHO+CH3CHO+OH	2.50E+10	0.0	0.0	18860.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2958. C6H12OH-3<=>C6H12-3+OH	3.90E+15	-0.9	0.0	29420.0
Reverse Arrhenius coefficients:	1.00E+12	0.0	-1042.0	
2959. O2C6H12OH-3<=>C6H12OH-3+O2	3.82E+21	-2.0	0.0	37830.0
Reverse Arrhenius coefficients:	2.00E+12	0.0	0.0	
2960. O2C6H12OH-3<=>OH+C2H5CHO+C2H5CHO	2.50E+10	0.0	0.0	18860.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2961. NC4H9CHO+O2<=>NC4H9CO+H2O	2.00E+13	0.5	42200.0	
Reverse Arrhenius coefficients:	1.00E+07	0.0	40000.0	
2962. NC4H9CHO+OH<=>NC4H9CO+H2O	2.69E+10	0.8	-340.0	
Reverse Arrhenius coefficients:	2.14E+10	0.7	31240.0	
2963. NC4H9CHO+H-<=>NC4H9CO+H2	4.00E+13	0.0	4200.0	
Reverse Arrhenius coefficients:	1.80E+13	0.0	24000.0	
2964. NC4H9CHO+O-<=>NC4H9CO+OH	5.00E+12	0.0	1790.0	
Reverse Arrhenius coefficients:	1.00E+12	0.0	19000.0	
2965. NC4H9CHO+H02<=>NC4H9CO+H2O2	2.80E+12	0.0	13600.0	
Reverse Arrhenius coefficients:	1.00E+12	0.0	10000.0	
2966. NC4H9CHO+CH3-<=>NC4H9CO+CH4	1.70E+12	0.0	8440.0	
Reverse Arrhenius coefficients:	1.50E+13	0.0	28000.0	
2967. NC4H9CHO+CH3O-<=>NC4H9CO+CH3OH	1.15E+11	0.0	1280.0	
Reverse Arrhenius coefficients:	3.00E+11	0.0	18000.0	
2968. NC4H9CHO+CH3O2-<=>NC4H9CO+CH3O2H	1.00E+12	0.0	9500.0	
Reverse Arrhenius coefficients:	2.50E+10	0.0	10000.0	
2969. NC4H9CHO+OH<=>C4H8CHO-1+H2O	5.27E+09	1.0	1586.0	
Reverse Arrhenius coefficients:	1.23E+09	0.9	21040.0	
2970. NC4H9CHO+OH<=>C4H8CHO-2+H2O	4.67E+07	1.6	-35.0	
Reverse Arrhenius coefficients:	6.84E+05	1.9	21920.0	
2971. NC4H9CHO+OH<=>C4H8CHO-3+H2O	4.67E+07	1.6	-35.0	
Reverse Arrhenius coefficients:	6.84E+05	1.9	21920.0	
2972. NC4H9CHO+H4O<=>C4H8CHO-4+H2O	4.67E+07	1.6	-35.0	
Reverse Arrhenius coefficients:	1.20E+09	1.3	2870.0	
2973. NC4H9CO-<=>P-C4H9+CO	1.00E+11	0.0	9600.0	
Reverse Arrhenius coefficients:	1.00E+11	0.0	7800.0	
2974. C4H8CHO-1<=>C2H4+CH2CH2CHO	5.98E-18	-1.6	30730.0	
Reverse Arrhenius coefficients:	2.50E+11	0.0	7800.0	
2975. C4H8CHO-2<=>C3H6+CH2CHO	2.98E-14	-0.8	23320.0	
Reverse Arrhenius coefficients:	1.00E+11	0.0	7800.0	
2976. C4H8CHO-3<=>C4H8-1+HCO	4.80E+14	-0.7	24350.0	
Reverse Arrhenius coefficients:	1.00E+11	0.0	7800.0	
2977. C4H8CHO-3<=>AC3H5CO+CH3	3.64E+13	-0.4	30330.0	
Reverse Arrhenius coefficients:	1.00E+11	0.0	7800.0	
2978. C4H8CHO-4<=>C2H3CHO+C2H5	1.86E-18	-1.3	30830.0	
Reverse Arrhenius coefficients:	1.00E+11	0.0	7800.0	
2979. AC3H5CHO-<=>C3H5-A+HCO	1.81E+19	-1.1	68480.0	
Reverse Arrhenius coefficients:	1.00E+13	0.0	0.0	
2980. AC3H5CHO+OH<=>AC3H5CO+H2O	2.69E+10	0.8	-340.0	
Reverse Arrhenius coefficients:	1.74E+10	0.8	3120.0	
2981. AC3H5CHO+OH<=>C2H3CH3CHO+C2H5	3.12E+06	2.0	-298.0	
Reverse Arrhenius coefficients:	1.25E+08	1.8	34930.0	
2982. AC3H5CHO+H02<=>AC3H5CO+H2O2	3.00E+12	0.0	11920.0	
Reverse Arrhenius coefficients:	1.15E+13	-0.3	11990.0	
2983. AC3H5CHO+H02<=>C2H3CH3CHO+H2O2	9.63E+03	2.6	13910.0	
Reverse Arrhenius coefficients:	2.28E+06	2.1	17670.0	
2984. AC3H5CHO+CH3O2-<=>AC3H5CO+CH3O2H	1.00E+12	0.0		11920.0
Reverse Arrhenius coefficients:	1.58E-13	-0.5	11270.0	
2985. AC3H5CHO+CH3O2-<=>C2H3CH3CHO+CH3O2H	1.99E+12	0.0		
2986. Reverse Arrhenius coefficients:	1.94E+15	-0.7	20090.0	
2987. Reverse Arrhenius coefficients:	6.20E+15	-1.1	-330.0	
2988. C2H3CH3CHO+H02<=>C2H3CH3CHO+HCO+OH	1.50E+11	0.0	4810.0	
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0	
2989. NC3H7COCH3+OH<=>C3H6COCH3-1+H2O2	2.06E+07	1.7	753.0	
Reverse Arrhenius coefficients:	3.60E-06	1.8	20170.0	
2990. NC3H7COCH3+OH<=>C3H6COCH3-2+H2O	3.62E-07</td			

3006. C2H5COC2H5+HO2=>C2H5COC2H4P+H2O2	4.76E+04	2.5	Reverse Arrhenius coefficients: 3.20E+04 2.2 4472.0	4.98E-01 3.7 2562.0
16490.0 Reverse Arrhenius coefficients:			3.007. C2H5COC2H5+HO2=>C2H5COC2H4S+H2O2 4.00E+11 0.0 8698.0	6.32E+01 3.4 13720.0
Reverse Arrhenius coefficients: 4.63E+13 -0.7 6200.0			3055. NC7H16+CH3<=>C7H15-4+H2O2 4.95E-01 3.7 2562.0	
3008. C2H5COC2H5+O2=>C2H5COC2H4P+HO2 4.10E+13 0.0 51310.0			3056. NC7H16+CH3<=>C7H15-1+CH4 9.04E-01 3.6 7154.0	
Reverse Arrhenius coefficients: 1.95E+13 0.3 -1882.0			3057. NC7H16+CH3<=>C7H15-2+CH4 8.93E-02 3.8 11030.0	
3009. C2H5COC2H5+O2=>C2H5COC2H4S+HO2 3.10E+13 0.0 41970.0			3058. NC7H16+CH3<=>C7H15-3+CH4 5.41E+04 2.3 7287.0	
Reverse Arrhenius coefficients: 2.54E+12 0.0 -1702.0			3059. NC7H16+CH3<=>C7H15-4+CH4 3.43E+02 2.8 13670.0	
3010. C2H5COC2H5+H<=>C2H5COC2H4P+H2 1.83E+07 2.0 7700.0			3059. NC7H16+CH3<=>C7H15-4+CH4 3.42E+02 2.8 13670.0	
Reverse Arrhenius coefficients: 4.79E+05 2.0 11990.0			3060. NC7H16+O2=>C7H15-1+H2O 4.20E+13 0.0 52800.0	
3011. C2H5COC2H5+H<=>C2H5COC2H4S+H2 8.96E+06 2.0 3200.0			Reverse Arrhenius coefficients: 2.39E+10 0.3 453.0	
Reverse Arrhenius coefficients: 4.04E+07 1.7 17010.0			3061. NC7H16+O2=>C7H15-2+H2O 2.80E+13 0.0 50150.0	
3012. C2H5COC2H5+C2H3<=>C2H5COC2H4P+C2H4 1.00E+12 0.0 10400.0			Reverse Arrhenius coefficients: 1.00E+09 0.6 309.0	
Reverse Arrhenius coefficients: 3.85E+08 0.8 14040.0			3062. NC7H16+O2=>C7H15-3+H2O 2.80E+13 0.0 50150.0	
3013. C2H5COC2H5+C2H3<=>C2H5COC2H4S+C2H4 6.00E+11 0.0 5600.0			Reverse Arrhenius coefficients: 1.00E+09 0.6 309.0	
Reverse Arrhenius coefficients: 3.98E+10 0.5 18760.0			3063. NC7H16+O2=>C7H15-4+H2O 1.40E+13 0.0 50150.0	
3014. C2H5COC2H5+C2H3<=>C2H5COC2H4S+C2H6 1.00E+11 0.0 13400.0			Reverse Arrhenius coefficients: 9.94E+08 0.6 309.0	
Reverse Arrhenius coefficients: 1.07E+13 -0.6 14000.0			3064. NC7H16+C2H5<=>C7H15-1+C2H6 1.00E+11 0.0 13400.0	
3015. C2H5COC2H5+C2H5<=>C2H5COC2H4S+C2H6 6.00E+10 0.0 8600.0			Reverse Arrhenius coefficients: 3.20E+11 0.0 12300.0	
Reverse Arrhenius coefficients: 1.10E+15 -0.9 18720.0			3065. NC7H16+C2H5<=>C7H15-2+C2H6 1.00E+11 0.0 10400.0	
3016. C2H5COC2H5+CH3O<=>C2H5COC2H4P+CH3OH 4.34E+11 0.0 6460.0			Reverse Arrhenius coefficients: 1.00E+11 0.0 12900.0	
Reverse Arrhenius coefficients: 5.48E+09 0.0 9020.0			3066. NC7H16+C2H5<=>C7H15-3+C2H6 1.00E+11 0.0 10400.0	
3017. C2H5COC2H5+CH3O<=>C2H5COC2H4S+CH3OH 2.90E+11 0.0 2771.0			Reverse Arrhenius coefficients: 1.00E+11 0.0 12900.0	
Reverse Arrhenius coefficients: 6.30E+11 -0.3 14850.0			3067. NC7H16+C2H5<=>C7H15-4+C2H6 5.00E+10 0.0 10400.0	
3018. C2H5COC2H5+CH3O2=>C2H5COC2H4P+CH3O2H 6.02E+12 0.0 19380.0			Reverse Arrhenius coefficients: 1.00E+11 0.0 12900.0	
Reverse Arrhenius coefficients: 1.66E+13 -0.5 6642.0			3068. NC7H16+CH3O<=>C7H15-1+CH3OH 3.16E+11 0.0 7000.0	
3019. C2H5COC2H5+CH3O2=>C2H5COC2H4S+CH3O2H 4.00E+12 0.0 15250.0			Reverse Arrhenius coefficients: 1.20E+10 0.0 9200.0	
Reverse Arrhenius coefficients: 1.90E+15 -0.8 12030.0			3069. NC7H16+CH3O<=>C7H15-2+CH3OH 2.19E+11 0.0 5000.0	
3020. C2H5COC2H4P<=>C2H5CO+C2H4 1.77E+17 -1.5 29540.0			Reverse Arrhenius coefficients: 8.90E+09 0.0 7200.0	
Reverse Arrhenius coefficients: 8.00E+10 0.0 11300.0			3070. NC7H16+CH3O<=>C7H15-3+CH3OH 2.19E+11 0.0 5000.0	
3021. C2H5COC2H4S<=>C2H5COC2H3+H 8.70E+16 -0.8 42130.0			Reverse Arrhenius coefficients: 8.90E+09 0.0 7200.0	
Reverse Arrhenius coefficients: 1.30E+13 0.0 1560.0			3071. NC7H16+CH3O<=>C7H15-4+CH3OH 1.10E+11 0.0 5000.0	
3022. C2H5COC2H3+OH<=>C2H5COCH2+CH2O 1.00E+10 0.0 0.0			Reverse Arrhenius coefficients: 8.90E+09 0.0 7200.0	
Reverse Arrhenius coefficients: 1.67E+11 -0.4 18220.0			3072. NC7H16+C2H3<=>C7H15-1+C2H4 1.00E+12 0.0 18000.0	
3023. C2H5COC2H3+OH<=>PC2H4+COC2H3+H2O 7.55E+09 1.0 1586.0			Reverse Arrhenius coefficients: 2.57E+12 0.0 25400.0	
Reverse Arrhenius coefficients: 1.28E+08 2.5 20210.0			3073. NC7H16+C2H3<=>C7H15-2+C2H4 8.00E+11 0.0 16800.0	
3024. C2H5COC2H3+OH<=>SC2H4+COC2H3+H2O 8.45E+11 0.0 -228.0			Reverse Arrhenius coefficients: 2.00E+12 0.0 24200.0	
Reverse Arrhenius coefficients: 1.35E+13 -0.2 28600.0			3074. NC7H16+C2H3<=>C7H15-3+C2H4 8.00E+11 0.0 16800.0	
3025. C2H5COC2H3+H2O2=>C2H5CO+CH2CHO+OH 6.03E+09 0.0 7949.0			Reverse Arrhenius coefficients: 2.00E+12 0.0 24200.0	
Reverse Arrhenius coefficients: 1.00E+00 0.0 0.0			3075. NC7H16+C2H3<=>C7H15-4+C2H4 4.00E+11 0.0 16800.0	
3026. C2H5COC2H3+H2O2=>PC2H4+COC2H3+H2O 2.38E+04 2.5 16490.0			Reverse Arrhenius coefficients: 2.00E+12 0.0 24200.0	
Reverse Arrhenius coefficients: 2.40E+03 3.8 3652.0			3076. NC7H16+CH3O2=>C7H15-1+CH3O2H 1.39E+00 4.0 18280.0	
3027. C2H5COC2H3+H2O2=>SC2H4+COC2H3+H2O2 2.00E+11 0.0 8698.0			Reverse Arrhenius coefficients: 1.69E+00 3.5 3024.0	
Reverse Arrhenius coefficients: 1.90E+13 -0.5 6605.0			3077. NC7H16+CH3O2=>C7H15-2+CH3O2H 2.04E+01 3.6 14810.0	
3028. C2H5COC2H3+CH3O2=>C2H5CO+CH2CHO+CH3O 3.97E+11 0.0 17050.0			Reverse Arrhenius coefficients: 1.56E+00 3.4 2054.0	
Reverse Arrhenius coefficients: 1.00E+00 0.0 0.0			3078. NC7H16+CH3O2=>C7H15-3+CH3O2H 2.04E+01 3.6 14810.0	
3029. C2H5COC2H3+CH3O2=>PC2H4+COC2H3+CH3O2H 3.01E+12 0.0 19380.0			Reverse Arrhenius coefficients: 1.56E+00 3.4 2054.0	
Reverse Arrhenius coefficients: 1.25E+12 1.1 5822.0			3079. NC7H16+CH3O2=>C7H15-4+CH3O2H 1.02E+01 3.6 14810.0	
3030. C2H5COC2H3+CH3O2=>SC2H4+COC2H3+CH3O2H 2.00E+12 0.0 15250.0			Reverse Arrhenius coefficients: 1.55E+00 3.4 2054.0	
Reverse Arrhenius coefficients: 7.79E+14 -0.7 119000.0			3080. NC7H16+O2CHO=>C7H15-1+H2O2CHO 1.68E-13 0.0 20440.0	
3031. PC2H4+COC2H3=>C2H3CO+C2H4 5.26E+14 0.4 21460.0			Reverse Arrhenius coefficients: 1.17E+03 2.2 3057.0	
Reverse Arrhenius coefficients: 8.00E+10 0.0 11300.0			3081. NC7H16+O2CHO=>C7H15-2+H2O2CHO 1.12E+13 0.0 17690.0	
3032. SC2H4+COC2H3=>CH3CHO+C2H3 1.64E+16 -0.7 54590.0			Reverse Arrhenius coefficients: 2.48E+01 2.6 2823.0	
Reverse Arrhenius coefficients: 8.00E+10 0.0 12600.0			3082. NC7H16+O2CHO=>C7H15-3+H2O2CHO 1.12E+13 0.0 17690.0	
3033. NC7H16<=>C7H15-1 2.68E+88 -21.2 142800.0			Reverse Arrhenius coefficients: 2.48E+01 2.6 2823.0	
Reverse Arrhenius coefficients: 7.26E+88 -20.8 41560.0			3083. NC7H16+O2CHO=>C7H15-4+H2O2CHO 5.60E+12 0.0 17690.0	
3034. NC7H16<=>C7H15-2 1.30E+88 -21.0 139500.0			Reverse Arrhenius coefficients: 2.47E+01 2.6 2823.0	
Reverse Arrhenius coefficients: 2.26E+83 -20.3 40830.0			3084. NC7H16+C7H1502-1=>C7H15-1+C7H1502H-1 1.21E+13 0.0 20430.0	
3035. NC7H16<=>C7H15-3 1.30E+88 -21.0 139500.0			Reverse Arrhenius coefficients: 1.44E+10 0.0 15000.0	
Reverse Arrhenius coefficients: 2.26E+83 -20.3 40830.0			3085. NC7H16+C7H1502-2=>C7H15-1+C7H1502H-2 1.21E+13 0.0 20430.0	
3036. NC7H16<=>C7H15-4 6.50E+87 -21.0 139500.0			Reverse Arrhenius coefficients: 1.44E+10 0.0 15000.0	
Reverse Arrhenius coefficients: 2.25E+83 -20.3 40830.0			3086. NC7H16+C7H1502-3=>C7H15-1+C7H1502H-3 1.21E+13 0.0 20430.0	
3037. NC7H16(6-M)<=>C6H13-1+CH3(+M) 4.32E+24 -2.1 89900.0			Reverse Arrhenius coefficients: 1.44E+10 0.0 15000.0	
Low pressure limit: 0.496300E+43 -0.077800E+01 4.02800E+05			3087. NC7H16+C7H1502-4=>C7H15-1+C7H1502H-4 1.21E+13 0.0 20430.0	
TROE centering: 0.89200E+00 0.10000E+11 0.22280E+01 0.17980E+10			Reverse Arrhenius coefficients: 1.44E+10 0.0 15000.0	
3038. NC7H16(6-M)<=>C5H11-1+C2H5(+M) 6.82E+26 -2.7 88910.0			3088. NC7H16+C7H1502-5=>C7H15-2+C7H1502H-5 8.06E+12 0.0 17700.0	
Low pressure limit: 0.37530E+09 -0.094600E+01 0.41310E+05			Reverse Arrhenius coefficients: 1.44E+10 0.0 15000.0	
TROE centering: 0.9000E+01 -0.36556E+01 0.10000E+11 0.93300E+10			3089. NC7H16+C7H1502-6=>C7H15-2+C7H1502H-6 8.06E+12 0.0 17700.0	
3039. NC7H16(6-M)<=>PC4H9-N-C3H7(+M) 1.36E+26 -2.5 88760.0			Reverse Arrhenius coefficients: 1.44E+10 0.0 15000.0	
Low pressure limit: 0.6509E+09 -0.05700E+01 0.41290E+05			3090. NC7H16+C7H1502-7=>C7H15-2+C7H1502H-7 8.06E+12 0.0 17700.0	
TROE centering: 0.91100E+00 0.10000E+11 0.22382E+02 0.50000E+10			Reverse Arrhenius coefficients: 1.44E+10 0.0 15000.0	
3040. NC7H16<=>C7H15-1+H2 1.88E+05 2.8 6280.0			3091. NC7H16+C7H1502-8=>C7H15-1+C7H1502H-8 8.06E+12 0.0 17700.0	
Reverse Arrhenius coefficients: 2.04E+01 3.4 8618.0			Reverse Arrhenius coefficients: 1.44E+10 0.0 15000.0	
3041. NC7H16<=>C7H15-2+H2 2.60E+05 2.4 4471.0			3092. NC7H16+C7H1502-9=>C7H15-2+C7H1502H-9 8.06E+12 0.0 17700.0	
Reverse Arrhenius coefficients: 1.81E+01 3.4 9318.0			Reverse Arrhenius coefficients: 1.44E+10 0.0 15000.0	
3042. NC7H16<=>C7H15-3+H2 2.60E+05 2.4 4471.0			3093. NC7H16+C7H1502-10=>C7H15-2+C7H1502H-10 8.06E+12 0.0 17700.0	
Reverse Arrhenius coefficients: 1.81E+01 3.4 9318.0			Reverse Arrhenius coefficients: 1.44E+10 0.0 15000.0	
3043. NC7H16<=>C7H15-4+H2 1.30E+06 2.4 4471.0			3094. NC7H16+C7H1502-11=>C7H15-3+C7H1502H-11 8.06E+12 0.0 17700.0	
Reverse Arrhenius coefficients: 1.80E+01 3.4 9318.0			Reverse Arrhenius coefficients: 1.44E+10 0.0 15000.0	
3044. NC7H16<=>C7H15-5+OH 1.93E+05 2.7 3716.0			3095. NC7H16+C7H1502-12=>C7H15-3+C7H1502H-12 8.06E+12 0.0 17700.0	
Reverse Arrhenius coefficients: 1.08E+01 3.3 4642.0			Reverse Arrhenius coefficients: 1.44E+10 0.0 15000.0	
3045. NC7H16<=>C7H15-2+OH 9.54E+04 2.7 2106.0			3096. NC7H16+C7H1502-13=>C7H15-4+C7H1502H-13 8.06E+12 0.0 17700.0	
Reverse Arrhenius coefficients: 3.48E+01 3.7 5541.0			Reverse Arrhenius coefficients: 1.44E+10 0.0 15000.0	
3046. NC7H16<=>C7H15-3+OH 9.54E+04 2.7 2106.0			3097. NC7H16+C7H1502-14=>C7H15-5+C7H1502H-14 4.03E+12 0.0 17700.0	
Reverse Arrhenius coefficients: 3.48E+01 3.7 5541.0			Reverse Arrhenius coefficients: 1.44E+10 0.0 15000.0	
3047. NC7H16<=>C7H15-4+OH 4.77E+04 2.7 2106.0			3098. NC7H16+C7H1502-15=>C7H15-6+C7H1502H-15 4.03E+12 0.0 17700.0	
Reverse Arrhenius coefficients: 3.47E+01 3.7 5541.0			Reverse Arrhenius coefficients: 1.44E+10 0.0 15000.0	
3048. NC7H16<=>C7H15-1+H20 2.57E+07 1.8 954.0			3099. NC7H16+C7H1502-16=>C7H15-7+C7H1502H-16 4.03E+12 0.0 17700.0	
Reverse Arrhenius coefficients: 2.95E+04 2.3 18180.0			Reverse Arrhenius coefficients: 1.44E+10 0.0 15000.0	
3049. NC7H16<=>C7H15-2+H20 4.90E+06 2.0 -596.0			3100. NC7H16+C7H1502-17=>C7H15-8+C7H1502H-17 4.03E+12 0.0 17700.0	
Reverse Arrhenius coefficients: 3.62E+02 2.9 19140.0			Reverse Arrhenius coefficients: 1.44E+10 0.0 15000.0	
3050. NC7H16<=>C7H15-3+H20 4.90E+06 2.0 -596.0			3101. NC7H16+C7H1502-18=>C7H15-9+N-CH7H16 1.00E+11 0.0 10400.0	
Reverse Arrhenius coefficients: 3.62E+02 2.9 19140.0			Reverse Arrhenius coefficients: 1.50E+11 0.0 12300.0	
3051. NC7H16<=>C7H15-4+H20 2.45E+06 2.0 -596.0			3102. NC7H16+C7H1502-19=>C7H15-10+N-CH7H16 5.00E+10 0.0 10400.0	
Reverse Arrhenius coefficients: 3.61E+02 2.9 19140.0			Reverse Arrhenius coefficients: 1.50E+11 0.0 12300.0	
3052. NC7H16<=>C7H15-1+H20 4.08E+01 3.6 17160.0			3103. NC7H16+C7H1502-20=>C7H15-11+N-CH7H16 1.00E+11 0.0 10400.0	
Reverse Arrhenius coefficients: 2.56E+00 3.5 3498.0			Reverse Arrhenius coefficients: 1.50E+11 0.0 12300.0	
3053. NC7H16<=>C7H15-2+H20 1.26E+02 3.4 13720.0			3104. NC7H16+C7H1502-21=>C7H15-12+N-CH7H16 5.00E+10 0.0 10400.0	
Reverse Arrhenius coefficients: 4.98E-01 3.7 2562.0			Reverse Arrhenius coefficients: 1.00E+11 0.0 10400.0	
3054. NC7H16<=>C7H15-3+H20 1.26E+02 3.4 13720.0			3105. NC7H16+C7H1502-22=>C7H15-13+N-CH7H16 5.00E+10 0.0 10400.0	
Reverse Arrhenius coefficients: 3.61E+02 2.9 19140.0			Reverse Arrhenius coefficients: 1.00E+11 0.0 10400.0	
3106. C7H11-1<=>C5H11-1+C2H4 1.23E+19 -1.9 31400.0			3106. C7H11-1<=>C5H11-1+C2H4 1.23E+19 -1.9 31400.0	

Reverse Arrhenius coefficients:	1.00E+11	0.0	7700.0	Reverse Arrhenius coefficients:	1.26E+03	3.0	24860.0
3112. C7H15-3<=>C6H12-1+CH3	2.70E+17	-1.4	31480.0	3169. C7H14-2+CH3<=>C7H132-5+CH4	1.51E+00	3.5	5481.0
Reverse Arrhenius coefficients:	1.75E+11	0.0	7200.0	3170. C7H14-2+CH3<=>C7H132-6+CH4	1.51E+00	3.5	5481.0
3113. C7H15-3<=>C7H14-2+H	1.23E+13	-0.1	35640.0	Reverse Arrhenius coefficients:	1.17E-01	3.8	13010.0
Reverse Arrhenius coefficients:	1.00E+13	0.0	2900.0	3171. C7H14-2+CH3<=>C7H132-7+CH4	1.17E-01	3.8	13010.0
3114. C7H15-3<=>C7H14-3+H	9.15E+12	0.0	35730.0	Reverse Arrhenius coefficients:	4.52E-01	3.6	7154.0
Reverse Arrhenius coefficients:	1.00E+13	0.0	2900.0	3172. C7H14-2+HO2<=>C7H131-3+H2O2	5.59E-01	3.6	12170.0
3115. C7H15-4<=>C2H5+C5H10-1	1.14E+18	-1.3	31430.0	Reverse Arrhenius coefficients:	9.64E+03	2.6	13910.0
Reverse Arrhenius coefficients:	1.00E+11	0.0	8200.0	3173. C7H14-2+HO2<=>C7H132-4+H2O2	6.53E+06	1.8	15140.0
3116. C7H15-4<=>C7H14-3+H	1.82E+13	0.0	35730.0	Reverse Arrhenius coefficients:	4.82E+03	2.5	10530.0
Reverse Arrhenius coefficients:	1.00E+13	0.0	2900.0	3174. C7H14-2+HO2<=>C7H132-5+H2O2	1.62E+06	2.0	14600.0
3117. C7H15-1+O2<=>C7H14-1+HO2	3.00E-09	0.0	3000.0	Reverse Arrhenius coefficients:	9.64E+03	2.6	13910.0
Reverse Arrhenius coefficients:	6.52E-10	0.2	18760.0	3175. C7H14-2+HO2<=>C7H132-6+H2O2	7.32E+02	2.6	4652.0
3118. C7H15-2+O2<=>C7H14-1+HO2	4.50E-09	0.0	5020.0	Reverse Arrhenius coefficients:	9.64E+03	2.6	13910.0
Reverse Arrhenius coefficients:	1.53E-08	-0.2	18270.0	3176. C7H14-2+HO2<=>C7H132-7+H2O2	7.32E+02	2.6	4652.0
3119. C7H15-2+O2<=>C7H14-2+HO2	3.00E-09	0.0	3000.0	Reverse Arrhenius coefficients:	2.38E+04	2.5	16490.0
Reverse Arrhenius coefficients:	5.04E-09	0.0	19120.0	3177. C7H14-2+CH3O2<=>C7H131-3+CH3O2H	5.90E+04	2.2	4726.0
3120. C7H15-3+O2<=>C7H14-2+HO2	3.00E-09	0.0	3000.0	Reverse Arrhenius coefficients:	9.64E+03	2.6	13910.0
Reverse Arrhenius coefficients:	5.04E-09	0.0	19120.0	3178. C7H14-2+CH3O2<=>C7H132-4+CH3O2H	1.36E+07	1.7	12120.0
3121. C7H15-3+O2<=>C7H14-3+HO2	3.00E-09	0.0	3000.0	Reverse Arrhenius coefficients:	4.82E+03	2.5	10530.0
Reverse Arrhenius coefficients:	6.77E-09	-0.1	19030.0	Reverse Arrhenius coefficients:	3.36E+06	1.8	11580.0
3122. C7H15-4+O2<=>C7H14-3+HO2	6.00E-09	0.0	3000.0	3179. C7H14-2+CH3O2<=>C7H132-5+CH3O2H	9.64E+03	2.6	13910.0
Reverse Arrhenius coefficients:	6.79E-09	-0.1	19030.0	Reverse Arrhenius coefficients:	1.52E+03	2.4	1632.0
3123. C7H15-1<=>C7H15-3	1.39E+09	1.0	33760.0	3180. C7H14-2+CH3O2<=>C7H132-6+CH3O2H	9.64E+03	2.6	13910.0
Reverse Arrhenius coefficients:	8.72E+07	1.3	36270.0	Reverse Arrhenius coefficients:	1.52E+03	2.4	1632.0
3124. C7H15-1<=>C7H15-4	2.54E+09	0.3	19760.0	3181. C7H14-2+CH3O2<=>C7H132-7+CH3O2H	2.38E+04	2.5	16490.0
Reverse Arrhenius coefficients:	3.18E+08	0.7	22270.0	Reverse Arrhenius coefficients:	6.03E+04	2.0	1706.0
3125. C7H15-2<=>C7H15-3	9.59E+08	1.4	39700.0	3182. C7H14-2+CH3O2<=>C7H131-3+CH3OH	9.00E+01	3.0	11990.0
Reverse Arrhenius coefficients:	5.95E+08	1.4	39700.0	Reverse Arrhenius coefficients:	1.14E+03	2.5	27800.0
3126. C7H15-1<=>C7H15-2	5.48E+08	1.6	38760.0	3183. C7H14-2+CH3O2<=>C7H132-4+CH3OH	4.00E+01	2.9	8609.0
Reverse Arrhenius coefficients:	3.44E+07	2.0	41270.0	Reverse Arrhenius coefficients:	2.51E+02	2.7	27260.0
3127. C7H14-1+H<=>C7H131-3+H2	3.38E+05	2.4	207.0	3184. C7H14-2+CH3O2<=>C7H132-5+CH3OH	1.45E+11	0.0	4571.0
Reverse Arrhenius coefficients:	4.39E+06	2.1	20620.0	Reverse Arrhenius coefficients:	2.07E+08	0.4	9891.0
3128. C7H14-1+H<=>C7H131-4+H2	1.30E+06	2.4	4471.0	3185. C7H14-2+CH3O2<=>C7H132-6+CH3OH	1.45E+11	0.0	4571.0
Reverse Arrhenius coefficients:	3.83E+03	2.7	11540.0	Reverse Arrhenius coefficients:	2.07E+08	0.4	9891.0
3129. C7H14-1+H<=>C7H131-5+H2	1.30E+06	2.4	4471.0	3186. C7H14-2+CH3O2<=>C7H132-7-CH3OH	2.17E+11	0.0	6458.0
Reverse Arrhenius coefficients:	3.83E+03	2.7	11540.0	Reverse Arrhenius coefficients:	4.95E+09	0.0	9268.0
3130. C7H14-1+H<=>C7H131-6+H2	1.30E+06	2.4	4471.0	3187. C7H14-3+H<=>C7H131-1+H2	6.65E+05	2.5	6756.0
Reverse Arrhenius coefficients:	3.83E+03	2.7	11540.0	Reverse Arrhenius coefficients:	3.10E+04	2.5	11260.0
3131. C7H14-1+H<=>C7H131-7+H2	6.65E+05	2.5	6756.0	3188. C7H14-3+H<=>C7H132-4+H2	3.38E+05	2.4	207.0
Reverse Arrhenius coefficients:	3.06E+04	2.5	11300.0	Reverse Arrhenius coefficients:	3.28E+06	2.2	20680.0
3132. C7H14-1+OH<=>C7H131-3+H2O	2.76E+04	2.6	-1919.0	3189. C7H14-3+H<=>C7H133-5+H2	3.38E+05	2.4	207.0
Reverse Arrhenius coefficients:	1.56E+06	2.4	33650.0	Reverse Arrhenius coefficients:	4.38E+06	2.1	20560.0
3133. C7H14-1+OH<=>C7H131-4+H2O	4.67E+07	1.6	-35.0	3190. C7H14-3+H<=>C7H133-6+H2	1.30E+06	2.4	4471.0
Reverse Arrhenius coefficients:	5.96E+05	1.9	22190.0	Reverse Arrhenius coefficients:	3.92E+03	2.7	11490.0
3134. C7H14-1+OH<=>C7H131-5+H2O	4.67E+07	1.6	-35.0	3191. C7H14-3+H<=>C7H133-7+H2	6.65E+05	2.5	6756.0
Reverse Arrhenius coefficients:	5.96E+05	1.9	22190.0	Reverse Arrhenius coefficients:	3.10E+04	2.5	11260.0
3135. C7H14-1+OH<=>C7H131-6+H2O	4.67E+07	1.6	-35.0	3192. C7H14-3+OH<=>C7H133-1+H2O	1.05E+10	1.0	1586.0
Reverse Arrhenius coefficients:	5.96E+05	1.9	22190.0	Reverse Arrhenius coefficients:	2.12E+09	1.0	21240.0
3136. C7H14-1+OH<=>C7H131-7+H2O	5.27E+09	1.0	1586.0	3193. C7H14-3+OH<=>C7H132-4+H2O	2.76E+04	2.6	-1919.0
Reverse Arrhenius coefficients:	1.05E+09	1.0	21300.0	Reverse Arrhenius coefficients:	1.16E+06	2.4	33710.0
3137. C7H14-1+CH3<=>C7H131-3+CH4	3.69E+00	3.3	4002.0	3194. C7H14-3+OH<=>C7H133-5+H2O	2.76E+04	2.6	-1919.0
Reverse Arrhenius coefficients:	1.25E+03	3.0	24890.0	Reverse Arrhenius coefficients:	1.55E+06	2.4	33590.0
3138. C7H14-1+CH3<=>C7H131-4+CH4	1.51E+00	3.5	5481.0	3195. C7H14-3+OH<=>C7H133-6+H2O	4.67E+07	1.6	-35.0
Reverse Arrhenius coefficients:	1.16E-01	3.8	13030.0	Reverse Arrhenius coefficients:	6.09E+05	1.9	22140.0
3139. C7H14-1+CH3<=>C7H131-5+CH4	1.51E+00	3.5	5481.0	3196. C7H14-3+OH<=>C7H133-7+H2O	1.05E+10	1.0	1586.0
Reverse Arrhenius coefficients:	1.16E-01	3.8	13030.0	Reverse Arrhenius coefficients:	2.12E+09	1.0	21240.0
3140. C7H14-1+CH3<=>C7H131-6+CH4	1.51E+00	3.5	5481.0	3197. C7H14-3+CH3<=>C7H133-1+CH4	9.04E-01	3.6	7154.0
Reverse Arrhenius coefficients:	1.16E-01	3.8	13030.0	Reverse Arrhenius coefficients:	1.10E+00	3.6	12130.0
3141. C7H14-1+CH3<=>C7H131-7+CH4	4.52E+01	3.6	7154.0	3198. C7H14-3+CH3<=>C7H132-4+CH4	3.69E+00	3.3	4002.0
Reverse Arrhenius coefficients:	5.43E-01	3.6	12190.0	Reverse Arrhenius coefficients:	9.36E+02	3.1	24950.0
3142. C7H14-1+H2O<=>C7H131-3+H2O2	4.82E+03	2.5	10530.0	Reverse Arrhenius coefficients:	3.69E+00	3.3	4002.0
Reverse Arrhenius coefficients:	1.61E+06	2.0	14630.0	Reverse Arrhenius coefficients:	1.25E+03	3.0	24830.0
3143. C7H14-1+H2O<=>C7H131-4+H2O2	9.64E+03	2.6	13910.0	3200. C7H14-3+CH3<=>C7H133-6+CH4	1.51E+00	3.5	5481.0
Reverse Arrhenius coefficients:	7.31E+02	2.6	46720.0	Reverse Arrhenius coefficients:	1.19E-01	3.8	12980.0
3144. C7H14-1+H2O<=>C7H131-5+H2O2	9.64E+03	2.6	13910.0	3201. C7H14-3+CH3<=>C7H133-7+CH4	9.04E-01	3.6	7154.0
Reverse Arrhenius coefficients:	7.31E+02	2.6	46720.0	Reverse Arrhenius coefficients:	1.10E+00	3.6	12130.0
3145. C7H14-1+H2O<=>C7H131-6+H2O2	9.64E+03	2.6	13910.0	3202. C7H14-3+H2O<=>C7H133-1+H2O2	4.76E+04	2.5	16490.0
Reverse Arrhenius coefficients:	7.31E+02	2.6	46720.0	Reverse Arrhenius coefficients:	5.70E+04	2.2	4686.0
3146. C7H14-1+H2O<=>C7H131-7+H2O2	2.38E+04	2.5	16490.0	Reverse Arrhenius coefficients:	4.82E+03	2.5	10530.0
Reverse Arrhenius coefficients:	2.81E+04	2.2	47460.0	3203. C7H14-3+H2O2<=>C7H132-4+H2O2	1.20E+06	2.0	14690.0
3147. C7H14-1+CH3O2<=>C7H131-3+CH3O2H	4.82E+03	2.5	10530.0	Reverse Arrhenius coefficients:	4.82E+03	2.5	10530.0
Reverse Arrhenius coefficients:	3.36E+06	1.8	11610.0	Reverse Arrhenius coefficients:	1.61E+06	2.0	14570.0
3148. C7H14-1+CH3O2<=>C7H131-4+CH3O2H	9.64E+03	2.6	13910.0	3205. C7H14-3+H2O<=>C7H133-6+H2O2	9.64E+03	2.6	13910.0
Reverse Arrhenius coefficients:	1.52E+03	2.4	16520.0	Reverse Arrhenius coefficients:	7.46E+02	2.6	4622.0
3149. C7H14-1+CH3O2<=>C7H131-5+CH3O2H	9.64E+03	2.6	13910.0	3206. C7H14-3+H2O2<=>C7H133-7+H2O2	4.76E+04	2.5	16490.0
Reverse Arrhenius coefficients:	1.52E+03	2.4	16520.0	Reverse Arrhenius coefficients:	5.70E+04	2.2	4686.0
3150. C7H14-1+CH3O2<=>C7H131-6+CH3O2H	9.64E+03	2.6	13910.0	Reverse Arrhenius coefficients:	1.19E-01	3.8	12980.0
Reverse Arrhenius coefficients:	1.52E+03	2.4	16520.0	3207. C7H14-3+CH3O2<=>C7H133-7+CH3O2H	4.76E+04	2.5	16490.0
3151. C7H14-1+CH3O2<=>C7H131-7-CH3O2H	2.38E+04	2.5	16490.0	Reverse Arrhenius coefficients:	1.19E+05	2.0	1666.0
Reverse Arrhenius coefficients:	5.85E+04	2.0	17260.0	3208. C7H14-3+CH3O2<=>C7H132-4+CH3O2H	4.82E+03	2.5	10530.0
3152. C7H14-1+CH3O2<=>C7H131-3+CH3OH	4.00E+01	2.9	8609.0	Reverse Arrhenius coefficients:	2.50E+06	1.9	11670.0
Reverse Arrhenius coefficients:	2.51E+02	2.7	27290.0	3209. C7H14-3+CH3O2<=>C7H133-5+CH3O2H	4.82E+03	2.5	10530.0
3153. C7H14-1+CH3O2<=>C7H131-4+CH3OH	1.45E+11	0.0	4571.0	Reverse Arrhenius coefficients:	3.35E+06	1.8	11550.0
Reverse Arrhenius coefficients:	2.06E+08	0.4	9911.0	3210. C7H14-3+CH3O2<=>C7H133-6+CH3O2H	9.64E+03	2.6	13910.0
3154. C7H14-1+CH3O2<=>C7H131-5+CH3OH	1.45E+11	0.0	4571.0	Reverse Arrhenius coefficients:	1.55E+03	2.4	1602.0
Reverse Arrhenius coefficients:	2.06E+08	0.4	9911.0	3211. C7H14-3+CH3O2<=>C7H133-7+CH3O2H	4.76E+04	2.5	16490.0
3155. C7H14-1+CH3O2<=>C7H131-6+CH3OH	1.45E+11	0.0	4571.0	Reverse Arrhenius coefficients:	1.19E+05	2.0	1666.0
Reverse Arrhenius coefficients:	2.06E+08	0.4	9911.0	3212. C7H14-3+CH3O2<=>C7H133-1+CH3OH	4.34E+11	0.0	6458.0
3156. C7H14-1+CH3O2<=>C7H131-7+CH3OH	2.17E+11	0.0	4580.0	Reverse Arrhenius coefficients:	9.74E+09	0.0	9228.0
Reverse Arrhenius coefficients:	4.81E+09	0.0	9288.0	3213. C7H14-3+CH3O2<=>C7H134-2+CH3OH	4.00E+01	2.9	8609.0
3157. C7H14-2+H<=>C7H131-3+H2	1.73E+05	2.5	2492.0	Reverse Arrhenius coefficients:	1.87E+02	2.7	2735.0
Reverse Arrhenius coefficients:	4.56E+06	2.1	20300.0	3214. C7H14-3+CH3O2<=>C7H133-5+CH3OH	4.00E+01	2.9	8609.0
3158. C7H14-2+H<=>C7H132-4+H2	3.38E+05	2.4	207.0	Reverse Arrhenius coefficients:	2.50E+02	2.7	27230.0
Reverse Arrhenius coefficients:	4.40E+06</td						

Reverse Arrhenius coefficients:	1.00E+11	0.0	8300.0		Reverse Arrhenius coefficients:	1.93E+16	-0.8	32310.0
3226. C7H132+4+HO2<=>C7H13O2-4+OH	9.64E+12	0.0	0.0		3283. C7H15O2-1<=>C7H14+1+HO2	5.04E+38	-8.1	41490.0
Reverse Arrhenius coefficients:	4.27E+15	-1.0	15430.0		3284. C7H15O2-2<=>C7H14+1+HO2	9.29E+29	-6.2	20860.0
3227. C7H132-4+CH3O2<=>C7H13O2-4+CH3O	9.64E+12	0.0	0.0		3285. C7H15O2-2<=>C7H14+2+HO2	5.07E+42	-9.4	42490.0
Reverse Arrhenius coefficients:	4.17E+17	-1.6	20190.0		3286. C7H15O2-3<=>C7H14+2+HO2	9.60E+32	-7.2	17070.0
3228. C7H132+4+C2H5O2<=>C7H13O2-4+C2H5O	9.64E+12	0.0	0.0		3287. C7H15O2-3<=>C7H14+2+HO2	5.04E+38	-8.1	41490.0
Reverse Arrhenius coefficients:	2.73E+14	-0.7	18030.0		3288. C7H15O2-4<=>C7H14+3+HO2	4.71E+28	-5.7	18940.0
3229. C7H132-5<=>C4H8-1+C3H5-S	9.42E+17	-1.5	44260.0		3289. C7H15O2-4<=>C7H14+3+HO2	5.04E+38	-8.1	41490.0
Reverse Arrhenius coefficients:	1.00E+11	0.0	8300.0		3290. C7H15O2-1<=>C7H14O0H1-3	4.71E+28	-5.7	18940.0
3230. C7H132-6<=>C3H6+C4H7I-3	2.19E+14	-0.7	17740.0		3291. C7H15O2-1<=>C7H14O0H1-4	5.04E+38	-8.1	41490.0
Reverse Arrhenius coefficients:	1.00E+11	0.0	8300.0		3292. C7H15O2-1<=>C7H14O0H1-5	3.91E+08	0.0	21650.0
3231. C7H132-7<=>C2H4+CSH92-5	9.79E+17	-1.6	31160.0		3293. C7H15O2-2<=>C7H14O0H2-1	3.00E+11	0.0	29000.0
Reverse Arrhenius coefficients:	1.00E+11	0.0	8300.0		3294. C7H15O2-2<=>C7H14O0H2-3	2.00E+11	0.0	26450.0
3232. C7H133-1<=>C2H4+CSH91-1	1.01E+17	-1.3	43990.0		3295. C7H15O2-2<=>C7H14O0H2-4	2.50E+10	0.0	20450.0
Reverse Arrhenius coefficients:	1.00E+11	0.0	8300.0		3296. C7H15O2-2<=>C7H14O0H2-5	3.12E+09	0.0	18650.0
3233. C7H133-5+HO2<=>C7H13O3-5+OH	9.64E+12	0.0	0.0		3297. C7H15O2-2<=>C7H14O0H2-6	3.91E+08	0.0	21650.0
Reverse Arrhenius coefficients:	1.18E+15	-0.8	15270.0		3298. C7H15O2-3<=>C7H14O0H3-1	3.75E+10	0.0	24000.0
3234. C7H133-5+CH3O2<=>C7H13O3-5+CH3O	9.64E+12	0.0	0.0		3299. C7H15O2-3<=>C7H14O0H3-2	2.00E+11	0.0	26450.0
Reverse Arrhenius coefficients:	1.16E+17	-1.4	20300.0		3300. C7H15O2-3<=>C7H14O0H3-4	2.00E+11	0.0	26450.0
3235. C7H133-5+C2H5O2<=>C7H13O3-5+C2H5O	9.64E+12	0.0	0.0		3301. C7H15O2-3<=>C7H14O0H3-5	2.50E+10	0.0	20450.0
Reverse Arrhenius coefficients:	7.56E+13	-0.5	17870.0		3302. C7H15O2-3<=>C7H14O0H3-6	3.12E+09	0.0	18650.0
3236. C7H133-6<=>C3H6+C4H7I-1	1.35E+16	-0.9	43560.0		3303. C7H15O2-3<=>C7H14O0H3-7	5.86E+08	0.0	25150.0
Reverse Arrhenius coefficients:	1.00E+11	0.0	8300.0		3304. C7H15O2-4<=>C7H14O0H4-1	9.38E+09	0.0	21950.0
3237. C7H133-7<=>C2H4+CSH91-3	2.27E+15	-1.2	18050.0		3305. C7H15O2-4<=>C7H14O0H4-2	5.00E+10	0.0	20450.0
Reverse Arrhenius coefficients:	1.00E+11	0.0	8300.0		3306. C7H15O2-4<=>C7H14O0H4-3	4.00E+11	0.0	26450.0
3238. C7H130-1<=>C2H3CHO-P-C4H9	9.62E+19	-2.0	10850.0		3307. C7H15O2-1+HO2<=>C7H15O2-1+O2	1.75E+10	0.0	-3275.0
Reverse Arrhenius coefficients:	1.00E+11	0.0	9600.0		Reverse Arrhenius coefficients:	3.78E+13	-0.8	34010.0
3239. C7H130-1-3<=>NC4H9CHO+C2H3	1.03E+18	-1.5	23300.0		3308. C7H15O2-2+HO2<=>C7H15O2-2+O2	1.75E+10	0.0	-3275.0
Reverse Arrhenius coefficients:	1.00E+11	0.0	9600.0		Reverse Arrhenius coefficients:	4.50E+13	-0.8	34040.0
3240. C7H1302-4<=>SC3H5CHO+N-C3H7	6.32E+19	-1.9	11130.0		3309. C7H15O2-3+HO2<=>C7H15O2H-3+O2	1.75E+10	0.0	-3275.0
Reverse Arrhenius coefficients:	1.00E+11	0.0	9600.0		Reverse Arrhenius coefficients:	4.50E+13	-0.8	34040.0
3241. C7H1302-4<=>NC3H7CHO+C3H5-S	1.01E+22	-2.5	29190.0		3310. C7H15O2-4+HO2<=>C7H15O2H-4+O2	1.75E+10	0.0	-3275.0
Reverse Arrhenius coefficients:	1.00E+11	0.0	9600.0		Reverse Arrhenius coefficients:	2.40E+12	0.0	10000.0
3242. C7H1303-5<=>C4H7CHO1+C2H5	6.03E+18	-1.6	10450.0		3311. H2O2+C7H15O2-2<=>HO2+C7H15O2H-1	2.40E+12	0.0	10000.0
Reverse Arrhenius coefficients:	1.00E+11	0.0	9600.0		3312. H2O2+C7H15O2-2<=>HO2+C7H15O2H-2	2.40E+12	0.0	10000.0
3243. C7H1303-5<=>C2H5CHO+C4H7I-1	6.42E+21	-2.4	30090.0		Reverse Arrhenius coefficients:	2.40E+12	0.0	10000.0
Reverse Arrhenius coefficients:	1.00E+11	0.0	9600.0		3313. H2O2+C7H15O2-3<=>HO2+C7H15O2H-3	2.40E+12	0.0	10000.0
3244. C7H14-1+OH<=>C2H2O+C6H13-I	1.00E+11	0.0	-4000.0		Reverse Arrhenius coefficients:	2.40E+12	0.0	10000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		3314. H2O2+C7H15O2-4<=>HO2+C7H15O2H-4	2.40E+12	0.0	10000.0
3245. C7H14-1+OH<=>C3H3CHO+C5H11-I	1.00E+11	0.0	-4000.0		Reverse Arrhenius coefficients:	2.40E+12	0.0	10000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		3315. C7H15O2-1+CH3O2<=>C7H15O-1+CH3O-2	1.40E+16	-1.6	1860.0
3246. C7H14-2+OH<=>C3H3CHO+C5H11-I	1.00E+11	0.0	-4000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		3316. C7H15O2-2+CH3O2<=>C7H15O-2+CH3O-2	1.40E+16	-1.6	1860.0
3247. C7H14-2+OH<=>C2H5CHO+P-C4H9	1.00E+11	0.0	-4000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		3317. C7H15O2-3+CH3O2<=>C7H15O-3+CH3O-2	1.40E+16	-1.6	1860.0
3248. C7H14-3+OH<=>C2H5CHO+P-C4H9	1.00E+11	0.0	-4000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		3318. C7H15O2-4+CH3O2<=>C7H15O-4+CH3O-2	1.40E+16	-1.6	1860.0
3249. C7H14-1-O<=>C2H2CHO+C5H11-I	1.00E+11	0.0	-1050.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		3319. C7H15O2-1+C7H15O2-1<=>O2+C7H15O-1+C7H15O-1	1.40E+16	-1.6	1860.0
3250. C7H14-2-O<=>C3H3CHO+C5H10-I	1.00E+11	0.0	-1050.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		3320. C7H15O2-1+C7H15O2-2<=>C7H15O-1+C7H15O-2+O2	1.40E+16	-1.6	1860.0
3251. C7H14-3-O<=>C3H3CHO+C5H10-I	1.00E+11	0.0	-1050.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0		3321. C7H15O2-1+C7H15O2-3<=>C7H15O-1+C7H15O-3+O2	1.40E+16	-1.6	1860.0
3252. C7H14-1-O<=>P-C4H9+C5H5-A	3.17E+21	-1.6	75330.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	1.00E+13	0.0	0.0		3322. C7H15O2-1+C7H15O2-4<=>C7H15O-1+C7H15O-4+O2	1.40E+16	-1.6	1860.0
3253. C7H14-2-C<=C4H7I-3+N-C3H7	3.74E+21	-1.7	75710.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	1.00E+13	0.0	0.0		3323. C7H15O2-1+C7H15O2-2<=>C7H15O-1+C7H15O-2+O2	1.40E+16	-1.6	1860.0
3254. C7H14-3-C<=C5H91-3+C2H5	5.95E+21	-1.9	75790.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	1.00E+13	0.0	0.0		3324. C7H15O2-1<=>C7H15I-1+O2	0.00E+00	0.0	0.0
3255. C7H15O2-1<=>C7H15I-1+O2	2.66E+20	-1.7	35400.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	4.52E+12	0.0	0.0		3325. C7H15O2-2<=>C7H15I-2+O2	1.36E+23	-2.4	37670.0
3256. C7H15O2-2<=>C7H15I-2+O2	7.54E+12	0.0	0.0		Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0
Reverse Arrhenius coefficients:	1.36E+23	-2.4	37670.0		3326. C7H15O2-4<=>C7H15I-2+O2	1.36E+23	-2.4	37670.0
3257. C7H15O2-3<=>C7H15I-3+O2	1.36E+23	-2.4	37670.0		Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0
Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0		3327. C7H15I-1+C7H15I-2<=>C7H15I-1+C7H15I-2+O2	1.36E+23	-2.4	37670.0
3258. C7H15O2-4<=>C7H15I-4+O2	1.36E+23	-2.4	37670.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0		3328. C7H15I-2+C7H15I-3<=>C7H15I-2+C7H15I-3+O2	1.36E+23	-2.4	37670.0
3259. C7H15I-1+C7H15I-2<=>C7H15I-1+C7H15I-2+O2	5.51E+15	-0.7	31790.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	6.35E+13	-0.2	29880.0		3329. C7H15I-2+C7H15I-3<=>C7H15I-2+C7H15I-3+O2	1.36E+23	-2.4	37670.0
3260. C7H15I-1+C7H15I-2<=>C7H15I-1+C7H15I-2+O2	7.00E+12	0.0	-1000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	6.35E+13	-0.2	29880.0		3330. C7H15I-1+C7H15I-2+C7H15I-2+O2	1.36E+23	-2.4	37670.0
3261. C7H15I-1+C7H15I-3<=>C7H15I-1+C7H15I-3+O2	7.00E+12	0.0	-1000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	6.35E+13	-0.2	29880.0		3331. C7H15I-2+C7H15I-3<=>C7H15I-2+C7H15I-3+O2	1.36E+23	-2.4	37670.0
3262. C7H15I-1+C7H15I-4<=>C7H15I-1+C7H15I-4+O2	7.00E+12	0.0	-1000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	6.35E+13	-0.2	29880.0		3332. C7H15I-3+C7H15I-4<=>C7H15I-3+C7H15I-4+O2	1.36E+23	-2.4	37670.0
3263. C7H15I-2+C7H15I-5<=>C7H15I-2+C7H15I-5+O2	7.00E+12	0.0	-1000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	9.69E+15	-0.8	32160.0		3333. C7H15I-2+C7H15I-6<=>C7H15I-2+C7H15I-6+O2	1.36E+23	-2.4	37670.0
3264. C7H15I-2+C7H15I-5<=>C7H15I-2+C7H15I-5+O2	7.00E+12	0.0	-1000.0		Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
Reverse Arrhenius coefficients:	5.51E+15	-0.7	31790.0		3334. C7H15I-1+C7H15I-7<=>C7H15I-1+C7H15I-7+O2	1.36E+23	-2.4	37670.0
3265. C7H15I-2+C7H15I-3<=>C7H15I-2+C7H15I-3+O2	7.00E+12	0.0	-1000.0		Reverse Arrhenius coefficients:	1.00E+11	0.0	11900.0
Reverse Arrhenius coefficients:	5.51E+15	-0.7	31790.0		3335. C7H15I-2+C7H15I-4<=>C7H15I-2+C7H15I-4+O2	1.36E+23	-2.4	37670.0
3266. C7H15I-2+C7H15I-4<=>C7H15I-2+C7H15I-4+O2	7.00E+12	0.0	-1000.0		Reverse Arrhenius coefficients:	1.00E+11	0.0	11900.0
Reverse Arrhenius coefficients:	5.51E+15	-0.7	31790.0		3336. C7H15I-4+C7H15I-5<=>C7H15I-4+C7H15I-5+O2	1.36E+23	-2.4	37670.0
3267. C7H15I-3+C7H15I-4<=>C7H15I-3+C7H15I-4+O2	7.00E+12	0.0	-1000.0		Reverse Arrhenius coefficients:	1.00E+11	0.0	11900.0
Reverse Arrhenius coefficients:	5.51E+15	-0.7	31790.0		3337. C7H15I-4+HO2=C7H15O0H1-2	2.50E+03	2.5	11200.0
3268. C7H15I-3+C7H15I-5<=>C7H15I-3+C7H15I-5+O2	7.00E+12	0.0	-1000.0		3338. C7H15I-4+HO2=C7H15O0H2-1	2.70E+03	2.5	10500.0
Reverse Arrhenius coefficients:	5.51E+15	-0.7	31790.0		33			

Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3347. C7H14OOH2-1<=>C7H14O1-2+OH	6.00E+11	0.0	22000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3348. C7H14OOH2-3<=>C7H14O2-3+OH	6.00E+11	0.0	22000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3349. C7H14OOH2-4<=>C7H14O2-4+OH	7.50E+10	0.0	15250.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3350. C7H14OOH2-5<=>C7H14O2-5+OH	9.38E+09	0.0	7000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3351. C7H14OOH2-6<=>C7H14O2-6+OH	1.17E+09	0.0	1800.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3352. C7H14OOH3-1<=>C7H14O1-3+OH	7.50E+10	0.0	15250.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3353. C7H14OOH3-2<=>C7H14O2-3+OH	6.00E+11	0.0	22000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3354. C7H14OOH3-4<=>C7H14O3-4+OH	6.00E+11	0.0	22000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3355. C7H14OOH3-5<=>C7H14O3-5+OH	7.50E+10	0.0	15250.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3356. C7H14OOH3-6<=>C7H14O2-5+OH	9.38E+09	0.0	7000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3357. C7H14OOH3-7<=>C7H14O1-5+OH	1.17E+09	0.0	1800.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3358. C7H14OOH4-1<=>C7H14O1-4+OH	9.38E+09	0.0	7000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3359. C7H14OOH4-2<=>C7H14O2-4+OH	7.50E+10	0.0	15250.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3360. C7H14OOH4-3<=>C7H14O3-4+OH	6.00E+11	0.0	22000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3361. C7H14OOH1-3<=>OH+CH2O+C6H12-1	2.15E+09	1.2	30370.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3362. C7H14OOH2-4<=>OH+CH3CHO+CSH1-1	1.55E+12	0.6	30090.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3363. C7H14OOH3-1<=>OH+NC4H9CHO+CH24	8.18E+13	-0.1	31330.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3364. C7H14OOH3-5<=>OH+CH25CHO+CH48-1	2.66E+13	0.1	30430.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3365. C7H14OOH4-2<=>OH+NC3H7CHO+CH3H6	6.19E+13	0.1	30840.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3366. C7H14OOH1-3<=>C4H7OOH1-4+N-C3H7	1.61E+12	0.5	27740.0
Reverse Arrhenius coefficients:	2.20E+03	2.5	6130.0
3367. C7H14OOH1-4<=>C5H10-1+C2H4+H2O	1.45E+11	0.7	30820.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3368. C7H14OOH1-4<=>C5H9OOH1-5+C2H5	1.72E+12	0.5	27900.0
Reverse Arrhenius coefficients:	2.20E+03	2.5	6130.0
3369. C7H14OOH2-4<=>C5H9OOH1-4+C2H5	4.08E+12	0.3	29230.0
Reverse Arrhenius coefficients:	2.20E+03	2.5	6130.0
3370. C7H14OOH2-5<=>C4H8-1+C3H6OOH2-1	6.86E+13	0.0	31380.0
Reverse Arrhenius coefficients:	2.20E+03	2.5	6130.0
3371. C7H14OOH2-5<=>C6H11-1+OHOH1-5+CH3	7.42E+10	0.8	30260.0
Reverse Arrhenius coefficients:	2.20E+03	2.5	6130.0
3372. C7H14OOH3-5<=>C6H11OOH1-4+CH3	7.42E+10	0.8	30260.0
Reverse Arrhenius coefficients:	2.20E+03	2.5	6130.0
3373. C7H14OOH3-6<=>C4H8OOH2-1+C3H6	4.58E+11	0.6	29170.0
Reverse Arrhenius coefficients:	2.20E+03	2.5	6130.0
3374. C7H14OOH4-1<=>C5H10OOH2-1+C2H4	1.64E+12	0.4	29320.0
Reverse Arrhenius coefficients:	2.20E+03	2.5	6130.0
3375. C7H14OOH1-20<=>C7H14OOH1-2+O2	1.37E+23	-2.4	37640.0
Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0
3376. C7H14OOH1-30<=>C7H14OOH1-3+O2	1.37E+23	-2.4	37640.0
Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0
3377. C7H14OOH1-40<=>C7H14OOH1-4+O2	1.37E+23	-2.4	37640.0
Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0
3378. C7H14OOH1-50<=>C7H14OOH1-5+O2	1.37E+23	-2.4	37640.0
Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0
3379. C7H14OOH2-102<=>C7H14OOH2-1+O2	3.32E+20	-1.6	35280.0
Reverse Arrhenius coefficients:	4.52E+12	0.0	0.0
3380. C7H14OOH2-302<=>C7H14OOH2-3+O2	1.39E+23	-2.4	37600.0
Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0
3381. C7H14OOH2-402<=>C7H14OOH2-4+O2	1.39E+23	-2.4	37600.0
Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0
3382. C7H14OOH2-502<=>C7H14OOH2-5+O2	1.39E+23	-2.4	37600.0
Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0
3383. C7H14OOH2-602<=>C7H14OOH2-6+O2	1.39E+23	-2.4	37600.0
Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0
3384. C7H14OOH3-102<=>C7H14OOH3-1+O2	3.32E+20	-1.6	35280.0
Reverse Arrhenius coefficients:	4.52E+12	0.0	0.0
3385. C7H14OOH3-202<=>C7H14OOH3-2+O2	1.39E+23	-2.4	37600.0
Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0
3386. C7H14OOH3-402<=>C7H14OOH3-4+O2	1.39E+23	-2.4	37600.0
Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0
3387. C7H14OOH3-502<=>C7H14OOH3-5+O2	1.39E+23	-2.4	37600.0
Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0
3388. C7H14OOH3-602<=>C7H14OOH3-6+O2	1.39E+23	-2.4	37600.0
Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0
3389. C7H14OOH3-702<=>C7H14OOH3-7+O2	3.32E+20	-1.6	35280.0
Reverse Arrhenius coefficients:	4.52E+12	0.0	0.0
3390. C7H14OOH4-102<=>C7H14OOH4-1+O2	1.67E+20	-1.6	35280.0
Reverse Arrhenius coefficients:	4.52E+12	0.0	0.0
3391. C7H14OOH4-202<=>C7H14OOH4-2+O2	6.97E+22	-2.4	37600.0
Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0
3392. C7H14OOH4-302<=>C7H14OOH4-3+O2	6.97E+22	-2.4	37600.0
Reverse Arrhenius coefficients:	7.54E+12	0.0	0.0
3393. C7H14OOH1-20<=>NC7KET1+2+OH	2.00E+11	0.0	26000.0
3394. C7H14OOH1-30<=>NC7KET1+3+OH	2.50E+10	0.0	21000.0
3395. C7H14OOH1-40<=>NC7KET1+4+OH	3.12E+09	0.0	18950.0
3396. C7H14OOH1-50<=>NC7KET1+5+OH	3.91E+08	0.0	22150.0
3397. C7H14OOH2-102<=>NC7KET21+OH	1.00E+11	0.0	23450.0
3398. C7H14OOH2-302<=>NC7KET23+OH	1.00E+11	0.0	23450.0
3399. C7H14OOH2-402<=>NC7KET24+OH	1.25E+10	0.0	17450.0
3400. C7H14OOH2-502<=>NC7KET25+OH	1.56E+09	0.0	15650.0
3401. C7H14OOH2-602<=>NC7KET26+OH	1.95E+08	0.0	18650.0
3402. C7H14OOH3-102<=>NC7KET31+OH	1.25E+10	0.0	17450.0
3403. C7H14OOH3-202<=>NC7KET32+OH	1.00E+11	0.0	23450.0
3404. C7H14OOH3-402<=>NC7KET34+OH	1.00E+11	0.0	23450.0
3405. C7H14OOH3-502<=>NC7KET35+OH	1.25E+10	0.0	17450.0
3406. C7H14OOH3-602<=>NC7KET36+OH	1.56E+09	0.0	15650.0
3407. C7H14OOH3-702<=>NC7KET37+OH	1.95E+08	0.0	18650.0
3408. C7H14OOH4-102<=>NC7KET41+OH	1.56E+09	0.0	15650.0
3409. C7H14OOH4-202<=>NC7KET42+OH	1.25E+10	0.0	17450.0
3410. C7H14OOH4-302<=>NC7KET43+OH	1.00E+11	0.0	23450.0
3411. NC7KET12<=>NC5H11CHO+HCO+OH	1.00E+16	0.0	39000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3412. NC7KET13<=>NC4H9CHO+CH2CHO+OH	1.00E+16	0.0	39000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3413. NC7KET14<=>NC3H7CHO+CH2CH2CHO+OH	1.00E+16	0.0	
39000.0			
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3414. NC7KET15<=>C2H5CHO+C3H6CHO-1+OH	1.00E+16	0.0	39000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3415. NC7KET21<=>CH2O+NC5H11CO+OH	1.00E+16	0.0	39000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3416. NC7KET23<=>NC4H9CHO+CH3CO+OH	1.00E+16	0.0	39000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3417. NC7KET24<=>NC3H7CHO+CH3COCH2+OH	1.00E+16	0.0	
39000.0			
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3418. NC7KET25<=>C2H5CHO+CH2CH2COCH3+OH	1.00E+16	0.0	
39000.0			
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3419. NC7KET26<=>CH3CHO+CH36COCH3-1+OH	1.00E+16	0.0	39000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3420. NC7KET31<=>CH2O+NC4H9COCH2+OH	1.00E+16	0.0	39000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3421. NC7KET32<=>CH3CHO+NC4H9CO+OH	1.00E+16	0.0	39000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3422. NC7KET34<=>NC3H7CHO+CH2H5CO+OH	1.00E+16	0.0	39000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3423. NC7KET35<=>C2H5CHO+CH2H5COCH2+OH	1.00E+16	0.0	39000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3424. NC7KET46<=>CH3CHO+CH3H7COCH2+OH	1.00E+16	0.0	
39000.0			
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3425. NC7KET37<=>CH2O+C3H6COCH2H5-1+OH	1.00E+16	0.0	39000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3426. NC7KET41<=>CH2O+NC3H7COC2H4P+OH	1.00E+16	0.0	39000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3427. NC7KET42<=>CH3CHO+NC3H7COCH2+OH	1.00E+16	0.0	
39000.0			
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3428. NC7KET43<=>C2H5CHO+NC3H7CO+OH	1.00E+16	0.0	39000.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3429. C7H14O1-2+OH<=>C4H9+CH2H3CHO+H2O	2.50E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3430. C7H14O1-3+OH<=>C6H12-1+HCO+H2O	2.50E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3431. C7H14O1-4+OH<=>C5H10-1+CH2CHO+H2O	2.50E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3432. C7H14O1-5+OH<=>C4H8-1+H2O	2.50E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3433. C7H14O2-6+OH<=>C2H2O+C3H6+H2O	2.50E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3434. C7H14O3-4+OH<=>C2H5CO+C2H5+H2O	2.50E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3435. C7H14O3-5+OH<=>C2H5CO+C4H8-1+H2O	2.50E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3436. C7H14O2-6+OH<=>C2H2O+C3H6+H2O	2.50E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3437. C7H14O2-7+OH<=>C2H2O+C5H11-1+H2O	2.50E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3438. C7H14O2-8+OH<=>C2H2O+C5H11-2+H2O	2.50E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3439. C7H14O1-2+OH<=>C4H8-1+H2O	2.50E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3440. C7H14O1-3+OH<=>C2H4+NC4H9CO+H2O	2.50E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3441. C7H14O1-4+OH<=>C2H4+NC3H7COCH2+H2O	2.50E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3442. C7H14O1-5+OH<=>C2H4+NC3H7COCH2+H2O	2.50E+12	0.0	0.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3443. C7H14O2-3+OH2<=>C2H3COCH3-N-C3H7+H2O	5.00E+12	0.0	17700.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3451. C7H14O1-4+H2O<=>C5H10-1+CH2CHO+H2O	5.00E+12	0.0	17700.0
Reverse Arrhenius coefficients:	0.00E+00	0.0	0.0
3452. C7H14O1-5+H2O<=>C4H8-1+CH2CH2CHO+H2O	5.00E+12	0.0	

3463. C7H14O2-3+HO<=>CH3CHCO+P-C4H9+H2O2 17700.0	5.00E+12 0.0		
Reverse Arhenius coefficients:	0.00E+00 0.0	0.0	
3464. C7H14O2-4+HO2<=>C3H6+NC3H7CO+H2O2 17700.0	5.00E+12 0.0	17700.0	
Reverse Arhenius coefficients:	0.00E+00 0.0	0.0	
3465. C7H14O2-5+HO2<=>C3H6+C2H5COCH2+H2O2 17700.0	5.00E+12 0.0		
Reverse Arhenius coefficients:	0.00E+00 0.0	0.0	
3466. C7H14O2-6+HO2<=>CH3CHO+C5H9I-4+H2O2 17700.0	5.00E+12 0.0	17700.0	
Reverse Arhenius coefficients:	0.00E+00 0.0	0.0	
3467. C7H14O3-4+HO2<=>C2H5CHCO+N-C3H7+H2O2 17700.0	5.00E+12 0.0		
Reverse Arhenius coefficients:	0.00E+00 0.0	0.0	
3468. C7H14O3-5+HO2<=>C2H5CHCO+C4H7-1+H2O2 17700.0	5.00E+12 0.0		
Reverse Arhenius coefficients:	0.00E+00 0.0	0.0	
3469. C7H14OH-1<=>C7H14-1+OH 17050.0	5.43E+14 -0.5	27830.0	
Reverse Arhenius coefficients:	1.00E+12 0.0	-1042.0	
3470. O2C7H14OH-1<=>C7H14OH-1+O2 17050.0	2.98E+21 -2.0	37820.0	
Reverse Arhenius coefficients:	2.00E+12 0.0	0.0	
3471. O2C7H14OH-1<=>NC5H11CHO+CH2O+OH 17050.0	2.50E+10 0.0	18860.0	
Reverse Arhenius coefficients:	0.00E+00 0.0	0.0	
3472. C7H14OH-2<=>C7H14-2+OH 17050.0	1.04E+16 -1.0	29400.0	
Reverse Arhenius coefficients:	1.00E+12 0.0	-1042.0	
3473. O2C7H14OH-2<=>C7H14OH-2+O2 17050.0	4.78E+21 -2.1	37860.0	
Reverse Arhenius coefficients:	2.00E+12 0.0	0.0	
3474. O2C7H14OH-1<=>NC4H9CHO+CH3CHO+OH 18860.0	2.50E+10 0.0		
Reverse Arhenius coefficients:	0.00E+00 0.0	0.0	
3475. C7H14OH-3<=>C7H14-3+OH 17050.0	7.77E+15 -0.9	29490.0	
Reverse Arhenius coefficients:	1.00E+12 0.0	-1042.0	
3476. O2C7H14OH-3<=>C7H14OH-3+O2 17050.0	4.78E+21 -2.1	37860.0	
Reverse Arhenius coefficients:	2.00E+12 0.0	0.0	
3477. O2C7H14OH-3<=>NC3H7CHO+C2H5CHO+OH 18860.0	2.50E+10 0.0		
Reverse Arhenius coefficients:	0.00E+00 0.0	0.0	
3478. NC5H11CHO+O<=>NC5H11CO+OH 17050.0	2.00E+13 0.5	42200.0	
Reverse Arhenius coefficients:	1.00E+07 0.0	40000.0	
3479. NC5H11CHO+OH<=>NC5H11CO+H2O 17050.0	2.69E+10 0.8	-340.0	
Reverse Arhenius coefficients:	1.74E+10 0.8	31200.0	
3480. NC5H11CHO+H<=>NC5H11CO+H2 17050.0	4.00E+13 -0.0	4200.0	
Reverse Arhenius coefficients:	1.80E+13 0.0	24000.0	
3481. NC5H11CHO+O<=>NC5H11CO+OH 17050.0	5.00E+12 0.0	1790.0	
Reverse Arhenius coefficients:	1.00E+12 0.0	190000.0	
3482. NC5H11CHO+H2O<=>NC5H11CO+H2O2 17050.0	2.80E+12 0.0	13600.0	
Reverse Arhenius coefficients:	1.00E+12 0.0	100000.0	
3483. NC5H11CHO+CH3<=>NC5H11CO+CH4 17050.0	1.70E+12 0.0	8440.0	
Reverse Arhenius coefficients:	1.50E+13 0.0	28000.0	
3484. NC5H11CHO+CH3O<=>NC5H11CO+CH3OH 17050.0	1.15E+11 0.0	1280.0	
Reverse Arhenius coefficients:	3.00E+11 0.0	18000.0	
3485. NC5H11CHO+CH3O2<=>NC5H11CO+CH3O2H 17050.0	1.00E+12 0.0		
Reverse Arhenius coefficients:	2.50E+06 0.0	10000.0	
3486. NC5H11CHO+OH<=>C5H10CHO-1+H2O 17050.0	5.27E+09 1.0	1586.0	
Reverse Arhenius coefficients:	1.07E+09 1.0	21010.0	
3487. NC5H11CHO+OH<=>C5H10CHO-2+H2O 17050.0	4.67E+07 1.6	-35.0	
Reverse Arhenius coefficients:	1.75E+06 1.9	23880.0	
3488. NC5H11CHO+OH<=>C5H10CHO-3+H2O 17050.0	4.67E+07 1.6	-35.0	
Reverse Arhenius coefficients:	1.75E+06 1.9	23880.0	
3489. NC5H11CHO+OH<=>C5H10CHO-4+H2O 17050.0	4.67E+07 1.6	-35.0	
Reverse Arhenius coefficients:	1.75E+06 1.9	23880.0	
3490. NC5H11CHO+OH<=>C5H10CHO-5+H2O 17050.0	4.67E+07 1.6	-35.0	
Reverse Arhenius coefficients:	3.32E+09 1.2	30840.0	
3491. NC5H11CHO<=>C5H11-1+CO 17050.0	1.00E+11 0.0	9600.0	
Reverse Arhenius coefficients:	1.00E+11 0.0	0.0	
3492. NC5H11CHO+H2O<=>C5H10CHO-1+H2O2 17050.0	2.76E+04 2.5	16480.0	
Reverse Arhenius coefficients:	3.33E+04 2.2	44420.0	
3493. NC5H11CHO+H2O<=>C5H10CHO-2+H2O2 17050.0	1.48E+04 2.6	13910.0	
Reverse Arhenius coefficients:	3.28E+03 2.5	63620.0	
3494. NC5H11CHO+H2O<=>C5H10CHO-3+H2O2 17050.0	1.48E+04 2.6	13910.0	
Reverse Arhenius coefficients:	3.28E+03 2.5	63620.0	
3495. NC5H11CHO+H2O<=>C5H10CHO-4+H2O2 17050.0	1.48E+04 2.6	13910.0	
Reverse Arhenius coefficients:	3.28E+03 2.5	63620.0	
3496. NC5H11CHO+H2O<=>C5H10CHO-5+H2O2 17050.0	2.95E+04 2.6	13910.0	
Reverse Arhenius coefficients:	1.24E+07 1.9	13320.0	
3497. NC5H11CHO+CH3O2<=>C5H10CHO-1+CH3O2H 17050.0	6.03E+12 0.0		
Reverse Arhenius coefficients:	2.99E+13 -0.5	6617.0	
3498. NC5H11CHO+CH3O2<=>C5H10CHO-2+CH3O2H 17050.0	1.99E+12 0.0		
Reverse Arhenius coefficients:	1.82E+12 -0.3	8784.0	
3499. NC5H11CHO+CH3O2<=>C5H10CHO-3+CH3O2H 17050.0	1.99E+12 0.0		
Reverse Arhenius coefficients:	1.82E+12 -0.3	8784.0	
3500. NC5H11CHO+CH3O2<=>C5H10CHO-4+CH3O2H 17050.0	1.99E+12 0.0		
Reverse Arhenius coefficients:	1.82E+12 -0.3	8784.0	
3501. NC5H11CHO+CH3O2<=>C5H10CHO-5+CH3O2H 17050.0	3.98E+12 0.0		
Reverse Arhenius coefficients:	6.90E+15 -0.9	15740.0	
3502. C5H10CHO-1<=>C2H4+C3H6CO-1 17050.0	2.68E+18 -1.6	30410.0	
Reverse Arhenius coefficients:	2.50E+11 0.0	7800.0	
3503. C5H10CHO-2<=>C3H6+CH2CH2CHO 17050.0	9.38E+17 -1.3	31970.0	
Reverse Arhenius coefficients:	1.00E+11 0.0	7800.0	
3504. C5H10CHO-3<=>C4H8-1+CH2CHO 17050.0	6.27E+16 -1.4	25990.0	
Reverse Arhenius coefficients:	1.00E+11 0.0	7800.0	
3505. C5H10CHO-3<=>C4H7CHO-1+CH3 17050.0	2.37E+14 -0.6	31320.0	
Reverse Arhenius coefficients:	1.00E+11 0.0	7800.0	
3506. C5H10CHO-4<=>AC3H5CHO+C2H5 17050.0	7.19E+17 -1.4	33230.0	
Reverse Arhenius coefficients:	1.00E+11 0.0	7800.0	
3507. C5H10CHO-4<=>C5H10-1+HCO 17050.0	1.06E+14 -0.4	26330.0	
Reverse Arhenius coefficients:	1.00E+11 0.0	7800.0	
3508. C5H10CHO-5<=>C2H3CHO+N-C3H7 17050.0	1.56E+19 -1.5	33310.0	
Reverse Arhenius coefficients:	1.00E+11 0.0	7800.0	
3509. C4H7CHO-1+OH<=>C4H7CO1-4+H2O 17050.0	3.37E+12 0.0	-616.0	
Reverse Arhenius coefficients:	2.40E+12 0.0	30940.0	
3510. C4H7CHO-1+OH<=>C4H6CHO1-4+H2O 17050.0	2.08E+06 2.0	-298.0	
Reverse Arhenius coefficients:	1.19E+08 1.7	34980.0	
3511. C4H7CHO-1+OH<=>C4H6CHO1-4+H2O 17050.0	4.67E+07 1.6	-35.0	
Reverse Arhenius coefficients:	1.50E+09 1.3	28900.0	
3512. C4H7CHO-1+OH<=>C3H3CHO+CH2CH2CHO 17050.0	1.00E+11 0.0	0.0	
Reverse Arhenius coefficients:	5.34E+06 1.0	19260.0	
3513. C4H7CHO-1+OH2<=>C4H7CO1-4+H2O2 17050.0	1.00E+12 0.0	11920.0	
Reverse Arhenius coefficients:	4.22E+12 -0.3	12010.0	
3514. C4H7CHO1-4+HO2<=>C4H6CHO1-43+H2O2 17050.0	9.64E+03 2.6	13910.0	
Reverse Arhenius coefficients:	3.26E+06 2.0	17730.0	
3515. C4H7CHO1-4+HO2<=>C4H6CHO1-44+H2O2 17050.0	1.48E+04 2.6	13910.0	
Reverse Arhenius coefficients:	2.82E+06 2.0	11380.0	
3516. C4H7CHO1-4+CH3O2<=>C4H7CO1-4+CH3O2H 17050.0	2.80E+12 0.0		
Reverse Arhenius coefficients:	4.86E+13 -0.5	12970.0	
3517. C4H7CHO1-4+CH3O2<=>C4H6CHO1-43+CH3O2H 17050.0	1.99E+12 0.0		
Reverse Arhenius coefficients:	2.77E+15 -0.8	20150.0	
3518. C4H7CHO1-4+CH3O2<=>C4H6CHO1-44+CH3O2H 17050.0	1.99E+12 0.0		
Reverse Arhenius coefficients:	1.56E+15 -0.8	13800.0	
3519. C4H7CO1-4<=>C4H7-1+CO 17050.0	7.37E+18 -1.8	15230.0	
Reverse Arhenius coefficients:	1.50E+11 0.0	4810.0	
3520. C4H6CHO1-4<=>C4H6-HCO 17050.0	4.83E+15 -0.8	33540.0	
Reverse Arhenius coefficients:	1.00E+11 0.0	7800.0	
3521. C4H6CHO1-4<=>C2H3CHO+C2H3 17050.0	2.12E+14 -0.4	37160.0	
Reverse Arhenius coefficients:	1.00E+11 0.0	7800.0	
3522. NC4H9COCH3-OH<=>C4H8COCH3-1+H2O 17050.0	2.06E-07 1.7	753.0	
Reverse Arhenius coefficients:	4.28E+06 1.7	20190.0	
3523. NC4H9COCH3-OH<=>C4H8COCH3-2+H2O 17050.0	3.62E-07 1.6	-247.0	
Reverse Arhenius coefficients:	3.07E+05 2.0	21630.0	
3524. NC4H9COCH3-OH<=>C4H8COCH3-3+H2O 17050.0	3.62E-07 1.6	-247.0	
Reverse Arhenius coefficients:	3.07E+05 2.0	21630.0	
3525. NC4H9COCH3-OH<=>C4H8COCH3-4+H2O 17050.0	8.45E+11 0.0	-228.0	
Reverse Arhenius coefficients:	1.63E+13 -0.2	28640.0	
3526. NC4H9COCH3-OH<=>NC4H9COCH2+H2O 17050.0	5.10E+11 0.0	1192.0	
Reverse Arhenius coefficients:	6.79E+13 -0.7	27680.0	
3527. NC4H9COCH3+HO2<=>C4H8COCH3-1+H2O2 17050.0	2.38E+04 2.5		
Reverse Arhenius coefficients:	2.93E+04 2.2	4462.0	
3528. NC4H9COCH3+HO2<=>C4H8COCH3-2+H2O2 17050.0	5.60E+12 0.0		
Reverse Arhenius coefficients:	2.82E+11 0.1	8112.0	
3529. NC4H9COCH3+HO2<=>C4H8COCH3-3+H2O2 17050.0	5.60E+12 0.0		
Reverse Arhenius coefficients:	2.82E+11 0.1	8112.0	
3530. NC4H9COCH3+HO2<=>C4H8COCH3-4+H2O2 17050.0	2.00E+11 0.0	8698.0	
Reverse Arhenius coefficients:	2.29E+13 -0.6	6100.0	
3531. NC4H9COCH3+HO2<=>NC4H9COCH2+H2O2 17050.0	2.38E+04 2.5		
Reverse Arhenius coefficients:	1.52E+13 -0.5	6627.0	
3532. NC4H9COCH3+CH3O2<=>C4H8COCH3-2+CH3O2H 17050.0	1.99E+12 0.0		
Reverse Arhenius coefficients:	4.12E+11 -0.1	6744.0	
3533. NC4H9COCH3+CH3O2<=>C4H8COCH3-3+CH3O2H 17050.0	9.43E+14 -0.7	11950.0	
Reverse Arhenius coefficients:	9.43E+14 -0.7	11950.0	
3534. NC4H9COCH3+CH3O2<=>NC4H9COCH2+CH3O2H 17050.0	3.01E+12 0.0		
Reverse Arhenius coefficients:	9.77E+15 -1.2	11880.0	
3535. C4H8COCH3-1<=>C2H2COCH3+C2H4 17050.0	1.13E+18 -1.6	30910.0	
Reverse Arhenius coefficients:	1.00E+11 0.0	8300.0	
3536. C4H8COCH3-2<=>C3H6+CH3COCH2 17050.0	3.18E+15 -0.8	26220.0	
Reverse Arhenius coefficients:	1.00E+11 0.0	8300.0	
3537. C4H8COCH3-3<=>C4H8-1+CH3CO 17050.0	1.71E+18 -1.6	28250.0	
Reverse Arhenius coefficients:	1.00E+11 0.0	9800.0	
3538. C4H8COCH3-4<=>C2H3COCH3+C2H5 17050.0	4.69E+19 -1.6	33750.0	
Reverse Arhenius coefficients:	1.00E+11 0.0	8300.0	
3539. NC4H9COCH2+CH3O2<=>C4H8COCH2+C2H2O 17050.0	1.55E+18 -1.4	43140.0	
Reverse Arhenius coefficients:	1.00E+11 0.0	11600.0	
3540. C4H7HO1-4<=>C2H2+CH2COH 17050.0	1.00E+11 0.0	47040.0	
Reverse Arhenius coefficients:	2.00E+13 0.0	0.0	
3541. C5H9OOH1-5<=>C5H9O1-4+OH 17050.0	1.18E+20 -1.4	46050.0	
Reverse Arhenius coefficients:	2.00E+13 0.0	0.0	
3542. C5H9OOH1-5<=>C5H9O1-4+OH 17050.0	1.59E+20 -1.5	46990.0	
Reverse Arhenius coefficients:	2.00E+13 0.0	0.0	
3543. C5H9OOH1-5<=>C5H9O1-4+OH 17050.0	1.23E+20 -1.4	46050.0	
Reverse Arhenius coefficients:	2.00E+13 0.0	0.0	
3544. C5H9OOH1-5<=>C5H9O1-5+OH 17050.0	1.18E+20 -1.4	46050.0	
Reverse Arhenius coefficients:	2.00E+13 0.0	0.0	
3545. C5H9OOH1-4<=>C5H9O1-4+OH 17050.0	5.00E+10 0.0	9600.0	
Reverse Arhenius coefficients:	1.11E+17 -1.2	17960.0	
3546. C5H9OOH1-5<=>C5H9O1-5+OH 17050.0	4.31E-17 -1.3	17940.0	
Reverse Arhenius coefficients:	1.00E+11 0.0	9600.0	
3547. C5H9O1-4<=>C2H2+C3H5-A 17050.0	7.27E+20 -2.1	18870.0	
Reverse Arhenius coefficients:	1.00E+11 0.0	9600.0	
3548. C5H9O1-4<=>C2H5COH+C3H5-A 17050.0	1.21E+21 -2.5	5641.0	
Reverse Arhenius coefficients:	5.00E+10 0.0	9600.0	
3549. C5H9O1-5<=>C4H7CHO1-4+CH3 17050.0			

3564. C4H7CHO1-1+CH3O2<=>C4H6CHO1-14+CH3O2H	6.03E+12	0.0	3638. C6H111-5+O2=C6H111O2-5	7.54E+12	0.0	0.0
19380.0 Reverse Arrhenius coefficients:	2.98E+13 -0.5	6627.0	3639. C6H111-6+O2=C6H111O2-6	4.52E+12	0.0	0.0
3565. C4H7CHO1-1+CH3O2<=>C4H6CHO1-13+CH3O2H	1.99E+12	0.0	3640. C6H112-4+O2=C6H113O2-2	2.00E+12	0.0	0.0
17050.0 Reverse Arrhenius coefficients:	1.95E+15 -0.7	20100.0	3641. C6H112-4+O2=C6H112O2-4	2.00E+12	0.0	0.0
3566. C4H7CO1-1<->C4H7-1+CO	8.51E+20 -2.1	40320.0	3642. C6H112-5+O2=C6H112O2-5	7.54E+12	0.0	0.0
Reverse Arrhenius coefficients:	1.50E+11 0.0	4810.0	3643. C6H112-6+O2=C6H112O2-6	4.52E+12	0.0	0.0
3567. C4H6CHO1-14<->C2H4+CHCHCHO	9.05E+16 -1.3	46870.0	3644. C6H113-1+O2=C6H113O2-1	4.52E+12	0.0	0.0
Reverse Arrhenius coefficients:	8.00E+10 0.0	11400.0	3645. C6H111O2-3->C6H101-3+HO2	1.00E+39 -8.1	40500.0	
3568. C4H6CHO1-13<->C4H6+HCO	8.95E+17 -1.3	46230.0	3646. C6H111O2-4->C6H101-3+HO2	2.04E+38 -8.1	38500.0	
Reverse Arrhenius coefficients:	8.00E+10 0.0	11400.0	3647. C6H111O2-5->C6H101-4+HO2	1.00E+39 -8.1	40500.0	
3569. NC3H7COOC2H5-OH<->C3H6COC2H5-1+H2O	2.06E+07 1.7	753.0	3648. C6H111O2-6->C6H101-5+HO2	1.00E+39 -8.1	40500.0	
Reverse Arrhenius coefficients:	5.17E+06 1.7	20220.0	3649. C6H111O2-5->C6H101-5+HO2	1.01E+43 -9.4	41500.0	
3570. NC3H7COOC2H5-OH<->C3H6COC2H5-2+H2O	3.62E+07 1.6	-247.0	3650. C6H112O2-4->C6H101-3+HO2	5.04E+38 -8.1	40500.0	
Reverse Arrhenius coefficients:	7.23E+05 1.9	21760.0	3651. C6H112O2-5->C6H102-4+HO2	1.04E+38 -8.1	37500.0	
3571. NC3H7COOC2H5-OH<->C3H6COC2H5-3+H2O	8.45E+11 0.0	-228.0	3652. C6H112O2-6->C6H101-4+HO2	5.04E+38 -8.1	40500.0	
Reverse Arrhenius coefficients:	3.31E+13 -0.3	28740.0	3653. C6H113O2-2->C6H101-3+HO2	5.08E+42 -9.4	41500.0	
3572. NC3H7COOC2H5-OH<->NC3H7COC2H4P+H2O	5.10E+11 0.0	1192.0	3654. C6H113O2-1->C6H101-3+HO2	1.04E+38 -8.1	37500.0	
Reverse Arrhenius coefficients:	1.28E+11 0.0	20660.0	3655. C6H111O2-3->C6H101OHOH-3	2.00E+11 0.0	26450.0	
3573. NC3H7COC2H5+HO2<->C3H6COC2H5-1+H2O	8.45E+11 0.0	228.0	3656. C6H111O2-3-C6H101OHOH-3	2.50E+10 0.0	20450.0	
Reverse Arrhenius coefficients:	3.31E+13 -0.3	28740.0	3657. C6H111O2-3-C6H101OHOH-3	9.38E-09 0.0	21950.0	
3574. NC3H7COC2H5+HO2<->C3H6COC2H5-1+H2O	2.38E+04 2.5	16490.0	3658. C6H111O2-4-C6H101OHOH-3	2.00E+11 0.0	24500.0	
Reverse Arrhenius coefficients:	3.54E+04 2.2	4492.0	3659. C6H111O2-4-C6H101OHOH-5	2.00E+11 0.0	26450.0	
3575. NC3H7COC2H5+H2O<->C3H6COC2H5-2+H2O	5.60E+12 0.0	17700.0	3660. C6H111O2-4-C6H101OHOH-6	3.75E+10 0.0	24000.0	
Reverse Arrhenius coefficients:	6.65E+11 -0.1	8242.0	3661. C6H111O2-5-C6H101OHOH-5	2.50E+10 0.0	18450.0	
3576. NC3H7COC2H5+H2O<->C3H6COC2H5-3+H2O	2.00E+11 0.0	8698.0	3662. C6H111O2-5-C6H101OHOH-4	2.00E+11 0.0	26450.0	
Reverse Arrhenius coefficients:	4.65E+13 -0.7	6200.0	3663. C6H111O2-5-C6H101OHOH-6	3.00E+11 0.0	29000.0	
3577. NC3H7COC2H5+H2O<->NC3H7COC2H4P+H2O	2.38E+04 2.5	14690.0	3664. C6H111O2-6-C6H101OHOH-3	3.12E+09 0.0	16650.0	
Reverse Arrhenius coefficients:	3.54E+04 2.2	2692.0	3665. C6H111O2-6-C6H101OHOH-4	2.50E+10 0.0	20450.0	
3578. NC3H7COC2H5+H2O<->NC3H7COC2H4S+H2O	2.00E+11 0.0	8698.0	3666. C6H111O2-6-C6H101OHOH-5	2.00E+11 0.0	26450.0	
Reverse Arrhenius coefficients:	4.65E+13 -0.7	6200.0	3667. C6H111O2-4-C6H102OOH-4	2.00E+11 0.0	26450.0	
3579. NC3H7COC2H5+H2O<->NC3H7COC2H5-1+CH3O2H	3.01E+12 0.0	19380.0	3668. C6H111O2-4-C6H102OOH-5	3.75E+10 0.0	24000.0	
Reverse Arrhenius coefficients:	1.84E+13 -0.5	6657.0	3669. C6H111O2-5-C6H102OOH-4	2.00E+11 0.0	2450.0	
3580. NC3H7COC2H5+CH3O2<->C3H6COC2H5-2+CH3O2H	1.99E+12 0.0	17050.0	3670. C6H111O2-5-C6H102OOH-6	3.00E+11 0.0	29000.0	
Reverse Arrhenius coefficients:	9.71E+11 -0.2	6874.0	3671. C6H112O2-6-C6H102OOH-4	2.50E+10 0.0	18450.0	
3581. NC3H7COC2H5+CH3O2<->C3H6COC2H5-3+CH3O2H	2.00E+12 0.0	15250.0	3672. C6H112O2-6-C6H102OOH-5	2.00E+11 0.0	26450.0	
Reverse Arrhenius coefficients:	1.91E+13 -0.8	12030.0	3673. C6H113O2-1-C6H103OHOH-2	2.00E+11 0.0	2450.0	
3582. NC3H7COC2H5+CH3O2<->NC3H7COC2H4P+CH3O2H	3.01E+12 0.0	17580.0	3674. C6H113O2-2-C6H103OHOH-1	3.00E+11 0.0	29000.0	
Reverse Arrhenius coefficients:	1.84E+13 -0.5	4862.0	3675. C6H101OHOH-3->ETES1+OH	6.00E+11 0.0	22000.0	
3583. NC3H7COC2H5+CH3O2<->NC3H7COC2H4S+CH3O2H	2.00E+12 0.0	15250.0	3676. C6H101OHOH-3->MVVOX+OH	7.50E+10 0.0	15250.0	
Reverse Arrhenius coefficients:	1.91E+13 -0.8	12030.0	3677. C6H101OHOH-3->VTHF+OH	9.38E-09 0.0	7000.0	
3584. C3H6COC2H5-2<->C3H6COC2H5-3+C2H5COCH2	2.22E+15 -0.8	23590.0	3678. C6H101OHOH-3->EDHF+OH	9.38E-09 0.0	7000.0	
Reverse Arrhenius coefficients:	2.50E+11 0.0	7800.0	3679. C6H101OHOH-3->ETES1+OH	6.00E+11 0.0	22000.0	
3585. C3H6COC2H5-2<->C3H6COC2H5-3+C2H5CO	4.05E+16 -1.1	26150.0	3680. C6H101OHOH-4->ETES1+OH	6.00E+11 0.0	22000.0	
Reverse Arrhenius coefficients:	1.00E+11 0.0	8300.0	3681. C6H101OHOH-4->ETES1+OH	7.50E+10 0.0	15250.0	
3586. C3H6COC2H5-3<->C2H5COC2H3+CH3	2.92E+15 -0.7	32300.0	3682. C6H101OHOH-5->MVVOX+OH	7.50E+10 0.0	15250.0	
Reverse Arrhenius coefficients:	1.00E+11 0.0	7800.0	3683. C6H101OHOH-5->ETES1+OH	6.00E+11 0.0	22000.0	
3587. NC3H7COC2H4P<->NC3H7COC2H4+CH2H4	5.40E+17 -1.4	26040.0	3684. C6H101OHOH-5->ETES1+OH	6.00E+11 0.0	22000.0	
Reverse Arrhenius coefficients:	2.50E+11 0.0	7800.0	3685. C6H101OHOH-6->VTHF+OH	9.38E-09 0.0	7000.0	
3588. NC3H7COC2H4S<->C3H6CHCO+N-C3H7	1.97E+19 -1.5	42860.0	3686. C6H101OHOH-6->ETES1+OH	7.50E+10 0.0	15250.0	
Reverse Arrhenius coefficients:	1.00E+11 0.0	10600.0	3687. C6H101OHOH-6->ETES1+OH	6.00E+11 0.0	22000.0	
3589. CHHCHO+OH<->CH2CHO+HCO	1.00E+12 0.0	0.0	3688. C6H102OOH4-5->ETES1+OH	6.00E+11 0.0	22000.0	
Reverse Arrhenius coefficients:	2.72E+11 0.3	36200.0	3689. C6H102OOH4-6->ETES1+OH	7.50E+10 0.0	15250.0	
3590. C2+CH12-1<->CH2O2+NC4H9CHO	1.00E+14 0.0	37000.0	3690. C6H102OOH4-6->ETES1+OH	6.00E+11 0.0	22000.0	
3591. C6H12-1<->C3H6-C3H6	4.00E+12 0.0	58000.0	3691. C6H102OOH5-6->ETES1+OH	6.00E+11 0.0	22000.0	
3592. C6H111-3+H<->C6H12-1	1.00E+14 0.0	0.0	3692. C6H102OOH6-4->ETES1+OH	7.50E+10 0.0	15250.0	
3593. C5H9J-5+CH3<->C6H12-1	1.00E+13 0.0	0.0	3693. C6H102OOH6-5->ETES1+OH	6.00E+11 0.0	22000.0	
3594. P-C4H9+2CH3<->C6H12-1	1.00E+13 0.0	0.0	3694. C6H103OOH1-1->ETES1+OH	6.00E+11 0.0	22000.0	
3595. C4H71-4+CH2H5<->C6H12-1	8.00E+12 0.0	0.0	3695. C6H103OOH1-2->ETES1+OH	6.00E+11 0.0	22000.0	
3596. C6H111-3+H<->C6H12-2	1.00E+14 0.0	0.0	3696. HO2+CH6H101-3-<->C6H101OHOH-3	4.85E+11 0.0	10000.0	
3597. C6H112-4+H<->C6H12-2	1.00E+14 0.0	0.0	3697. HO2+CH6H101-3-<->C6H101OHOH-3	4.85E+11 0.0	9000.0	
3598. C5H9J-5+CH3<->C6H12-2	1.00E+13 0.0	0.0	3698. HO2+CH6H101-4->C6H101OHOH-3	3.40E+11 0.0	11800.0	
3599. N-C3H7+C3H5-T<->C6H12-2	1.00E+13 0.0	0.0	3699. HO2+CH6H101-4->C6H101OHOH-4	3.40E+11 0.0	11800.0	
3600. C6H112-4+H<->C6H111-5+OH	1.00E+14 0.0	0.0	3700. HO2+CH6H101-5->C6H101OHOH-5	1.00E+12 0.0	13700.0	
3601. C4H71-1+CH2<->C6H12-3	1.00E+13 0.0	0.0	3701. HO2+CH6H101-5->C6H101OHOH-5	1.00E+12 0.0	13700.0	
3602. C6H112-1+O2<->C6H111-3+HO2	2.20E+12 0.0	3722.0	3702. HO2+CH6H102-4->C6H102OOH-4	3.80E+11 0.0	8800.0	
3603. C6H112-1+O2<->C6H111-4+HO2	2.00E+13 0.0	3703. HO2+CH6H102-4->C6H102OOH-5	3.80E+11 0.0	7800.0		
3604. C6H112-1+O2<->C6H111-5+HO2	2.00E+13 0.0	3704. HO2+CH6H101-4->C6H102OOH-5	1.00E+12 0.0	13700.0		
3605. C6H112-1+O2<->C6H111-6+HO2	3.00E+13 0.0	3705. HO2+CH6H101-4->C6H102OOH-6	1.00E+12 0.0	13700.0		
3606. C6H112-1+O2<->C6H111-3+OH	6.60E+05 2.4	3723.0	3706. HO2+CH6H101-3->C6H103OOH-1	4.85E+11 0.0	10000.0	
3607. C6H112-1+O2<->C6H111-4+OH	5.51E+05 2.5	3711. C6H12-2+HO2->C6H12OOH-3	6.80E+11 0.0	11800.0		
3608. C6H112-1+O2<->C6H111-5+OH	5.51E+05 2.5	3712. C6H12-3+HO2->C6H12OOH-3	6.80E+11 0.0	11800.0		
3609. C6H112-1+O2<->C6H111-6+OH	9.80E+05 2.4	3713. C6H101OHOH-3->C3H3AC3H5OOH+C2H2	3.00E+13 0.0	35500.0		
3610. C6H12-2+O2<->C6H111-3+HO2	5.50E+12 0.0	3714. C6H101OHOH-4->C6H101OHOH-3	3.00E+13 0.0	23000.0		
3611. C6H12-2+O2<->C6H112-4+HO2	2.20E+10 0.0	3715. C6H101OHOH-3->HO2+CH4H6+C2H4	3.00E+13 0.0	30000.0		
3612. C6H12-2+O2<->C6H112-5+HO2	2.00E+13 0.0	3716. C6H101OHOH-4->C2H5+CH3O2H+C3H2	1.00E+13 0.0	35000.0		
3613. C6H12-2+O2<->C6H112-6+HO2	3.00E+13 0.0	3717. C6H101OHOH-4->C3H5+A+AC3H5OOH	3.00E+13 0.0	23000.0		
3614. C6H12-2+O2<->C6H111-3+OH	4.41E+05 2.4	3718. C6H101OHOH-4->C6H101OHOH-3+C2H4	3.00E+13 0.0	30000.0		
3615. C6H12-2+O2<->C6H112-4+OH	6.60E+05 2.4	3719. C6H101OHOH-5->OH+C4H6+CH3CHO	1.00E+13 0.0	35000.0		
3616. C6H12-2+O2<->C6H112-5+OH	5.51E+05 2.5	3720. C6H101OHOH-4->C6H101OHOH-3+C2H2	3.00E+13 0.0	35500.0		
3617. C6H12-2+O2<->C6H112-6+OH	9.80E+05 2.4	3721. C6H101OHOH-5->C4H71-3+C2H3OOH	3.00E+13 0.0	30000.0		
3618. C6H12-3+O2<->C6H112-4+HO2	4.40E+12 0.0	3722. C6H101OHOH-6->C6H101OHOH-5+C2H4	1.00E+13 0.0	35000.0		
3619. C6H12-3+O2<->C6H113-1+HO2	6.00E+13 0.0	3723. C6H101OHOH-6->C6H101OHOH-4	3.00E+13 0.0	20000.0		
3620. C6H12-3+O2<->C6H112-4+OH	1.32E+06 2.4	3724. C6H101OHOH-6->C6H101OHOH-3	1.00E+13 0.0	29500.0		
3621. C6H12-3+O2<->C6H113-1+OH	1.96E+06 2.4	3725. C6H101OHOH-6->C6H101OHOH-5	3.00E+13 0.0	23000.0		
3622. C2H5+C4H6+C6H11-3	8.50E+10 0.4	3800.0	3726. C6H101OHOH-6->C6H101OHOH-6	3.00E+13 0.0	22000.0	
3623. C3H3-C5H8J-4-C6H11-4	1.00E+11 0.0	3700.0	3727. C6H101OHOH-6->C6H101OHOH-6	3.00E+13 0.0	22000.0	
3624. C3H5+A+CH6-C6H11-5	4.00E+11 0.0	3700.0	3728. C6H101OHOH-6->C6H101OHOH-6	3.00E+13 0.0	22000.0	
3625. C4H71-4+CH2H4-C6H11-6	1.00E+11 0.0	3700.0	3729. C6H101OHOH-6->C6H101O			

3752. C6H10IOOH3-6O2=>NC6D1KET36+OH	1.56E+09	0.0	13650.0	3825. CH3O+ETES1=>CH3OH+C2H3COCH3+C2H3	5.14E+05	2.0	1583.6
3753. C6H10IOOH4-3O2=>NC6D1KET43+OH	1.00E+11	0.0	23450.0	3826. CH3O2+ETES1=>CH3O2H+C2H3COCH3+C2H3	9.13E+05	2.0	12360.4
3754. C6H10IOOH4-5O2=>NC6D1KET45+OH	1.00E+11	0.0	23450.0	3827. O2+MVOX=>HO2+C2H3COCH3+C2H3	2.04E+07	2.0	40722.5
3755. C6H10IOOH4-6O2=>NC6D1KET46+OH	1.25E+10	0.0	17450.0	3828. H+MVOX=>H2+C2H3COCH3+C2H3	2.57E+07	2.0	3950.6
3756. C6H10IOOH5-3O2=>NC6D1KET53+OH	1.25E+10	0.0	17450.0	3829. OH+MVOX=>HO2+C2H3COCH3+C2H3	4.79E+06	2.0	-229.8
3757. C6H10IOOH5-4O2=>NC6D1KET54+OH	1.00E+11	0.0	23450.0	3830. O+MVOX=>HO2+C2H3COCH3+C2H3	1.62E+07	2.0	2579.5
3758. C6H10IOOH5-6O2=>NC6D1KET56+OH	1.00E+11	0.0	23450.0	3831. HO2+MVOX=>HO2+C2H3COCH3+C2H3	6.46E+05	2.0	11887.7
3759. C6H10IOOH6-3O2=>NC6D1KET63+OH	3.12E+09	0.0	22150.0	3832. HCO+MVOX=>CH2O+C2H3COCH3+C2H3	1.52E+06	2.0	12360.4
3760. C6H10IOOH6-4O2=>NC6D1KET64+OH	2.50E+10	0.0	21000.0	3833. CH3+MVOX=>CH4+C2H3COCH3+C2H3	4.68E+05	2.0	4871.3
3761. C6H10IOOH6-5O2=>NC6D1KET65+OH	2.00E+11	0.0	26150.0	3834. C2H5+MVOX=>C2H6+C2H3COCH3+C2H3	2.76E+05	2.0	7658.1
3762. C6H10IOOH6-4O2=>NC6D2KET45+OH	1.00E+11	0.0	21450.0	3835. CH3O2+MVOX=>CH3O2H+C2H3COCH3+C2H3	9.13E+05	2.0	12360.4
3763. C6H10IOOH4-6O2=>NC6D2KET46+OH	1.25E+10	0.0	15450.0	3836. C2H3+MVOX=>C2H4+C2H3COCH3+C2H3	8.14E+05	2.0	4871.3
3764. C6H10IOOH5-4O2=>NC6D2KET54+OH	1.00E+11	0.0	23450.0	3837. CH3O+MVOX=>CH3OH+C2H3COCH3+C2H3	5.14E+05	2.0	1583.6
3765. C6H10IOOH6-6O2=>NC6D2KET56+OH	1.00E+11	0.0	23450.0	3838. O2+VTHF=>HO2+C2H3COCH3+C2H3	2.04E+07	2.0	40722.5
3766. C6H10IOOH6-4O2=>NC6D2KET64+OH	2.50E+10	0.0	21000.0	3839. H+VTHF=>H2+C2H3COCH3+C2H3	2.57E+07	2.0	3950.6
3767. C6H10IOOH6-5O2=>NC6D2KET65+OH	2.00E+11	0.0	26000.0	3840. O+VTHF=>HO2+C2H3COCH3+C2H3	4.79E+06	2.0	-229.8
3768. C6H10IOOH2-1O2=>NC6D3KET21+OH	1.00E+11	0.0	21450.0	3841. O+VTHF=>HO2+C2H3COCH3+C2H3	1.62E+07	2.0	2579.5
3769. C6H10IOOH1-2O2=>NC6D3KET12+OH	2.00E+11	0.0	26000.0	3842. HO2+VTHF=>HO2+C2H3COCH3+C2H3	6.46E+05	2.0	11887.7
3770. NC6D1KET34=>OH+C2H3O+C2H3COCH3	1.00E+16	0.0	39000.0	3843. HCO+VTHF=>CH2O+C2H3COCH3+C2H3	1.52E+06	2.0	12360.4
3771. NC6D1KET35=>OH+C3H3-CO+C2H3COCH3	5.00E+15	0.0	39000.0	3844. CH3+VTHF=>CH4+C2H3COCH3+C2H3	4.68E+05	2.0	4871.3
3772. NC6D1KET36=>OH+C3H3-CO+C2H3COCH3	5.00E+15	0.0	39000.0	3845. C2H5+VTHF=>C2H6+C2H3COCH3+C2H3	2.76E+05	2.0	7658.1
3773. NC6D1KET37=>OH+C3H5O+C2H3CHO	1.00E+16	0.0	39000.0	3846. CH3O2+VTHF=>CH3OH+C2H3COCH3+C2H3	5.14E+05	2.0	1583.6
3774. NC6D1KET43=>OH+C3H5O+C2H3CHO	1.00E+16	0.0	39000.0	3847. CH3O2+VTHF=>CH3OH2H+C2H3COCH3+C2H3	9.13E+05	2.0	12360.4
3775. NC6D1KET45=>OH+C2H3+C3H3CHO-C2H2O	1.00E+16	0.0	39000.0	3848. C2H3+VTHF=>C2H4+C2H3COCH3+C2H3	8.14E+05	2.0	4871.3
3776. NC6D1KET46=>OH+C3H5A+C0+C3H3CHO	1.00E+16	0.0	39000.0	3849. O2+EDHF=>HO2+C2H3COCH3+C2H3	2.04E+07	2.0	40722.5
3777. NC6D1KET53=>OH+C2H5CO+C2H3CHO	1.00E+16	0.0	39000.0	3850. H+EDHF=>HO2+C2H3COCH3+C2H3	2.57E+07	2.0	3950.6
3778. NC6D1KET54=>OH+C3H5A+A+C0+C3H3CHO	1.00E+16	0.0	39000.0	3851. HO+EDHF=>HO2+C2H3COCH3+C2H3	4.79E+06	2.0	-229.8
3779. NC6D1KET56=>OH+C3H5A+A+CH2CO+C2H2O	1.00E+16	0.0	39000.0	3852. O+EDHF=>OH+C2H3COCH3+C2H3	1.62E+07	2.0	2579.5
3780. NC6D1KET63=>OH+C2H3CHO-HCO+C2H4	1.00E+16	0.0	39000.0	3853. HO2+EDHF=>HO2+C2H3COCH3+C2H3	6.46E+05	2.0	11887.7
3781. NC6D1KET64=>OH+C3H5A+A+CH3CHO-CO	5.00E+15	0.0	39000.0	3854. HCO+EDHF=>CH2O+C2H3COCH3+C2H3	1.52E+06	2.0	12360.4
3782. NC6D1KET64=>OH+C2H2O+AC3H5CHO	5.00E+15	0.0	39000.0	3855. CH3+EDHF=>CH4+C2H3COCH3+C2H3	4.68E+05	2.0	4871.3
3783. NC6D1KET65=>OH-HCO-C2H2O+C3H6	1.00E+16	0.0	39000.0	3856. C2H5+EDHF=>C2H6+C2H3COCH3+C2H3	2.76E+05	2.0	7658.1
3784. NC6D2KET45=>OH+C3H5-T+CO+C3H3CHO	1.00E+16	0.0	39000.0	3857. C2H3+EDHF=>C2H4+C2H3COCH3+C2H3	8.14E+05	2.0	4871.3
3785. NC6D2KET46=>OH+C3H5-T+C2H2O+C2H2O	1.00E+16	0.0	39000.0	3858. CH3O2+EDHF=>CH3OH2H+C2H3COCH3+C2H3	9.13E+05	2.0	12360.4
3786. NC6D2KET54=>OH+C2H3CO-C2H3COCH3	1.00E+16	0.0	39000.0	3859. CH3O+EDHF=>CH3OH+C2H3COCH3+C2H3	5.14E+05	2.0	1583.6
3787. NC6D2KET56=>OH+C3H5-T+C2H20+C2H2O	1.00E+16	0.0	39000.0	3860. C2H5+C5H8I4=>H2+C3H5-A+C2H2	5.11E+06	2.0	40722.5
3788. NC6D2KET64=>OH+C2H2O+C2H3COCH3	1.00E+16	0.0	39000.0	3861. H+C5H8I4=>H2+C3H5-A+C2H2	6.44E+06	2.0	3950.6
3789. NC6D2KET65=>OH+C4H71-T+CO+C2H2O	1.00E+16	0.0	39000.0	3862. OH+C5H8I4=>H2O+C3H5-A+C2H2	1.20E+06	2.0	-229.8
3790. NC6D3KET21=>OH+C4H71-T+CO+C2H2O	1.00E+16	0.0	39000.0	3863. O+C5H8I4=>H2O+C3H5-A+C2H2	4.06E+06	2.0	2579.5
3791. NC6D3KET12=>OH-HCO-C4H7CHO1-I	1.00E+16	0.0	39000.0	3864. HO2+C5H8I4=>H2O2+C3H5-A+C2H2	1.62E+05	2.0	11887.7
3792. C6H12OH-1=>CH3CHO-P-C4H9	1.50E+13	0.0	30000.0	3865. HCO+C5H8I4=>CH2O+C3H5-A+C2H2	3.79E+05	2.0	12360.4
3793. C6H12OH-1=>C2H5CHO-N-C2H7	1.50E+13	0.0	30000.0	3866. CH3+C5H8I4=>CH4+C3H5-A+C2H2	1.17E+03	2.0	4871.3
3794. C6H12OH-2=>NC3H7CHO-C2H5	1.50E+13	0.0	30000.0	3867. C2H5+C5H8I4=>C2H6+C3H5-A+C2H2	6.90E+04	2.0	7658.1
3795. C6H12OH-2=>NC4H9CHO+C2H3	1.50E+13	0.0	30000.0	3868. CH3O+C5H8I4=>C2H6+C3H5-A+C2H2	1.28E+05	2.0	1583.6
3796. C6H12OH-3=>NC3H7CHO-C2H5	3.00E+13	0.0	30000.0	3869. CH3O2+C5H8I4=>CH3O2H+C3H5-A+C2H2	2.28E+05	2.0	12360.4
3797. C6H12-3-O=>N-C3H7-C2H5CO	1.00E+11	0.0	-1050.0	3870. C2H3+C5H8I4=>C2H4+C3H5-A+C2H2	2.04E+05	2.0	4871.3
3798. C6H1114-4+HO2-C6H111O2H-4	9.00E+12	0.0	0.0	3871. C6H101-3+H=<C6H111-3	2.50E+11	0.5	2620.0
3799. C6H1114-5+HO2-C6H111O2H-5	9.00E+12	0.0	0.0	3872. C6H101-3+H=<C6H111-4	2.50E+11	0.5	2620.0
3800. C6H1114-6+HO2-C6H111O2H-6	9.00E+12	0.0	0.0	3873. C6H101-3+H=<C6H111-3	4.25E+11	0.5	230.0
3801. C6H112-5+HO2-C6H112O2H-5	9.00E+12	0.0	0.0	3874. C6H101-3+H=<C6H112-4	2.50E+11	0.5	2620.0
3802. C6H112-6+HO2-C6H112O2H-6	9.00E+12	0.0	0.0	3875. C6H101-4+H=<C6H111-4	2.50E+11	0.5	2620.0
3803. C6H112-4+HO2-C6H113O2H-2	4.00E+12	0.0	0.0	3876. C6H101-4+H=<C6H111-5	2.50E+11	0.5	2620.0
3804. C6H112-4+HO2-C6H112O2H-4	4.00E+12	0.0	0.0	3877. C6H101-4+H=<C6H112-5	4.25E+11	0.5	1230.0
3805. C6H113-1+HO2-C6H113O2H-1	9.00E+12	0.0	0.0	3878. C6H101-4+H=<C6H112-6	2.50E+11	0.5	2620.0
3806. C6H112O2-1=>C2H3COC3H7+OH	4.00E+12	0.0	38000.0	3879. C6H101-5+H=<C6H111-5	4.25E+11	0.5	1230.0
3807. C6H11O2-3=>C2H3COC3H7+OH	4.00E+12	0.0	38000.0	3880. C6H101-5+H=<C6H111-6	2.50E+11	0.5	2620.0
3808. C6H11O2OH3-6=>C2H3COC3H7+OH	1.00E+11	0.0	16700.0	3881. C6H101-3+O=>C5H91-3+HCO	2.00E+11	0.0	-1050.0
3809. C6H111O2H-4=>C2H5CHO+C3H5-A	1.00E+16	0.0	39000.0	3882. C6H101-4+O=>C5H92-5+HCO	2.00E+11	0.0	-1050.0
3810. C6H111O2H-5=>OH+C3H3CHO+C4H71-4	1.00E+16	0.0	39000.0	3883. C6H101-5+O=>C5H91-5+HCO	2.00E+11	0.0	-1050.0
3811. C6H111O2H-6=>OH+C2H20+C5H91-5	1.00E+16	0.0	39000.0	3884. C6H101-3+OH=>C5H91-3+CH2O	1.00E+12	0.0	0.0
3812. C6H112O2H-4=>C2H3COC3H7+C2H5	1.00E+16	0.0	39000.0	3885. C6H101-4+OH=>C5H92-5+CH2O	1.00E+12	0.0	0.0
3813. C6H112O2H-5=>OH+C3H3CHO+C4H71-3	1.00E+16	0.0	39000.0	3886. C6H101-5+OH=>C5H91-5+CH2O	1.00E+12	0.0	0.0
3814. C6H112O2H-6=>OH+C2H20+C5H91-5	1.00E+16	0.0	39000.0	3887. C6H101-3+OH=>C2H3-C4H6-H2O	2.76E+04	2.6	-1919.0
3815. C6H113O2H-2=>OH+C3H3CHO+C4H71-4	1.00E+16	0.0	39000.0	3888. C6H101-4+OH=>C2H3-C4H6-H2O	2.76E+04	2.6	-1919.0
3816. C6H113O2H-1=>OH+C2H20+C5H91-3	1.00E+16	0.0	39000.0	3889. C6H101-5+OH=>C2H3-C4H6-H2O	2.76E+04	2.6	-1919.0
3817. O2+ETES1=>H2+C2H3COCH3+C2H3	2.04E+07	2.0	40722.5	3890. C6H101-3+HO2=>C2H3-C4H6+H2O2	4.82E+03	2.5	10530.0
3818. H+ETES1=>H2+C2H3COCH3+C2H3	2.57E+07	2.0	3950.6	3891. C6H101-4+HO2=>C2H3+C4H6+H2O2	4.82E+03	2.5	10530.0
3819. OH+ETES1=>H2O+C2H3COCH3+C2H3	4.79E+06	2.0	-2259.8	3892. C6H101-5+HO2=>C2H3+C4H6+H2O2	4.82E+03	2.5	10530.0
3820. O+ETES1=>OH+C2H3COCH3+C2H3	1.62E+07	2.0	2579.5	3893. C6H101-3+H=>C2H3+C4H6+H2	3.38E+05	2.4	207.0
3821. HO2+ETES1=>H2O2+C2H3COCH3+C2H3	6.46E+05	2.0	11887.7	3894. C6H101-4+H=>C2H3+C4H6+H2	3.38E+05	2.4	207.0
3822. HCO+ETES1=>C2H20+C2H3COCH3+C2H3	4.68E+05	2.0	4871.3	3895. C6H101-5+H=>C2H3+C4H6+H2	3.38E+05	2.4	207.0
3823. CH3+ETES1=>CH4+C2H3COCH3+C2H3	2.76E+05	2.0	7658.1				

NOTE: A units mole-cm-sec-K, E units cal/mole