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The Instrumental Model

by

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Abstract

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The goal of this dissertation is to enable better predictive models by engaging raw experimental data through the Instrumental Model. The Instrumental Model captures the protocols and procedures of experimental data analysis. The approach is formalized by encoding the Instrumental Model in an XML record. Decoupling the raw experimental data from the data analysis procedure, the Instrumental Model provides means for rigorous uncertainty quantification of predictive model.

The concept of the Instrumental Model and its data model, which governs how the data is described, is discussed in this work. The Instrumental Model XML record is linked to raw experimental data records and calibration data records, providing a complete description of the experimental data.

The Instrumental Model approach is first demonstrated using a set of formaldehyde oxidation shock-tube experiments. In those experiments, the transmitted laser light intensity was measured by a photodiode and the produced voltages were recorded by a computer. The corresponding Instrumental Model transforms these raw data into CO concentration upon the user's request.

The Instrumental Model is expanded by performing uncertainty quantification of model predictions using raw data from a more complex experiment – a stoichiometric $C_2H_2/O_2/Ar$ premixed laminar flame mapped with VUV-photoionization molecular-beam mass spectrometry. The experimental signals were modeled with a premixed laminar flame code augmented with an Instrumental Model, designed to link raw signals to derived properties. The consistency of the model and raw experimental data are quantified and predictions for weak-signal observations of O, OH, C_2H_3 and unknown background H_2O mole fractions are made.

To Rachel

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Chapter 1

Introduction

1.1 Motivation

In our time, the global community is facing large challenges such as climate change, constrained natural resources, natural disasters, compromised national security, and financial crises. These challenges call for better predictive models, which may enable us to mitigate and act upon these imminent crises [1]. A "predictive model" is defined as a model that can reproduce a large set of well-defined experimental data and whose uncertainty bounds are quantified. Predictive models are improved by gaining more knowledge through proper uncertainty quantification. Uncertainty quantification is the field of study related to numerical characterization of uncertainties in various applications. Uncertainty quantification can be accomplished by a systematic analysis synthesizing both the model and experimental data.

In recent years, the chemical kinetics community has placed a large effort on advancing the state of building predictive models as discussed in several reviews [2-6]. Two main methods have been most popular: comprehensive hierarchical reaction set [6,7] and kinetic model optimization [8,9]. A *reaction set* is a list of possible elementary chemical reactions that can occur with their associated kinetic parameters.

The comprehensive hierarchical method of building reaction sets is based on the principle that chemical reaction sets for a given molecule are composed of reaction subsets of smaller molecules. Comprehensive hierarchical reaction sets are built by validating reaction subsets against experimental data. The new species are incorporated by "freezing" the parameters of the reaction subsets and again validating the augmented reaction set against additional experimental data. At each validation step kinetic parameters of the newly added reaction are chosen such that the reaction set reproduces the experimental data.

The method of kinetic model optimization poses the problem of determining kinetic parameters as constrained optimization. All known reactions are compiled into the reaction set with their respective parameter uncertainty bounds. Kinetic parameter values are identified in the least-squares sense such that the simulation by the reaction set reproduces chosen experimental data. It is recognized that the experimental data are not sensitive to each reaction, so only the select reactions which have the greatest impact are

chosen as optimization variables. Kinetic model optimization was demonstrated by creation of the GRI-Mech reaction set [8,9] which has become widely used in the research and industrial communities.

A more recent method to developing predictive kinetic models is called Data Collaboration, [10-14] which is a systems approach combining both model and data for uncertainty quantification. In Data Collaboration, the model and experiment, with respective uncertainties, which may describe diverse phenomena, are unified into a concept called a dataset. By constrained optimization the set of model parameter values is found such that the model reproduces the experiment within uncertainty bounds. Through this set of parameter values, called the feasible set, predictions with quantified uncertainties are made. Experimental and parameter uncertainties are propagated directly to model predictions through the feasible set.

It has been shown that experimental data play a critical in the building of predictive models for chemical kinetics. We have reached the point, with the advent of Data Collaboration, where the limit of our ability to build predictive models with quantified uncertainties lies in a more rigorous and consistent treatment of experimental data.

1.2 Analysis of Raw Experimental Data

Experimental data, particularly in the natural sciences, are observations of raw properties such as current or voltage. Typically experimenters employ elaborate procedures to transform the raw data into derived properties, such as concentration. Uncertainty quantification by means of derived properties leads to two problems. First, experimental data analysis often invokes unnecessary assumptions, which are propagated to the derived property, introducing additional errors. Next, the uncertainty of calibration parameters and experimental data become confounded. The addition of unnecessary error from data analysis and confounding of experimental and calibration errors hinders proper uncertainty quantification.

One approach to integrating the raw experimental data in uncertainty quantification is to predict raw signals by including the data analysis as part of the predictive model. By this approach the uncertainty of the raw data, model parameters, and data analysis are properly accounted. The uncertainty of the model parameters is propagated through to the model prediction uncertainty. The model uncertainty is employed in evaluating model predictiveness, the ability to predict the raw data within the bounds of experimental uncertainty.

Previous work simulating raw experiment signals with model derived properties is discussed in this paragraph. It is common in the validation of computational fluid dynamics (CFD) models to predict raw experimental data. Computational flow imaging (CFI) [15] is a technique for model validation, where the simulated flow images are compared to planar laser-induced fluorescence (PLIF) images. Several studies have been published demonstrating this approach for many flow structures such as past a blunt body

and wedge [16], in a shock tunnel [15], and in mixing flow fields [17]. Validation of the density field computed from CFD calculations has been done by comparison of simulated phase maps, representing line-of-sight integrated density, with interferometric data [18]. In reacting flows, model validation with OH and CO PLIF images and particle image velocimetry (PIV) was used to study extinction and edge flame phenomena of counter-flow diffusion flames [19-21]. NO formation pathways have been studied with model validation against simulated NO LIF images [22]. In a recent paper, Connelly et al. [23] compared measured and computed signals for the validation of NOx and soot models. They discussed a "paradigm shift" in data analysis whereby deriving signals from numerical results will result in simpler experiments with reduced uncertainties and fewer measurements. They argue that by this approach, greater information can be extracted from simulation to design more purposeful experiments.

Previous work of Frenklach and Wang [24] simulated the raw experimental data from model derived properties for soot model validation. The authors argued for benefits of a more direct analysis, comparing model predictions to the actual experimental observables, because calculations of derived properties from the raw data usually invoke additional assumptions.

1.3 Archival of Experimental Data

A primary imperative of advancing science is knowledge archival and sharing, which demands suitable archival of raw experimental data and data analysis procedures. The traditional method of archiving and sharing knowledge lacks transparency of the raw data and details of the data analysis procedure. Typically, all important experimental conditions, instrument settings, and observations are archived in a lab notebook. Instrument data acquisition is accomplished by commercial software such as LabVIEW or with custom computer programs. The raw data are typically archived in their original format on individual lab desktop computers or lab data servers. These data are then analyzed, perhaps with spreadsheet software, resulting in derived properties. The data analysis procedure is implicitly found within the formulae and coding of the data analysis software or spreadsheet. The knowledge about the experiment, data, and data analysis procedure is published in the form of a narrative, equations, and derived properties in scientific journals and presented at technical conferences.

If alternatively, an experimenter formally archives his raw data and data analysis procedure, derived properties can always be reconstructed. The data analysis procedure is the metadata, data that provides semantics, of the raw data. This understanding of the relationship of data and data analysis suggests archiving the raw data and data analysis procedure, providing a link between the two.

The need for better data archival is becoming widely recognized in the scientific community as evidenced by the February 2011 issue of *Science* dedicated to the topic of scientific data. Most scientists are experiencing a data deluge, where the bottleneck in scientific discovery is no longer quality sensors, but the management of large amounts of data [25-29]. One article in particular discussed how a major effort was required to

reconstruct data acquired 20 years prior [26]. In this case, the analysis of the recovered legacy data with new theoretical insights resulted in more than a dozen high-impact scientific publications. Looking forward, the author argues for greater data management and even advocates for employing a Data Archivist, a person who spends his time archiving and managing acquired data.

Current efforts to archive and share raw data and data analysis procedures are encouraging, yet fall short of providing standards and mandating compliance. Archival standards among a scientific community would encourage greater collaboration. National funding agencies, such as the NIH and NSF, have mandated that a data management plan be included for each proposal [30,31]. These policies require a principal investigator to set policies for archival and sharing of data and metadata. The mandate encourages data archival and sharing, but no standards to support interoperability are enforced.

Advances in technologies and standards in data collection and archival have been made over the past 40 years. Technologies such as Relational Database Management Systems (RDBMS) [32], Extensible Markup Language (XML), and Structured Query Language (SQL) have enabled the collection, archival, and retrieval of massive amounts of data in business settings. In the scientific community, efforts such as the National Nuclear Data center [33] have been successful in organizing, archiving, and managing repositories of nuclear data. In the chemical kinetics community, popular thermodynamic databases are available [34,35]. A recent effort of NIST has been the creation of an XML-based IUPAC standard for storage and exchange of experimental thermophysical and thermochemical property data [36]. The archiving and sharing of chemical kinetic reaction sets began with "mechanism files", which are stand-alone text files that include all of the species and reaction rate coefficient data of a reaction set. The format for these files became a defacto "standard" which also serves as input to the widely used CHEMKIN [37] kinetics codes. The text files are distributed through websites, and copied from one user to another. One example is the GRI-Mech reaction set [9], a model for natural gas combustion. A recently developed initiative for archival and management of data for the purpose of building predictive models is called Process Informatics Model (PrIMe – primekinetics.org) [1]. PrIMe consists of data models, a data warehouse for archival of XML data records, and a web-based workflow to link data and tools. PrIMe was used to accomplish the work of this dissertation and is discussed in greater detail in section 2.1.

1.4 Instrumental Model

An approach that provides a consistent treatment of experimental data leading to proper uncertainty quantification is the *Instrumental Model* [38]. This approach enables the integration of raw experimental data into predictive model uncertainty quantification, and allows the archival of raw data and metadata. The Instrumental Model approach, the major intellectual contribution of this dissertation, links the raw data and derived properties by capturing the experimenter's data analysis procedures and protocols. Conceptually, the Instrumental Model is a function or algorithm by which derived properties can be calculated from the raw data or vice-versa. The Instrumental Model is

encoded in an XML record allowing electronic archival of metadata, making it computer readable.

The Instrumental Model overcomes many of the limitations of previous approaches. With the Instrumental Model approach, uncertainty quantification is accomplished with both the raw data and model derived properties in their proper format. This approach properly accounts for uncertainty in the experimental data, data analysis procedure, and model. Archiving the data analysis procedure with an Instrumental Model allows more transparent documentation of the experiment and sources of uncertainty. Encoding the Instrumental Model with a computer readable format such as XML enables automatic data analysis. XML encoding enables one to easily apply an Instrumental model to many data sources, in addition to one's own.

1.5 Document Outline

This dissertation introduces the Instrumental Model and demonstrates its application to two different sets of experimental data. Chapter 2 discusses the technology and methods used in applying the Instrumental Model to actual experiments and performing uncertainty quantification. The details of the Instrumental Model are discussed in Chapter 3. The application of the Instrumental Model in Chapter 4 to a simple experiment, a shock tube, demonstrates archival of scientific data and automating the data analysis procedure. The second example, a laminar flame experiment, discussed in Chapter 5 demonstrates data analysis of complex experimental data by the Instrumental Model. It is also shown that the Instrumental Model enables proper uncertainty quantification by accounting for the experimental data and data analysis uncertainties separately. Finally, the Instrumental Model approach is summarized and future work is proposed in Chapter 6.

Chapter 2

Technologies and Methods

2.1 PrIMe: Predictive Model Building Through Process Informatics

Process Informatics Model (PrIMe – primekinetics.org) is a recently developed data-centric cyber-infrastructure for building predictive models [1]. PrIMe consists of *data models*, a *data warehouse*, and the *PrIMe Workflow Application*. The PrIMe infrastructure seeks to solve deficiencies of previous model building approaches through data archival, data management, and by linking data to tools.

2.1.1 PrIMe Warehouse

The PrIMe Warehouse is a repository of all scientific records which are archived in a native XML database. The warehouse consists of a depository and a library. The depository archives all data records which have been submitted to the warehouse. Anyone in the community is allowed to submit records to the depository. Previous versions of updated records remain in the depository and are archived in what is called the attic. The library is a subset of depository records which are identified as expert-recommended. A committee of experts selects records which are considered more reliable. The building predictive models can be automated by machine selection of expert-recommended training data and model parameters.

Different types of data records are archived in individual collections in the depository of the PrIMe Warehouse. The collections currently found in the PrIMe Warehouse are:

1. Bibliography
2. Elements
3. Species
4. Reactions
5. Experiments
6. Models

7. Datasets
8. Optimization Variables
9. Data Attributes

The bibliography collection stores bibliographic data for the experimental, model, and reaction rate records in the Warehouse. Data about each chemical element are stored in the elements collection. The species collection holds records containing data of chemical species. Records that describe chemical reactions are archived in the reactions collection, which is linked to the collection of reaction rate coefficients. The experiment collection houses the experimental data records. The models collection archives models both imported and created in PrIMe. Records of datasets, which will be discussed in section 2.2, are archived in the dataset collection. The optimization variables collection archives records of optimization variables. The records describing both targets and calibrations are kept in the data attributes collection. Targets are experimental features used for model development.

Each collection has both *catalog* and *data* folders. The catalog contains XML records belonging to the collection, which is identified by a unique identifier, called a PrIMe ID. The PrIMe ID is an 8 digit number preceded by a letter indicating the collection to which it belongs. The data folder contains a list of sub-folders, with a folder corresponding to each XML record in the catalog. Supplementary data such as raw experimental records, figures, or documentation are stored in the data folder.

2.1.2 PrIMe Data Models

The PrIMe data models [39-41] describe the structure of scientific data and models. Each collection in the PrIMe Warehouse has a corresponding data model. The data models are governed by schema, which ensure that data records conform to the data type for the collection to which they belong. In practice, PrIMe data models are implemented as XML schema. A newly submitted data record is automatically validated against the XML schema, ensuring the record conforms to the data model.

Data models play an important role in accomplishing a stated imperative of PrIMe, which is one record per entity. They provide a template by which data are archived and describe relationships among data records. For example, the PrIMe experiment data model requires that an experimental record properly attribute the data to a scientific publication with a link to a PrIMe bibliography record. In this way data models provide structure to the data.

2.1.3 PrIMe Workflow Application

The PrIMe Workflow Application (PWA) [42] is a web-based application that links the archived experimental data and models to tools for data analysis and building predictive models. The user interacts with the PrIMe Warehouse by means of the PWA to perform tasks such as submission of data, browsing the data, performing data analysis on archived data, and making predictions from models. The user builds a flow chart to describe the workflow of the intended task. Figure 2.1 is a screenshot of the PWA showing an example of a workflow which performs Data Collaboration on the GRI-Mech 3.0 dataset. The process elements, which are building blocks for the workflow, are on the left-hand side and the flow chart is on the right-hand side.

The PWA is extensible, allowing developers to add new tools through the Component Uploader (CU). With the CU, a developer can create a tool using MATLAB or C#, upload it to the PWA, define the user interface, and then publish it to the user base.

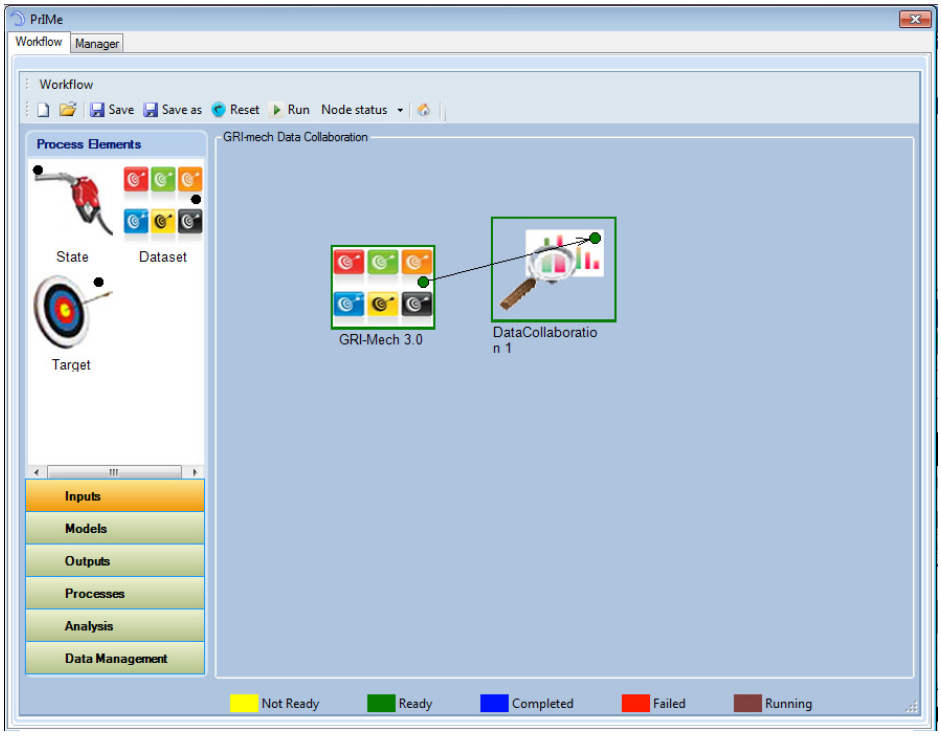

Figure 2.1. Screenshot of the PrIMe Workflow Application (PWA).

2.2 Data Collaboration

Data Collaboration is a mathematical framework for uncertainty quantification [10-14]. In data collaboration, experimental data and models are placed on equal footing. The Data Collaboration methodology has provisions for qualifying what is meant by "model predicts data" with quantitative metrics. Uncertainty quantification is performed with Data Collaboration by directly transferring the uncertainties of the model parameters and raw experimental data to the model predictions.

2.2.1 Dataset

The unification of experimental data and models is done through a concept called a *dataset*. For a given experiment *e*, the experimentally measured value of property Y_e is d_e with an uncertainty bounded by l_e from below and by u_e from above. M_e is a model predicting Y_e and has a functional dependence on a set of model parameters $\boldsymbol{\theta}_e$. Each experiment has associated with it a dataset unit, $\mathcal{U}_e$, defined by:

$$\mathcal{U}_e = (d_e, u_e, l_e, M_e)$$

A collection of dataset units, whose elements are indexed by *e* ranging from 1 to *m*, is referred to as a dataset, $\mathcal{D}_e$.

$$\mathcal{D}_e = \{\mathcal{U}_e\}_{\forall e}$$

All dataset parameter values, $\boldsymbol{\theta}$, span the prior-knowledge "hypercube" $H = \{\boldsymbol{\theta} \in \Re^n : \theta_{i,\min} \le \theta_i \le \theta_{i,\max},\ i = 1, 2, \ldots, n\}$. The subset of the hypercube satisfying

$$l_e \le M_e(\boldsymbol{\theta}) - d_e \le u_e \tag{2.1}$$

for all dataset units is referred to as the feasible set *F*. The dataset is said to be consistent if *F* is nonempty.

2.2.2 Dataset Consistency

A quantitative metric of dataset consistency, called the *consistency measure* C_D, identifies if values of $\boldsymbol{\theta}$ exist within the parameter uncertainty bounds that satisfy the constraints of the dataset given in eq. (2.1). The consistency measure, C_D, is defined as the maximum value of γ with the following constraints:

$$\begin{aligned} &\theta_j \le \theta_{j,max} \\ &-\theta_j \le -\theta_{j,min} \text{ (for } j = 1,2,..,n) \\ &-M_e(\boldsymbol{\theta}) + d_e \ \le -l_e - \gamma, \ \forall\, e \in \mathcal{E} \\ &M_e(\boldsymbol{\theta}) - d_e \ \le u_e - \gamma \end{aligned} \tag{2.2}$$

Here $\gamma$is a slack variable to identify how much the upper and lower experimental bounds could be tightened for the model to predict the data.

Both a lower and upper bound of the consistency measure, C_{D+} and C_{D-} respectively, are computed by solution of the optimization problem. There are three possibilities:

$C_{D-} > 0$, dataset is *consistent*.

$C_{D+} < 0$, dataset is *inconsistent*.

$C_{D-} < 0 < C_{D+}$, dataset is *inconclusive*.

If the dataset is consistent, the feasible set F is nonempty. Therefore a set of parameter values exists such that the model can make predictions within the experimental uncertainties. If the dataset is inconsistent or inconclusive, further evaluation is required to identify the source of inconsistency. A large parameter uncertainty bound or incorrectly specified bounds can lead to dataset inconsistency.

2.2.3 Sensitivity of the Consistency Measure

The sensitivity of the consistency measure to the experimental and parameter uncertainty bounds provides useful information about the contribution of experiment and parameter uncertainties to dataset consistency. The sensitivity of the consistency measure is estimated from Lagrange multipliers [11].

2.2.4 Model Predictions

In Data Collaboration, experimental uncertainties and model parameter uncertainties are transferred directly to the model prediction uncertainty through implicit exploitation of the feasible set. The upper and lower bounds of the model prediction, $\bar{M}_{\mathrm{P}}$ and $\underline{M}_{\mathrm{P}}$ respectively, are determined by the maximum and minimum model values over the feasible set. In mathematical terms,

$$\begin{aligned} \bar{M}_{\mathrm{P}} &= \max_{\mathbf{x}\in \boldsymbol{F}} M_{\mathrm{P}}(\boldsymbol{\theta}) \\ \underline{M}_{\mathrm{P}} &= \min_{\mathbf{x}\in \boldsymbol{F}} M_{\mathrm{P}}(\boldsymbol{\theta}) \end{aligned} \tag{2.3}$$

2.3 Chemical Kinetic Modeling

The evolution of chemical species in a reacting system is described by a system of ordinary differential equations of mass, species, and energy [43]. The PREMIX flame code [44] and CHEMKIN libraries [37] are used in this work to model the laboratory premixed laminar flame in Chapter 5. Chemical kinetic models, discussed in the introduction, are used to model the possible elementary reactions that occur in a system.

2.4 Dimensionality Reduction

Current reaction sets have 10^3 to 10^4 reaction parameters. However a given response, or model target, is sensitive to only a small subset of these parameters. This principal, called *effect sparsity*, states that only a small number of the variables will be statistically significant [45,46]. *Active variables* are those parameters to which a response is sensitive. Sensitivity analysis identifies the active variables over which the model is built. A method called *active subspace discovery* augments sensitivity analysis by identifying a subspace of the active variables. In this method, principal components analysis in the gradient space identifies the active subspace. The application of these two methods reduces the dimensionality of the parameter space and computational work significantly.

2.5 Response Sensitivity Analysis

Sensitivity analysis indicates how the output changes with respect to variation in the input parameters. The *response sensitivity* [47] of response η_i to parameter θ_j is defined as

$$S_i^j = \frac{\partial \eta_i}{\partial \theta_j}. \tag{2.4}$$

The sensitivity can be computed in two ways: 1) from a Taylor series approximation or 2) by so called “brute force”, both of which are described below.

The impact that each variable has on the model response is determined by calculating an impact factor [8], which is the product of the response sensitivity and the length of the parameter uncertainty interval. Parameters with higher uncertainty and sensitivity have potentially greater impact on the accuracy of the model and are selected as active variables.

2.5.1 Calculating Sensitivity from a Taylor Series Approximation

The sensitivity of mole fraction with respect to the rate coefficients is computed from the solution of the system of ordinary differential equations. The system of ordinary differential equations is set in terms of residuals by moving all terms to one side and is represented by

$$\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}) = 0 \tag{2.5}$$

where $\boldsymbol{\theta}$ is the vector of parameters and $\boldsymbol{x}$ is the vector of species concentrations [44]. Differentiating eq (2.6) with respect to $\boldsymbol{\theta}$ gives a matrix equation for sensitivity coefficients

$$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\frac{\partial \boldsymbol{x}}{\partial \boldsymbol{\theta}} + \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{\theta}} = 0 \tag{2.6}$$

where the matrix $\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}$ is the Jacobian, $\frac{\partial \boldsymbol{x}}{\partial \boldsymbol{\theta}}$ is the matrix of sensitivities of species concentration with respect to model parameters, and $\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{\theta}}$ is the matrix of partial derivatives of $\boldsymbol{f}$ with respect to the parameters. This linear system is readily solved for the sensitivity matrix, provided the Jacobian and matrix of partial derivatives of $\boldsymbol{f}$ with respect to the parameters have already been computed. The laminar flame code PREMIX normalizes the sensitivity in the form of logarithmic derivatives and reports the logarithmic sensitivities of the concentration of species *i* to parameter *j* computed by

$$E_{\log_{i,j}} = \frac{\partial \log x_i}{\partial \log \theta_j} = \frac{\partial x_i}{x_i}\frac{\theta_j}{\partial \theta_j}. \tag{2.7}$$

In this work we calculated the sensitivity to a modeling feature rather than the species sensitivity. To do this the sensitivity, $E_{i,j}$, is required. It is recovered from the logarithmic sensitivity by

$$E_{i,j} = \frac{\partial x_i}{\partial \theta_j} = \frac{x_i}{\theta_j} E_{log\,i,j}. \tag{2.8}$$

Calculating feature sensitivities from species concentration sensitivities follows the method of Goldenberg and Frenklach [48]. An example calculation of feature sensitivities for a laminar flame is shown in Appendix A.

2.5.2 Brute Force Method

The brute force method approximates eq (2.5) with a first-order Taylor series by

$$S_i^j \approx \frac{\Delta \eta_i}{\Delta \theta_j} = \frac{\tilde{\eta}_i - \eta_i}{\tilde{\theta}_j - \theta_j} \tag{2.9}$$

where $\tilde{\theta}_j$ is a perturbed value of parameter θ_j and $\tilde{\eta}_i$ is the perturbed response. These sensitivities are calculated by perturbing parameter θ_j while holding all other parameters constant.

2.6 Active Subspace Discovery

Reduction in dimensionality of the parameter space can be supplemented by *active-subspace discovery*, a recently developed method for identification of a lower-dimensional subspace introduced in the Ph.D. thesis of Trent Russi [49]. Active-subspace discovery is a technique for discovering the possible dependence of the response on a lower-dimensional active subspace of the parameters, uncovering possible correlations between parameters. This section will briefly describe the methodology following Russi.

The objective of active subspace discovery is to identify a low-rank subspace of the model parameters that approximate the full-rank parameter space. This is represented by

$$\boldsymbol{f}(\boldsymbol{\theta}) \approx \boldsymbol{g}(\mathbf{S}^{\mathsf{T}}\boldsymbol{\theta}). \tag{2.10}$$

We seek an $n \times r$ matrix $\mathbf{S}$ with $r < n$, where n is the dimension of the parameter space, r is the dimension of the active subspace, and $\boldsymbol{f}$ is a function in the full-rank parameter space. The matrix $\mathbf{S}$ is found by taking the derivatives of both sides,

$$\nabla\boldsymbol{f}(\boldsymbol{\theta}) \approx \nabla\boldsymbol{g}(\mathbf{S}^{\mathsf{T}}\boldsymbol{\theta}) \cdot \mathbf{S}^{\mathsf{T}}, \tag{2.11}$$

where $\nabla\boldsymbol{f}$ is the $1 \times n$ gradient vector at a point $\boldsymbol{\theta}$ in the parameter space. The gradient can be computed at several points by defining

$$\mathbf{F} \coloneqq \begin{bmatrix} \nabla\boldsymbol{f}(\boldsymbol{\theta}_1) \\ \vdots \\ \nabla\boldsymbol{f}(\boldsymbol{\theta}_{\mathrm{N}}) \end{bmatrix}, \quad \mathbf{G} \coloneqq \begin{bmatrix} \nabla\boldsymbol{g}(\mathbf{S}^{\mathsf{T}}\boldsymbol{\theta}_1) \\ \vdots \\ \nabla\boldsymbol{g}(\mathbf{S}^{\mathsf{T}}\boldsymbol{\theta}_{\mathrm{N}}) \end{bmatrix} \tag{2.12}$$

where each $\boldsymbol{\theta}_k$ is an n-dimensional vector at a different location in the parameter space. Eq (2.12) is now represented as

$$\mathbf{F} = \mathbf{G}\mathbf{S}^{\mathsf{T}}. \tag{2.13}$$

A matrix factorization of $\mathbf{F}$ is computed by singular value decomposition (SVD) by

$$\mathbf{F} = [\mathbf{U_1}\ \mathbf{U_2}] \begin{bmatrix} \mathbf{\Sigma_{11}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{V_1^{\mathsf{T}}} \\ \mathbf{V_2^{\mathsf{T}}} \end{bmatrix}. \tag{2.14}$$

The factorization leads to $\mathbf{G} = \mathbf{U_1}\mathbf{\Sigma_{11}}$ and $\mathbf{S} = \mathbf{V_1}$. The singular values given by the diagonal elements of $\mathbf{\Sigma_{11}}$ are in decreasing order and decay rapidly. The dimension of the active subspace r, is determined by the minimum number of singular values required to achieve a fitting error below a specified tolerance.

2.7 Solution Mapping Method

Solution mapping is the method of building an approximate model of a detailed chemical kinetic system given by a set of ODEs and then estimating kinetic model parameters with numerical optimization to experimental data [8,47,50]. This two-step procedure is a predecessor to Data Collaboration, which borrows the model building techniques of solution mapping. The approximating model, often called a *surrogate model* or *response surface model*, is built using the statistical technique of response surface methodology, by generating responses of carefully chosen points in the parameter space and then fitting an algebraic model of the responses [51].

2.7.1 Experimental Design

Many responses are generated to fit the surrogate model over the entire active variable space. Computer experiments are conducted to generate model responses at selected points in the active variable space. An experimental design distributes the experiments over the entire active parameter space to minimize the surrogate model error with the fewest possible runs.

The active variables are specified in terms of factorial variables which transform the active parameter space to be between the bounds [-1, 1]. The active parameters are transformed logarithmically following ref. [8] where the transformed variable becomes

$$X = \frac{\log\left(\theta/\theta_0\right)}{\log f} \tag{2.15}$$

where $f = \theta_{\max}/\theta_0 = \theta_0/\theta_{\min}$, $\theta_0 = (\theta_{\max}\theta_{\min})^{1/2}$. Here θ is the model parameter, $\theta_{\min}$ is the lower bound, and $\theta_{\max}$ is the upper bound. The upper bound of the model parameter, $\theta_{\max}$, corresponds to X = 1, while the lower bound of the model parameter, $\theta_{\min}$, corresponds to X = -1. An experimental design matrix is generated over the factorial variables.

The experimental design matrix is generated using Latin hypercube sampling (LHS) which is a commonly used space-filling design method [52]. Latin hypercube sampling divides the parameter space into n strata of equal marginal probability 1/n and samples once from each stratum. LHS is improved by applying an optimality criterion such as entropy [53], integrated mean square error [54], and maximin or minimax distance [55]. Latin hypercube sampling was applied using the **lhsdesign** command in MATLAB.

2.7.2 Model Responses

Surrogate models are used in the Data Collaboration framework for predictions of an experimental observation. An experimental feature, called a target, is a carefully selected property which summarizes the physics one would like to model. Examples of

targets are: peak value of a species profile, time/location of peak value, ignition delay time, location of ½ rise/decay, and laminar flame speed.

In chemical kinetics, it is common to make a $\log_{10}$ transformation of the model responses, or targets, in addition to a $\log_{10}$ transformation of the model parameters. This transformation of responses and parameters gives better fits, resulting in better surrogate models over the active variable space $\boldsymbol{\theta}$ [50].

2.7.3 Surrogate Model Building

Several types of surrogate models could be used to map the parameters to the response. Several methods such as response surface methodology [45], kriging [56], and support vector regression [57] are used for building approximate models. In modeling computer experiments, response surface methodology has enjoyed popularity [45,50,58,59]. Response surface models are polynomials, typically first or second-order, fit to responses of computer experiments. The second-order response surface model is given by the following general form

$$\hat{y}(\boldsymbol{\theta}) = \hat{\beta}_0 + \sum_{s=1}^{k} \hat{\beta}_s \theta_s + \sum_{s=1}^{k} \hat{\beta}_{ss} {\theta_s}^2 + \sum_{1 \le s < t \le k} \hat{\beta}_{st} \theta_s \theta_t. \tag{2.16}$$

where $\hat{y}(\boldsymbol{\theta})$ is the response for a set of parameters $\boldsymbol{\theta}$, $\hat{\beta}_0$ is the intercept, $\hat{\beta}_s$ is the linear coefficient for model parameter θ_s, $\hat{\beta}_{ss}$ is the quadratic coefficient, and $\hat{\beta}_{st}$ is the coefficient for the cross terms. The model coefficients are determined by fitting the surrogate model to computer experiment responses by ordinary least squares.

2.7.4 Model Checking

Surrogate model fits are checked by assessing the error compared to the in-sample and out-of-sample computer experiments. The in-sample errors evaluate how well the model fits the training data. Out-of-sample errors, which are computed from computer experiments conducted at random points in the parameter space, evaluate how well the model predicts validation data. One metric for evaluating error is the percent relative error, which computed as

$$\varepsilon_i = \frac{|\hat{y}_i - y_i|}{y_i} \tag{2.17}$$

where $\hat{y}_i$ is the surrogate model prediction and $y_i$is the response from the i^{th} computer experiment. The average and maximum relative errors are evaluated to determine goodness of fit. The relative error is a good metric for determining if the fitting error is below an error threshold. Relative error is used in evaluating the surrogate model fits in section 5.4.2.

2.8 MathML

MathML is a markup language, recommended by the World Wide Web Consortium (W3C) [60], used to describe mathematical relationships. Two types of mathML, presentation mathML and content mathML, are used to encode either the presentation or the semantics of a mathematical relationship respectively. Presentation mathML uses about 38 tags to describe notation, while content mathML uses about 120 tags to describe the meaning of a mathematical expression.

Content mathML is used in this work to describe the mathematical relationships within an Instrumental Model. An example of content mathML which describes the quadratic equation,

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}, \tag{2.18}$$

is shown in Figure 2.2. Content mathML begins with a `<math>` root node. Identifiers or variables, are indicated by `<ci>` nodes. Numbers, such as constants, are indicated by `<cn>` nodes. Operations are notated by an `<apply>` node followed by an operation such as `<times/>` for multiplication or `<minus/>` for subtraction. As shown in the example, the child nodes of an operation are its arguments. The operation A-B would be described by mathML as:

```
<apply><minus/>
   <ci>A</ci>
   <ci>B</ci>
</apply>.
```

```
<math xmlns="http://www.w3.org/1998/Math/MathML">
    <apply><in/>
        <ci>x</ci>
        <set>

            <apply><divide/>
                <apply><plus/> <!-- upper root -->
                    <apply><minus/>
                        <ci>b</ci>
                    </apply>
                    <apply><root/>
                        <apply><minus/>
                            <apply><power/>
                                <ci>b</ci>
                                <cn>2</cn>
                            </apply>
                            <apply><times/>
                                <cn>4</cn>
                                <ci>a</ci>
                                <ci>c</ci>
                            </apply>
                        </apply>
                    </apply>
                </apply>
                <apply><times/>
                    <cn>2</cn>
                    <ci>a</ci>
                </apply>
            </apply>

            <apply><divide/>
                <apply><minus/> <!-- lower root -->
                    <apply><minus/>
                        <ci>b</ci>
                    </apply>
                    <apply><root/>
                        <apply><minus/>
                            <apply><power/>
                                <ci>b</ci>
                                <cn>2</cn>
                            </apply>
                            <apply><times/>
                                <cn>4</cn>
                                <ci>a</ci>
                                <ci>c</ci>
                            </apply>
                        </apply>
                    </apply>
                </apply>
                <apply><times/>
                    <cn>2</cn>
                    <ci>a</ci>
                </apply>
            </apply>
        </set>
    </apply>
</math>
```

Figure 2.2. Content mathML markup of the quadratic equation [61].

Chapter 3

PrIMe Instrumental Model

In this chapter the concept of the PrIMe Instrumental Model is introduced. The mechanics of encoding the PrIMe Instrumental Model in XML is given and demonstrated with a simple example. The details of linking the PrIMe Instrumental Model to other PrIMe records are discussed. The foundation is given to demonstrate the application of the PrIMe Instrumental Model to actual experimental data in Chapter 4 and Chapter 5

3.1 Concept

The PrIMe Instrumental Model is an approach to capturing an experimenter's data analysis protocols and procedures to calculate derived properties from raw experimental data. It consists of the metadata of the experimental data. The PrIMe Instrumental Model allows the raw data to be archived separately from the data analysis procedures, which is in contrast to the typical method of archiving derived data only. This approach gives greater flexibility to the raw data, allowing scientists to apply alternative Instrumental Models to a given set of data. Moreover, an existing Instrumental Model can be easily applied to a new set of raw data. This approach has the potential to lead to greater scientific discovery by enabling the testing of new theories on previously-archived data. Additionally, it is shown in Chapter 5 how by this approach it is possible to perform uncertainty quantification of models with raw data.

A general experimental data analysis procedure is shown below in Figure 3.1. Not all data analysis procedures have each of the following steps, yet these can be found in many types of experimental data analysis. Generally, the analysis of raw data begins with evaluating the quality of the acquired data. Next, the data is cleaned in the case of missing data or outliers. Depending upon the nature of the data, it may be necessary to reduce the data by integration. The experimental data discussed in Chapter 5 provides one such case, where mass spectra at several locations in a flame are integrated to give a signal profile. Finally, the data are transformed into derived data using a constitutive relation, possibly with the use of calibration parameters.

The procedure in Figure 3.1 can be described by an Instrumental Model as shown by the dotted line enclosing the data analysis steps. By isolating the data analysis as an Instrumental Model, the elements of the process can be reduced to raw experimental data, calibration data, Instrumental Model, and derived data. From this abstraction it can be

seen that the derived data can always be reconstructed, provided that each of the raw experimental data, calibration data, and Instrumental Model are archived. Additionally, as will be shown in Chapter 5, uncertainty quantification can be done more rigorously with proper treatment of experimental uncertainties by isolating the data analysis procedure as an Instrumental Model from the raw experimental data and calibration data.

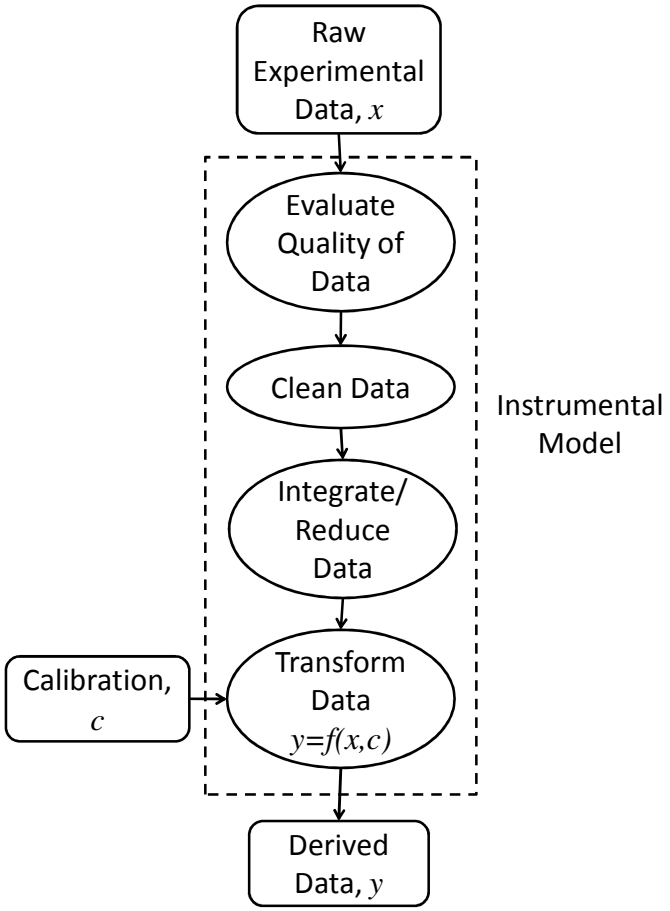

Figure 3.1. Flowchart of a general data analysis procedure, calculating derived data from raw data. The Instrumental Model describes the parts of the procedure within the dotted box.

3.2 XML Encoding

The PrIMe Instrumental Model is encoded by eXtensible Markup Language (XML) and is cataloged in the PrIMe data warehouse. Encoding the PrIMe Instrumental Model in XML provides two features: linking the Instrumental Model to experimental and calibration data, and automatic data analysis by machine processing. The XML language has provisions for linking different records to one another to form a database. The linking of an experimental record to an Instrumental Model gives the experimental record greater meaning by associating records that belong to each other. The ability to perform automatic data analysis allows the derived data to be computed on-the-fly.

Alternatively, model predictions can be computed in the raw data format, enabling uncertainty quantification with raw experimental data. The benefit of these features will be demonstrated in Chapter 4 and Chapter 5.

Figure 3.2 shows the general structure of a PrIMe Instrumental Model XML record. The related schema, which governs the structure of the model, is listed in Appendix B. The root node of the Instrumental Model XML is the `<instrumentalModel>` node which has attribute `primeid`. Members of the Instrumental Model collection are assigned PrIMe IDs which start with the prefix `im` followed by 8 digits, such as `im00000001`. The first block within the root node is the header block. The header block contains information about the Instrumental Model such as the preferred key, which is used to identify the record, and keywords.

The property block defines the properties, which are fundamental constants used in the Instrumental Model. The `<property>` node has attributes `description`, `name`, `units`, and `id`. The property's value is stored in the child node `<value>`.

The variable block defines external variables, those that are passed to and from the Instrumental Model, and internal variables, which are used to simplify the evaluation of the Instrumental Model. The external variables include, but are not limited to, raw experimental data and calibration parameters. Internal variables can also be defined to compute quantities from other variables. The variable identified by id `variable_4_ID` in this example shows how MathML can be used to calculate an internal variable value.

The Instrumental Model Expression block describes how all of the variables come together to form a single expression. The `<instrumentalModelExpression>` node has attributes `type` and `implicit`. The type attribute specifies the format by which the expression is represented. In this example the expression is described by MathML. The implicit attribute is a Boolean, specifying whether the expression is implicit or explicit. In this example, the variables labeled by `variable_3_ID` and `variable_4_ID` are subtracted from one another.

If an Instrumental Model Expression is implicit, the relationship is satisfied when the expression equals zero. Alternatively, if the Instrumental Model Expression is explicit, its result is the value of the Instrumental Model. Specifying an expression as implicit gives flexibility to numerically solve for any one of the variables in the instrumental model provided the remaining are known. This is useful when one wants to apply an Instrumental Model to calculate derived data from raw data or computing model predictions in the format of raw data.

The last block, Additional Data Item, lists data items which supplement the Instrumental Model. The example shown in Figure 3.2 has three such nodes: text, MATLAB function, and LaTeX expression. Additional data items that are of the type `MATLAB function` are used to link the record to a computer program which calculates the Instrumental Model for automatic data analysis. The specified MATLAB function is called and executes the Instrumental Model expression.

```
<?xml version="1.0" encoding="UTF-8"?>
<instrumentalModel … primeID="im00000001" >

<!--Header Block-->
    <preferredKey group="prime">Ideal Gas Law</preferredKey>
    <keyword>ideal Gas</keyword>
<!-- End Header Block -->

<!--Property Block-->
    <property description="Description of property" name="property name"
units="property units" id="property id">
        <value>8.3143</value>
    </property>
<!--End Property Block -->

<!--Variable Block-->
    <variable id="variable_1_ID" />
    <variable id="variable_2_ID" />
    <variable id="variable_3_ID" />
    <variable id="variable_4_ID" >
        <m:math>
            <!--MathML block-->
        </m:math>
    </variable>
<!--End Variable Block-->

<!--Instrumental Model Expression Block-->
    <instrumentalModelExpression type="MathML" implicit="Boolean: true or false">
        <m:math>
            <m:apply>
                <m:minus />
                <m:ci>variable_3_ID</m:ci>  <!--LHS-->
                <m:ci>variable_4_ID</m:ci>  <!--RHS-->
            </m:apply>
        </m:math>
    </instrumentalModelExpression>
<!--End Instrumental Model Expression Block-->

<!--Additional Data Item Block-->
    <additionalDataItem MIME=" " itemType="text" description="instrumental model
description">Description Text</additionalDataItem>
    <additionalDataItem MIME=" " itemType="MATLAB function" description="instrumental
model program">program_file_name.m</additionalDataItem>
    <additionalDataItem MIME=" " itemType="latex" description="latex expression of
instrumental model ">LaTeX expression</additionalDataItem>
<!--End Additional Data Item Block-->

</instrumentalModel>
```

Figure 3.2. Basic structure of the PrIMe Instrumental Model.

3.3 Instrumental Model XML – A Simple Real World Example

A simple real-world example of a PrIMe Instrumental Model XML record documenting the ideal-gas law is shown in Figure 3.3. The ideal gas law is given by the following equation

$$P = \frac{RT}{v}, \tag{3.1}$$

where P is pressure, R is the universal gas constant, T is the temperature, and v is the molar volume.

The universal gas constant is defined by a `<property>` node, establishing it as an internal constant with specified units of m^3*Pa*mol^{-1}*K^{-1} with id R. The external variables of the Instrumental Model are *T*, *v*, and *P* as shown in the property block. An internal variable, with id *RHS*, specifies the right-hand side of eq (3.1). The Instrumental Model expression for this example is an implicit expression, which is the subtraction of *RHS* from *P*. In the Additional Data Item section, a MATLAB function `iglaw.m` is specified for the computation of the ideal gas law. Also, an additional data item, specifying the LaTeX expression for the ideal gas law is given.

```
<?xml version="1.0" encoding="UTF-8"?>
<instrumentalModel … primeID="im00000001" >
    <preferredKey group="prime">Ideal Gas Law</preferredKey>
    <keyword>ideal Gas</keyword>
    <property description="Ideal Gas Constant" name="parameter" units="m^3*Pa*mol^-
1*K^-1" id="R">
        <value>8.3143</value>
    </property>
    <variable id="v" />
    <variable id="T" />
    <variable id="P" />
    <variable id="RHS" >
        <m:math>
            <m:apply>
                <m:divide>
                <m:apply>
                    <m:times>
                    <m:ci>R</m:ci>
                    <m:ci>T</m:ci>
                </m:apply>
                <m:ci>v</m:ci>
            </m:apply>
        </m:math>
    </variable>
    <instrumentalModelExpression type="MathML" implicit="true">
        <m:math>
            <m:apply>
                <m:minus />
                <m:ci>P</m:ci>
                <m:ci>RHS</m:ci>
            </m:apply>
        </m:math>
    </instrumentalModelExpression>
    <additionalDataItem MIME=" " itemType="text" description="instrumental model
description">Ideal Gas Law</additionalDataItem>
    <additionalDataItem MIME=" " itemType="MATLAB function" description="instrumental
model program">iglaw.m</additionalDataItem>
    <additionalDataItem MIME=" " itemType="latex" description="LaTeX expression of
Ideal Gas Law">$$P - \frac{\times{R}{T }}}{v} =0$$</additionalDataItem>
</instrumentalModel>
```

Figure 3.3. PrIMe Instrumental Model example showing the ideal gas law.

3.4 Linking Instrumental Model to Other Records

Encoding the Instrumental Model in XML provides the benefit that other records can link to it for the purpose of association with other data and to enable machine processing of the Instrumental Model. The PrIMe Experiment XML record provides links to the PrIMe Instrumental Model XML record, associating the metadata of the experiment to the record. The link to the Instrumental Model is done by defining a feature within a derived property node, which is a child of an experimental property.

The details of how the PrIMe Experiment XML record links to the PrIMe Instrumental Model XML record are outlined here with an example shown in Figure 3.4. The linking between the PrIMe Experiment XML and the PrIMe Instrumental Model

XML is shown graphically in Figure 3.5. The PrIMe Experiment XML data model is governed by the schema given in Appendix C. The <property> node, a child of the <dataGroup> node of a PrIMe Experiment XML record, is given an attribute derivedPropertyExists. When this attribute value, which is a Boolean, is true a <derivedProperty> child node exists. Within the <derivedProperty> node, a feature is defined, which provides the interface to a PrIMe Instrumental Model record. In the <feature> node, the Instrumental Model arguments are specified in <indicator> nodes while the output is specified in a single <observable> node. The <indicator> node can hold one of two nodes: a <propertyLink>, which links to an experimental property value within the experimental record or a <dataAttributeLink>, which links to a dataAttribute record. Calibration parameters or properties from other experimental data are specified in a dataAttribute record.

The Instrumental Model can also be employed to calculate derived properties within a dataAttribute. Recall that a data attribute record describes a feature calculated from experimental data such as an experimental target or calibration parameter. An example of a PrIMe Data Attribute XML record which links to an Instrumental Model XML record is shown in Figure 3.6. The linking between the Data Attribute XML record and the Instrumental Model XML record is shown graphically in Figure 3.7. In this example, <propertyLink> nodes specify properties that are later used in <feature> nodes to calculate experimental features. Within the <feature> node an <instrumentalModelLink> node specifies the instrumental model used to calculate the feature. The attribute instrumentalModelPrimeID indicates the PrIMe id of the instrumental model. Similar to linking from experimental XML records, the data attribute XML specifies input variables with <indicator> nodes. The propertyID attribute of each <indicator> node indicates which property from the <propertyLink> nodes is referenced. The result of the Instrumental Model is given in an <observable> node with a propertyID attribute which is referenced later in the <dataAttributeValue> node.

3.5 Summary

In this chapter, the concept of capturing the experimenter's protocols and procedures by the PrIMe Instrumental Model has been introduced. The mechanics of encoding the Instrumental Model in a PrIMe XML file has been given and a simple example has been shown. It has been shown how the PrIMe Instrumental Model provides a consistent treatment of experimental data, by formalizing the data analysis procedure. In the next chapter we apply the PrIMe Instrumental Model a shock-tube experiment. We will show how the PrIMe Instrumental Model enables one to view experimental data in either raw or derived format.

```
<dataGroup dataPointForm="HDF5" id="dg2" label="Experimental run 33">
    <dataGroupLink dataGroupID="" dataPointID=""/>
    <property description="time" id="x1" label="t" name="time" units="μs"/>
    <property derivedPropertyExists="true" description="Transient Voltage" id="x2"
label="V" name="voltage" units="mV">
        <derivedProperty description="CO concentration" id="CO" label="[CO]"
name="concentration" units="mol/m³">
            <feature id="C_CO" primeID="im00000001" type="instrumentalModel">
                <indicator id="V_inf" transformation="1" variableID="V_inf">
                    <propertyLink propertyID="V_inf"/>
                </indicator>
                <indicator id="V" transformation="1" variableID="V">
                    <propertyLink dataGroupID="dg2" propertyID="x2"/>
                </indicator>
                <indicator id="V_0" transformation="1" variableID="V_0">
                    <propertyLink propertyID="V_0"/>
                </indicator>
                <indicator id="gamma" transformation="1" variableID="gamma">
                    <dataAttributeLink id="gammaCalibration" primeID="a00000078"/>
                </indicator>
                <indicator id="L" transformation="1" variableID="L">
                    <propertyLink propertyID="D_internal"/>
                </indicator>
                <indicator id="C_tot" transformation="1" variableID="C_tot">
                    <propertyLink propertyID="C_tot"/>
                </indicator>
                <indicator id="T" transformation="1" variableID="T">
                    <propertyLink propertyID="T_5"/>
                </indicator>
                <observable id="C" variableID="C"/>
            </feature>
        </derivedProperty>
    </property>
</dataGroup>
```

Figure 3.4. A dataGroup block from a PrIMe Experiment XML record showing a link to an Instrumental Model record.

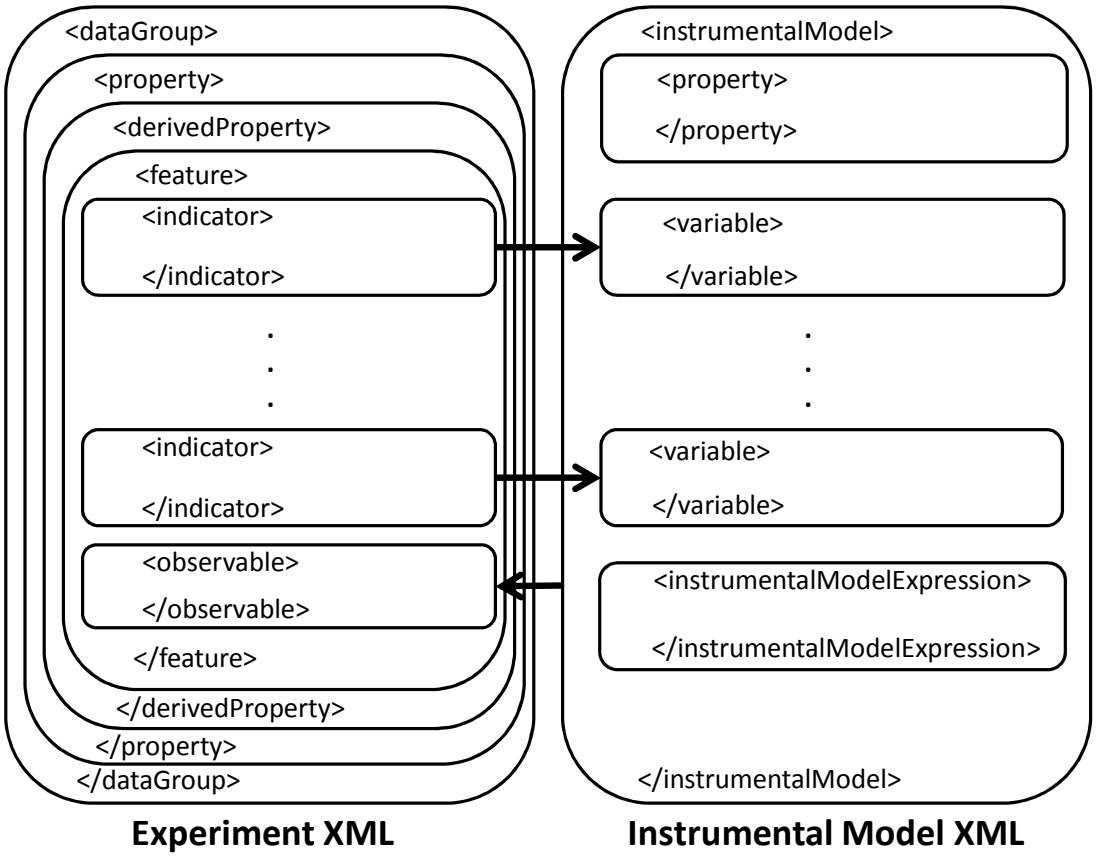

Figure 3.5. A schematic showing how the PrIMe Experiment XML links to the PrIMe Instrumental Model XML.

```
<?xml version="1.0" encoding="utf-8"?>
<dataAttribute type="calibration" primeID="a00000082"
xmlns="http://purl.org/NET/prime/" xmlns:xsi="http://www.w3.org/2001/XMLSchema-
instance" xmlns:m="http://www.w3.org/1998/Math/MathML"
xsi:schemaLocation="http://purl.org/NET/prime/
http://warehouse.primekinetics.org/schema/dataAttribute.xsd ">
    <copyright>primekinetics.org 2009</copyright>
    <origin type="primeID">b00014799</origin>
    <preferredKey group="prime">XH2/XAr Direct calibration factor</preferredKey>
    <propertyLink experimentPrimeID="x00000000" id="X_H2_1" propertyID="ic"
componentPrimeID="s00009809"/>
    <propertyLink experimentPrimeID="x00000000" id="X_Ar_1"  propertyID="ic"
componentPrimeID="s00000049"/>
    <propertyLink experimentPrimeID="x00000000" id="S_H2_1" dataGroupID="dg1"
propertyID="S_H2" dataPointID="15"/>
    <propertyLink experimentPrimeID="x00000000" id="S_Ar_1" dataGroupID="dg1"
propertyID="S_Ar" dataPointID="15"/>
    .
    .
    .
    <feature id="calibrationFactor_1" type="instrumentalModel">
        <instrumentalModelLink preferredKey="Direct Calibration Factor"
instrumentalModelPrimeID="im10000005" />
        <indicator id="X_H2_1" propertyID="X_H2_1" variableID="X_i"
transformation="1"/>
        <indicator id="X_Ar_1" propertyID="X_Ar_1" variableID="X_ref"
transformation="1"/>
        <indicator id="S_H2_1" propertyID="S_H2_1" variableID="S_i"
transformation="1"/>
        <indicator id="S_Ar_1" propertyID="S_Ar_1" variableID="S_ref"
transformation="1"/>
        <observable id="C_1" propertyID="C_1" transformation="1"/>
    </feature>
    .
    .
    .
    <dataAttributeValue type="derived">
        <indicator featureID="calibrationFactor_1" id="C_1" propertyID="C_1"
transformation="1" />
        <indicator featureID="calibrationFactor_2" id="C_2" propertyID="C_2"
transformation="1" />
        <observable featureID="meanCalibrationFactor" id="C_bar" propertyID="C_bar"
transformation="1" >
            <property name="parameter" units="" label="F_c_XH2/XAr"
description="XH2/XAr calibration factor">
                <value>0.15325</value>
            </property>
        </observable>
    </dataAttributeValue>
    <additionalDataItem MIME=" " itemType="text" description="Data Attribute
description">
        XH2/XAr Direct calibration factor
    </additionalDataItem>
</dataAttribute>
```

Figure 3.6. An example of a dataAttribute record which links to an Instrumental Model to calculate a derived property.

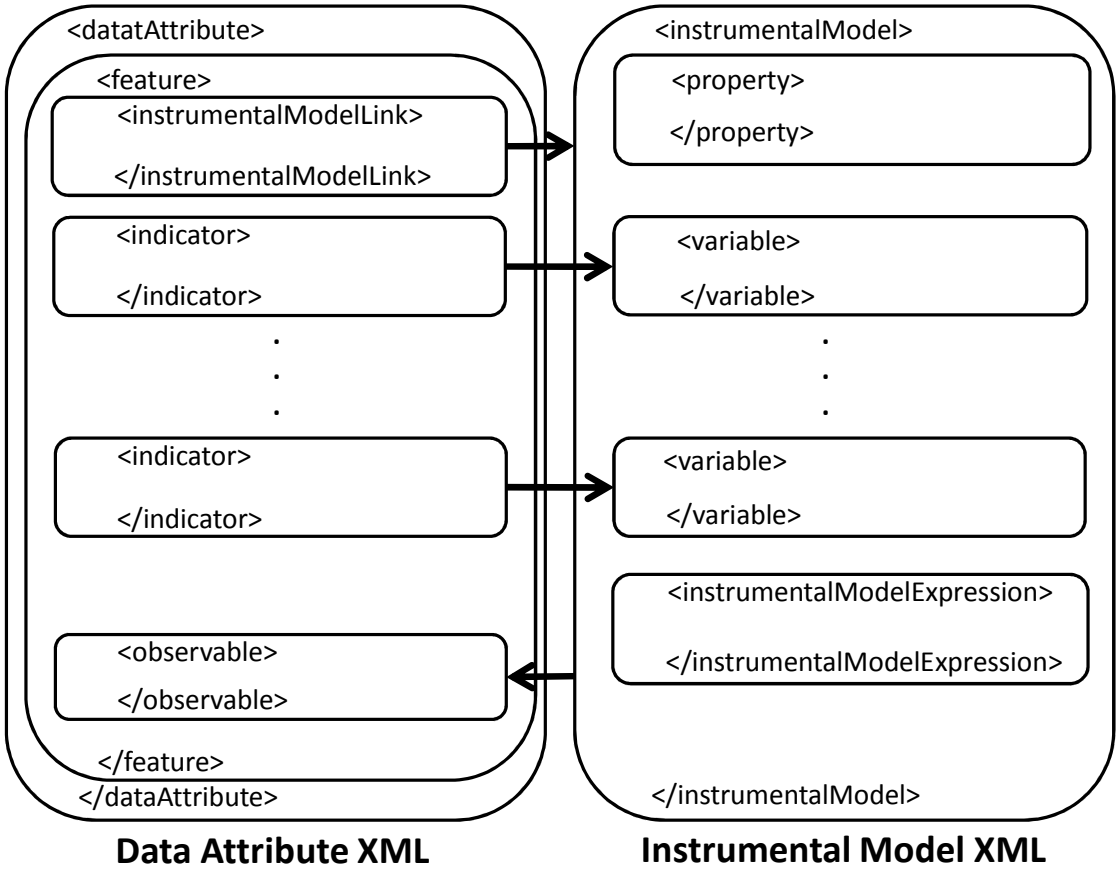

Figure 3.7. A schematic showing how the PrIMe Data Attribute XML links to the PrIMe Instrumental Model XML.

Chapter 4

Analysis of Experimental Shock Tube Data with the PrIMe Instrumental Model

4.1 Introduction

This chapter builds upon the foundation set in the previous chapter by applying the PrIMe Instrumental Model to the analysis of experimental data from shock tube measurements. Formalizing the data analysis procedure by the Instrumental Model, it is shown how the experimental data can be viewed in either raw or derived format by performing the data analysis on-the-fly.

4.2 Shock Tube Experiment

CO concentration as a function of reaction time was determined from a set of formaldehyde oxidation shock-tube experiments conducted by Eiteneer et al. [62,63]. In these experiments, seven mixtures of formaldehyde and oxygen diluted in argon were studied behind reflected shock waves from 1340 to 2270 K and pressures from 0.7 to 2.5 atm. The laser absorption of CO molecules was observed by measurement of transmitted laser light intensity with a photodiode and the produced voltages were recorded digitally. A schematic of the experimental setup and data acquisition is shown in Figure 4.1. The raw signal from the photodiode is reported in millivolts and is sampled once each microsecond. An example of the raw signal trace is shown in Figure 4.2

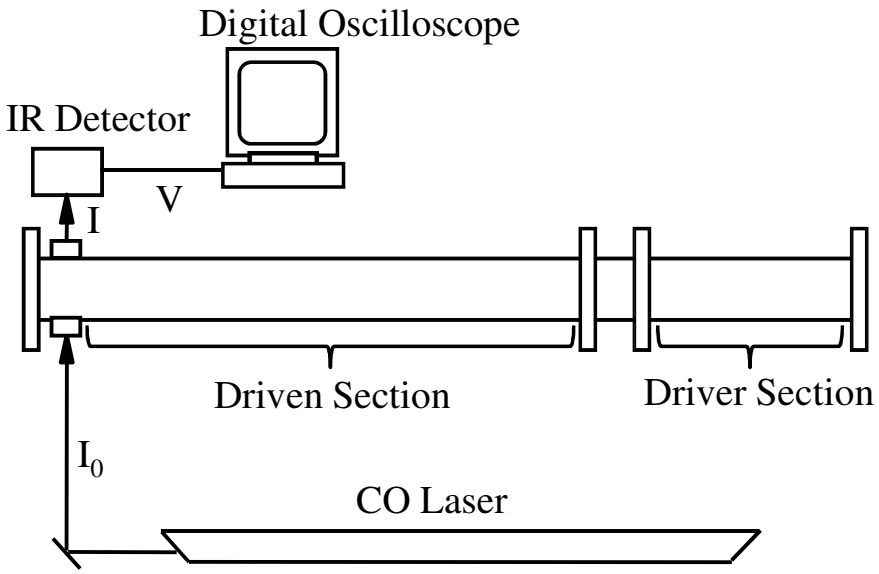

Figure 4.1. Schematic of shock tube experimental setup [63].

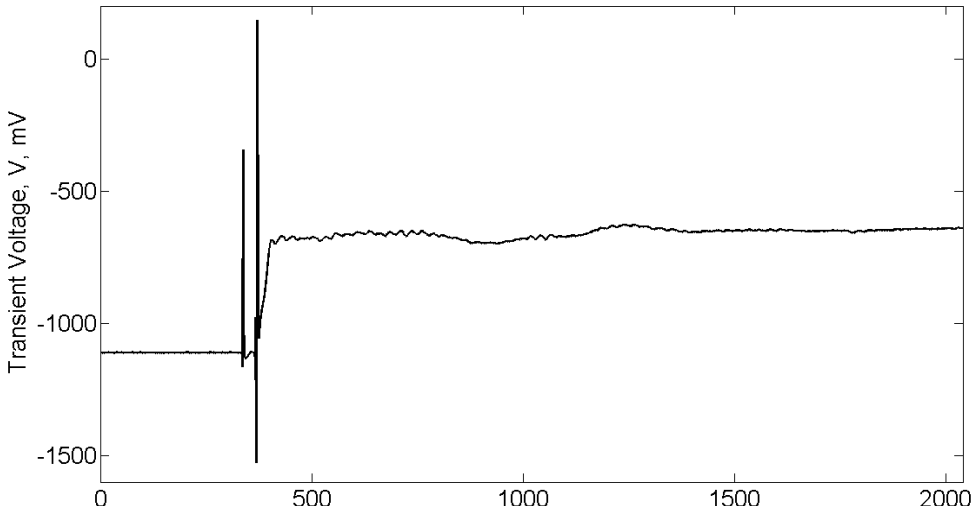

Figure 4.2. The raw experimental trace in millivolts from a photodiode representing the optical absorbance of CO in a shock tube experiment. The two sharp peaks on the left are artifacts from the shock wave passing through the detection window.

The shock tube experiment is conducted by pressurizing the driver section with an inert gas, while the driven section, filled with reactants, is maintained at low pressure. The diaphragm separating the two compartments is burst causing a shock wave to travel down the length of the shock tube, right to left in Figure 4.2. The shock wave nearly instantaneously raises the temperature and pressure of the gas in the driven section, initiating reaction. Once the shock wave hits the back wall it is reflected back leading to more pressure build up in the chamber. As the reaction proceeds the concentration of CO increases in the chamber leading to a change in voltage, signaling absorption of the laser light by the chemical species.

This experimental process can be seen in the raw experimental trace shown in Figure 4.2. The initial signal is flat, which corresponds to the data acquisition before the membrane between the driver and driven sections is burst. Two sharp peaks follow which represent the passing of the shock wave to the back wall and subsequently reflecting. The following gentler rise in voltage is due to the increase in CO concentration as the reaction progresses.

The CO concentration is computed from the voltage trace by the Beer-Lambert law defined as

$$\log\left(\frac{I}{I_0}\right) = \varepsilon_{\mathrm{CO}} \cdot C \cdot l, \tag{4.1}$$

where I_0 is the transmitted light intensity in absence of absorbing medium, I is the intensity of light attenuated by absorption, $\varepsilon_{\mathrm{CO}}$ is the molar absorptivity, C is the concentration of the absorbing species, and l is the optical length [64]. The intensity of light is measured by a photodiode, which gives voltages as an output. The difference in voltage of the transient signal and the infinite absorption gives the intensity of light attenuated by absorption, I. The molar absorptivity, $\varepsilon_{\mathrm{CO}}$, is obtained experimentally by performing calibration with known concentrations of the absorbing species.

The molar absorptivity as a function of temperature can be calculated by the following equations [63,65].

$$\varepsilon_{CO} = \frac{8\pi^3}{3hc}\nu_0 \frac{e^{\frac{-\Delta E_0^{\nu''}}{k_B T}}}{Q_{\mathrm{CO}}}\left(\frac{hcB_{\nu''}}{k_B T}e^{\frac{-B_{\nu''}J''(J''+1)hc}{k_B T}} - \frac{hcB_{\nu''+1}}{k_B T}e^{\frac{-\left(\Delta E_{\nu''}^{\nu''+1}+B_{\nu''+1}J''(J''-1)hc\right)}{k_B T}}\right) \times (|R_{\mathrm{CO}}|^2 J'') f(\nu_0) \tag{4.2}$$

$$f(\nu_0) = \frac{1}{\Delta\nu_D}\sqrt{\frac{\ln 2}{\pi}}\,\mathrm{e}^{a^2}\left(1 - \frac{2}{\sqrt{\pi}}\int_0^a \mathrm{e}^{-\mathrm{u}^2}\,\mathrm{du}\right) \tag{4.3}$$

$$a = \frac{\Delta\nu_c}{\Delta\nu_D}\sqrt{\ln 2} \tag{4.4}$$

$$\Delta\nu_D = \nu_0 \sqrt{\frac{2 \ln 2 \, k_B T}{mc^2}} \tag{4.5}$$

$$\Delta\nu_c = \gamma P \left(\frac{T_{ref}}{T}\right)^n \tag{4.6}$$

In eqs (4.2)-(4.6), T is the temperature in Kelvin and γ is the collisional broadening half-width. γ is an adjustable parameter obtained by performing experiments at known concentrations of CO in argon. The average value of γ reported from the calibration experiments is 4.8 x 10^{-2} $atm^{-1}cm^{-1}$. Since the present example is given only for the purpose of illustrating the PrIMe Instrumental Model, the remaining parameters of eqs (4.2)-(4.6) do not require further discussion.

The CO concentration derived from the data analysis using eqs (4.1) - (4.6) and the raw experimental signal in Figure 4.2 is shown in Figure 4.3. In addition to the transient voltages being transformed into CO concentration, the raw data was trimmed in the time axis to capture only the rise in CO concentration following the reflection of the shock. The time of ½ maximum CO concentration, which summarizes the profile, is used as one metric in the building of the GRI-Mech reaction set.

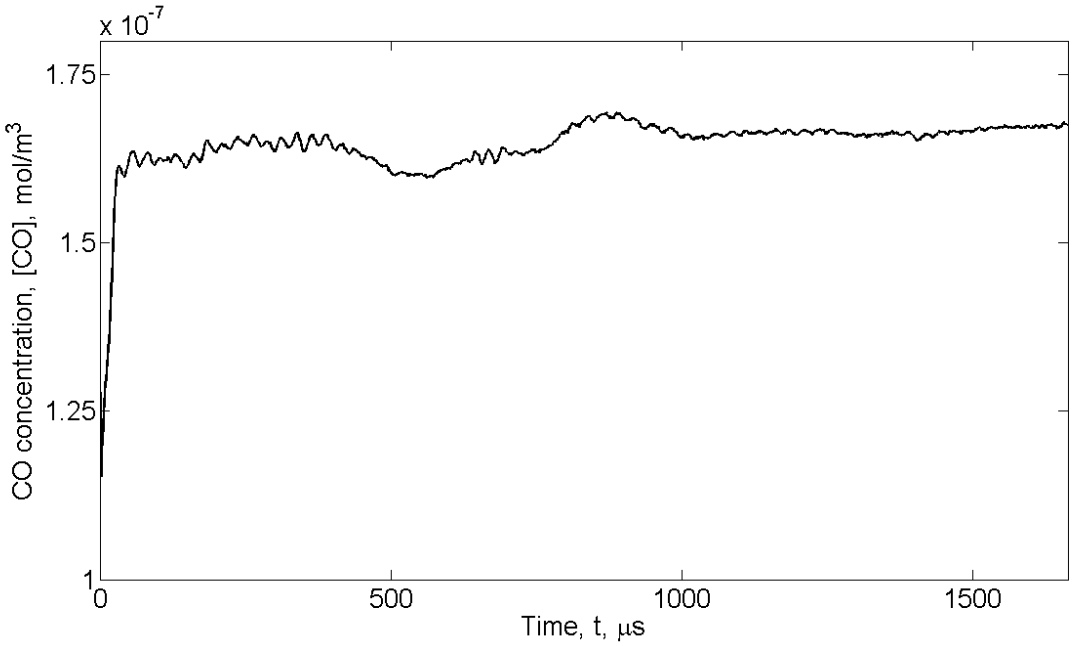

Figure 4.3. Graph of CO concentration derived from raw experimental signals of the shock tube data.

4.3 PrIMe XML Records

The raw experimental data is archived in a PrIMe Experiment XML record. The experiment XML record also links the experimental properties and raw data to the PrIMe Instrumental Model used to analyze the raw data. An abbreviated example of the PrIMe experiment XML file for the shock tube data is shown in Figure 4.4. An abbreviated version of the PrIMe Instrumental Model used to process the formaldehyde oxidation shock-tube data is shown in Figure 4.5. The PrIMe Calibration Data Attribute XML record (primeID a00000078) which specifies the collisional broadening half-width is given in Figure 4.6.

The entire PrIMe Instrumental Model (primeID i00000001) and experiment XML (primeID x00000010) records describing this particular experiment are located in the PrIMe Data Warehouse [66] and included in Appendix D and Appendix E respectively. The experimental feature, the time to ½ maximum CO concentration, is summarized in a PrIMe Target Data Attribute XML record (a00000044). This record is also found in the PrIMe Warehouse and Appendix F.

Figure 4.7 is a class diagram showing the relationship between the PrIMe target Data Attribute, PrIMe Experiment, PrIMe Instrumental Model, and PrIMe calibration Data Attribute files. The PrIMe target Data Attribute defines a modeling target from the characteristics of the PrIMe Experiment. The PrIMe Experiment uses the PrIMe Instrumental Model to interpret the experimental data. The PrIMe Instrumental Model requires a PrIMe calibration Data Attribute to define the calibration parameter γ; the

collisional broadening half-width in the case of the formaldehyde oxidation shock-tube experiments.

4.4 Hierarchical Data Format

For a given experimental run, the shock tube data contains over 2000 transient voltage observations. There was a need to archive the large number of experimental data points to allow efficient parsing of the data. The Hierarchical Data Format (HDF5) [67] a data model, which is similar to the hierarchical structure of XML, yet is better suited to efficiently store extremely large and complex data collections. The HDF5 Technology suite makes available tools for storing, viewing, and managing data in HDF5 format.

The PrIMe Experiment XML data model was extended to facilitate the use of HDF5 for experiments with large number of data points. A `dataPointForm` attribute was added to the `<dataGroup>` node. If the `dataPointForm` attribute has the value of `HDF5`, the data points are stored in an HDF5 file. Otherwise, the `dataPointForm` attribute can be assigned to XML or not assigned at all, indicating that the data points are stored in the XML file. When the data points are stored in HDF5, a file with the name of the data group id, followed by a .h5 extension, is located in the corresponding data sub-folder of the experiment collection. The HDF5 file has two child nodes, `dataPoints` and `propertyIDs`. The `dataPoints` node contains a list of the data points. The property IDs, assigned in the XML file, are specified in the `propertyIDs` node.

```
<experiment primeID="x00000010"… >
.
.
.
    <dataGroup id="dg2" label="Experimental run 24">
        <dataGroupLink dataGroupID="" dataPointID=""/>
            <property description="time" id="x1" label="t" name="time" units="μs"/>
            <property description="Transient Voltage" id="x2" label="V" name="voltage" units="mV" derivedPropertyExists="true">
                <derivedProperty method="instrumentalModel" description="CO concentration" id="CO" label="[CO]" name="concentration"
units="mol/m³" primeID="im00000001" >
                    <feature id="C_CO" type="instrumentalModel">
                    <indicator id="V_inf" instrumentalModelID="beersLaw" variableID="V_inf" propertyID="V_inf" transformation="1" />
                    <indicator id="V" instrumentalModelID="beersLaw" variableID="V" propertyID="x2" dataGroupID="dg1"
transformation="1" />
                    <indicator id="V_0" instrumentalModelID="beersLaw" variableID="V_0" propertyID="V_0" transformation="1" />
                    <indicator id="gamma"   instrumentalModelID="beersLaw" variableID="gamma" propertyID="gamma" transformation="1">
                        <dataAttributeLink id="gammaCalibration" primeID="a00000078" />
                    </indicator>
                    <indicator id="L" instrumentalModelID="beersLaw" variableID="L" propertyID="D_internal" transformation="1" />
                    <indicator id="C_tot" instrumentalModelID="beersLaw" variableID="C_tot" propertyID="C_tot" transformation="1" />
                    <indicator id="T" instrumentalModelID="beersLaw" variableID="T" propertyID="T_5" transformation="1" />
                    <observable id="C" instrumentalModelID="beersLaw" variableID="C" propertyID="C_CO" />
                </feature>
            </derivedProperty>
        </property>
    <dataPoint>
        <x1>1</x1>
        <x2>-1111</x2>
    </dataPoint>
    .
    .
    .
    </dataGroup>
.
.
.
</experiment>
```

Figure 4.4. An abbreviated PrIMe Experiment XML file (primeID – x00000010) describing the formaldehyde shock tube experiments of Eiteneer et al.

```
<instrumentalModel . . .  primeID="im00000001" >
    <copyright>primekinetics.org 2008</copyright>
    <preferredKey group="prime">Beer's Law for the P(10) 1->2 transition of CO</preferredKey>
    <keyword>laser absorption</keyword>
    <property description="Planck constant" name="parameter" units="erg*s" id="h">
        <value>6.6262e-27</value>
    </property>
    <property description="Speed of light" name="speed" units="cm/s" id="c_light">
        <value>2.997e10</value>
    </property>
    .
    .
    .
    <variable id="C" />
    <variable id="V_inf" />
    .
    .
    .
    <instrumentalModelExpression type="MathML" implicit="true">
        <m:math>
            <m:apply>
                <m:minus />
                <m:ci>LHS</m:ci>
                <m:ci>RHS</m:ci>
            </m:apply>
        </m:math>
    </instrumentalModelExpression>
    <additionalDataItem MIME=" " itemType="file" description="MATLAB code of instrumental model">BeerLawCO.m</additionalDataItem>
</instrumentalModel>
```

Figure 4.5. An abbreviated version of the PrIMe Instrumental Model (primeID -- im00000001) which describes the Beer-Lambert law using a complex expression for molar absorptivity used in the formaldehyde shock-tube experiments performed by Eiteneer et al.

```
<?xml version="1.0" encoding="utf-8" standalone="no" ?>
<dataAttribute xmlns="http://purl.org/NET/prime/" xmlns:xsi="http://www.w3.org/2001/XMLSchema-
instance" xmlns:m="http://www.w3.org/1998/Math/MathML" type="calibration" primeID="a00000078" xsi:schemaLocation="http://purl.org
/NET/prime/ http://warehouse.primekinetics.org/schema/dataAttribute.xsd ">
    <copyright>primekinetics.org 2008</copyright>
    <origin type="primeID">b00014778</origin>
    <preferredKey group="prime">Eiteneer CO Absorption Coefficient Calibration</preferredKey>
    <propertyLink dataGroupID="dg1" experimentPrimeID="x00000350" id="gamma" propertyID="x4"/>
    <feature id="gamma_bar" method="mean">
        <indicator id="gamma" propertyID="gamma" transformation="1"/>
        <observable id="gamma_bar" propertyID="gamma_bar" transformation="1"/>
    </feature>
    <dataAttributeValue type="derived">
        <observable id="gamma_bar" featureID="gamma_bar" propertyID="gamma_bar" transformation="1">
            <property name="parameter" units="atm^-1*cm^-1" label="gamma" description="collisional broadening half-width">
                <value>4.8e-2</value>
            </property>
        </observable>
    </dataAttributeValue>
    <additionalDataItem MIME=" " itemType="text" description="Data Attribute description">Determination of collisional half-
broadening width from calibration experiments.</additionalDataItem>
</dataAttribute>
```

Figure 4.6. Calibration Data Attribute XML record detailing the CO absorption coefficient parameter for the shock tube data.

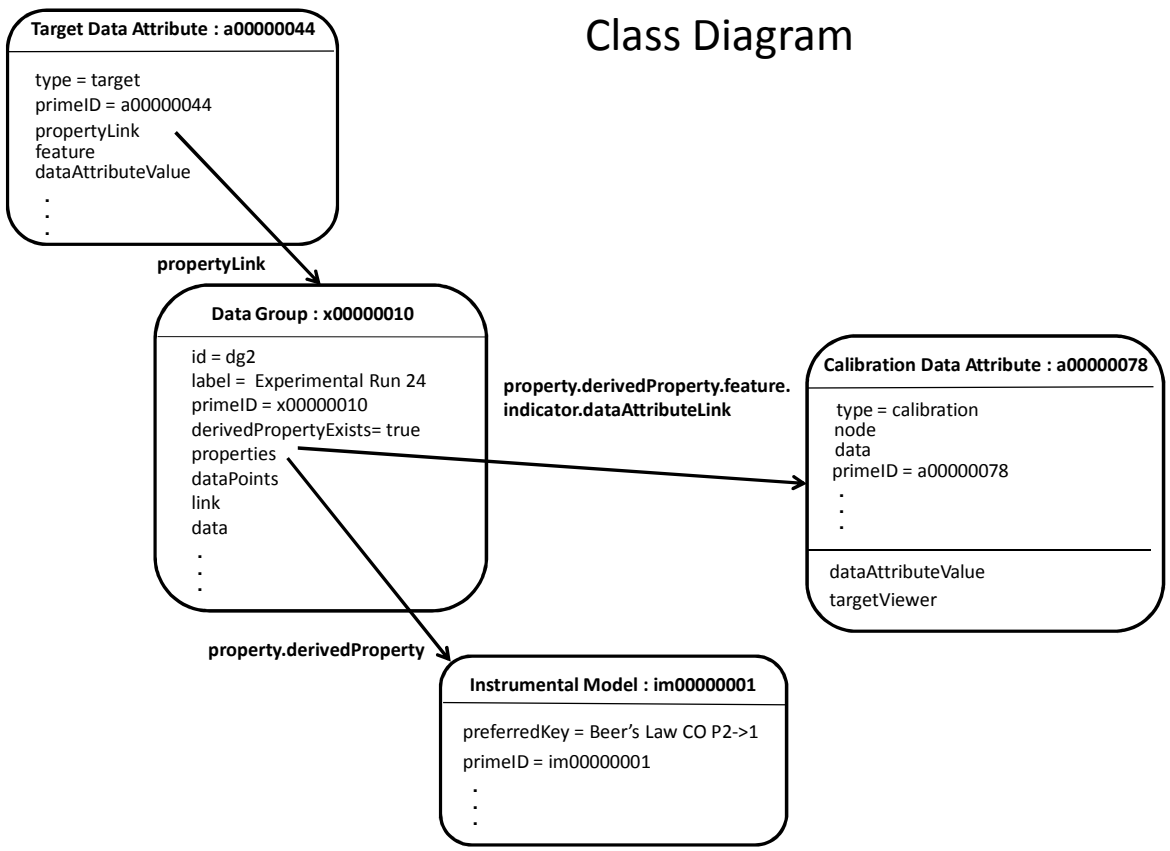

Figure 4.7. A class diagram showing the relationship between the PrIMe Target Data Attribute, PrIMe Experiment, PrIMe Instrumental Model, and PrIMe Calibration Data Attribute.

4.5 TargetViewer: Software to Display Raw Data in User-defined Format

A graphical user interface, called TargetViewer, has been developed to allow a user to select the format in which he or she wishes to view the experimental data. When the user wishes to view the data in raw format, the data are simply acquired from the experimental record and displayed. In the event that the user wishes to view the experimental data in the derived format, TargetViewer analyzes the raw data on-the-fly by means of the Instrumental Model that is linked to the experimental record. The application also displays calibration parameters and allows the user to input alternative values to perform data analysis in real time. The TargetViewer code is included in Appendix G.

A screenshot of TargetViewer is shown in Figure 4.8. The experimental data is plotted along with check boxes to select the format in which to display the experimental data. When the "Plot using Instrumental Model" box is checked, the data are presented in derived format; otherwise the raw data are displayed. On the left, the user can view the calibration parameter value and activate a button that will allow him to enter an alternative value. The user can get more details of the Instrumental Model by selecting "Instrumental Model" on the menu bar, which opens an additional window. Figure 4.9 shows a screenshot of the additional window giving Instrumental Model details. In this window, the Instrumental Model expression is displayed from the LaTeX encoding, if supplied in an `<additionalDataItem>` node. The properties, along with their descriptions and units, are also listed.

The MATLAB PrIMeInstrumentalModel class was created to enable the development of the TargetViewer application. The PrIMeInstrumentalModel class interacts with other classes of the PrIMe software to compute the derived data and display Instrumental Model information. The MATLAB code of the PrIMeInstrumentalModel class is included in Appendix H. The methods of this class perform the data analysis by the Instrumental Model and display properties and LaTeX representation of the Instrumental Model to the GUI.

4.6 Summary

In this chapter the PrIMe Instrumental Model has been applied to actual experimental data, a shock tube. It has been shown how by encoding the experimenters protocols and procedures by the Instrumental Model, the data analysis can be performed on-the-fly. An application, TargetViewer, was created to demonstrate this feature, by allowing the user to choose which format he or she views the experimental data.

In the next chapter, the Instrumental Model will be extended to a more complex experiment, a premixed laminar flame. The consistent treatment of experimental data by the Instrumental Model will allow us to integrate the raw experimental data in to

predictive models. The application of Data Collaboration and the Instrumental Model will facilitate uncertainty quantified predictions of species profile features.

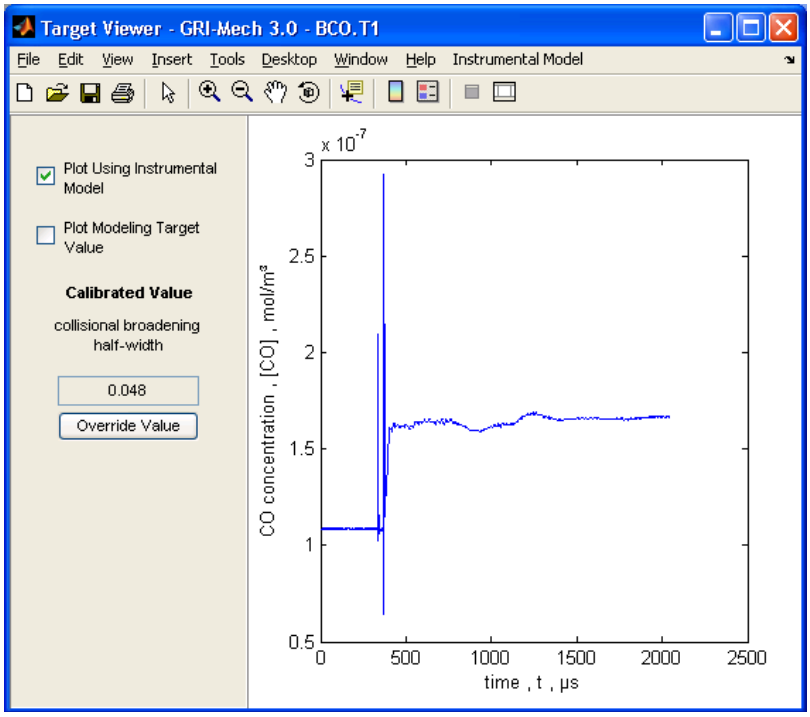

Figure 4.8. A snapshot from the TargetViewer GUI showing how the experimental data after analysis by the Instrumental Model.

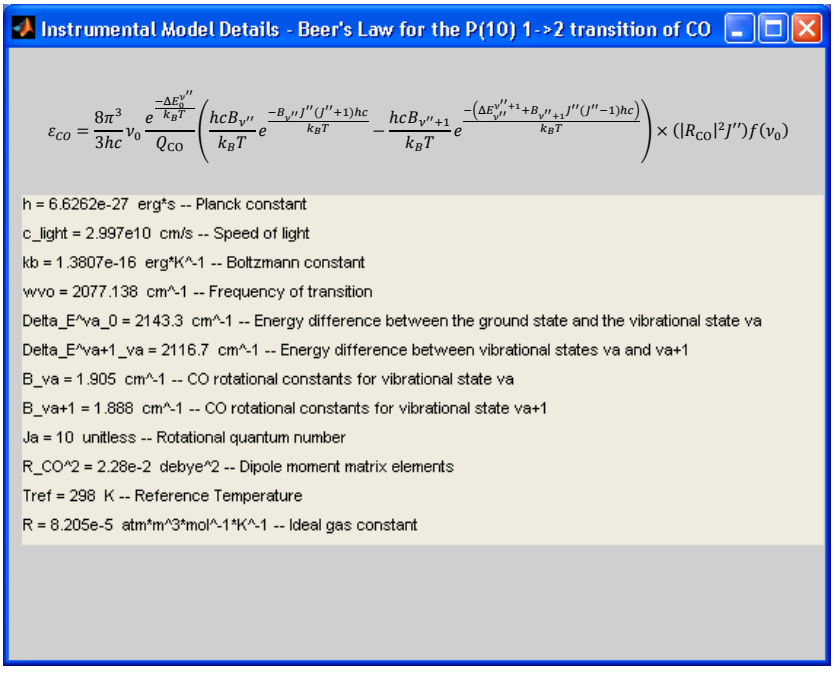

Figure 4.9. Details of the Instrumental Model given in the TargetViewer application.

Chapter 5

Application of the Instrumental Model to the Analysis of Complex Experimental Data

In this chapter, the Instrumental Model approach is extended from the work in the previous chapter to the analysis of a more complex system – an experimental premixed laminar flame mapped with VUV-photoionization molecular-beam mass spectrometry at the Advanced Light Source (ALS) of Lawrence Berkeley National Laboratory. The Instrumental Model improves the data analysis by reducing unnecessary assumptions and making uncertainty quantification more rigorous. It facilitates integration of model, calibration, and measurement uncertainties into a unified analysis. Expanding the scope of the Instrumental Model forced us to rethink the data analysis approach and choose an appropriate level of granularity to link data and model.

Typically, analysis of flame data is done by comparing derived properties, such as species concentration profiles, computed by a model to those derived from raw experimental data. Previous studies argued for benefits of a more direct analysis, extending model predictions to the actual experimental observables, because calculations of derived properties from the raw data usually invoke additional assumptions [23,24]. Yet, in a case like molecular-beam mass spectrometry, the raw data (mass spectra counts) are too granular, that is having a large amount of detail. The theoretical model and Instrumental Model lack sufficient information to predict the mass spectra counts directly. It is found here that meeting midway, at the integrated species signals, is a beneficial solution.

In this chapter it is shown how data analysis with the Instrumental Model and Data Collaboration delivers significant benefits over typical approaches. Predictions made by this approach consider information gained from experimental targets, the Instrumental Model, calibration parameters, and the theoretical model. This approach enables evaluation of dataset consistency using experimental signals. Furthermore, uncertainty estimates of the amount of background water, an unmeasured quantity, are made. Also uncertainty-quantified predictions of weak-signal quantities, in particular O, OH, and C_2H_3 signals, are estimated.

5.1 Experimental Flame

The present study employed the data from a fuel-lean acetylene premixed laminar flat flame: Φ = 0.96, 14 Torr, 11% C_2H_2–29% O_2–60% Ar, 70.5 cm/s gas velocity at burner surface and room temperature. The experimental flame data was acquired by Wenjun Li, Phil Westmoreland, and co-workers [68].

5.1.1 Description

The premixed laminar flat flame was measured using Photo-Ionization Molecular Beam Mass Spectrometry (PI-MBMS) at the Advanced Light Source of Lawrence Berkeley National Laboratory. The PI-MBMS experiment and procedures used for this work have been detailed in several previous papers [69-72]. A schematic of the experimental setup is shown in Figure 5.1. The main structure of the apparatus consists of a low-pressure flat-flame chamber, flame sampling system, molecular-beam photo-ionization region, and time-of-flight mass spectrometer. A premixed laminar flat flame was stabilized above the water-cooled, stainless-steel, porous McKenna-type burner. Flame species were sampled into a skimmer chamber through a quartz probe cone and were further collimated to form a molecular beam by a skimmer. The molecular beam was crossed and ionized by synchrotron-generated vacuum-ultraviolet light resolved to a specific energy with a monochromator.

Energy scans (signals as function of photon-ionization energy at fixed distance from burner surface) were acquired, which measure photo-ionization efficiency curves for species identification, and burner scans (signals as function of distance from burner surface with fixed photon-energy) were acquired, which measure species signal profiles. An example of a time-of-flight mass spectrum from a burner scan is shown in Figure 5.2. Species with high concentrations are shown as high peaks.

Typically the analysis of data from this flame is done by first integrating the mass spectra of each species of interest. The mass spectrum is integrated over intervals of time corresponding to the time-of-flight of the ionized molecule. These integrated signals are combined to form an integrated signal profile over the length of the physical domain. An example of the integrated signal profile for O_2 is shown in Figure 5.3.

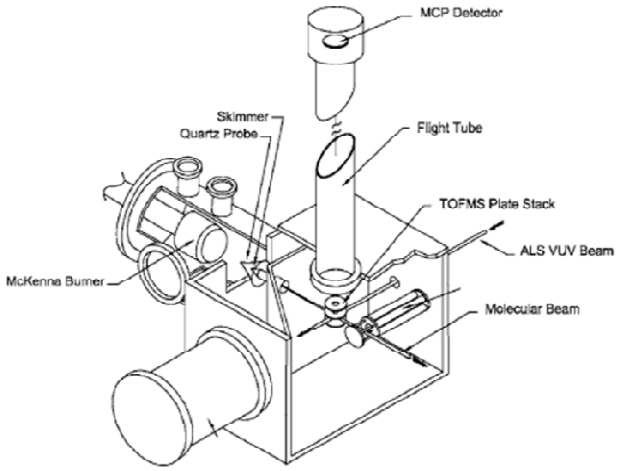

Figure 5.1. A schematic of the experimental flame and photoionization mass spectrometer [69].

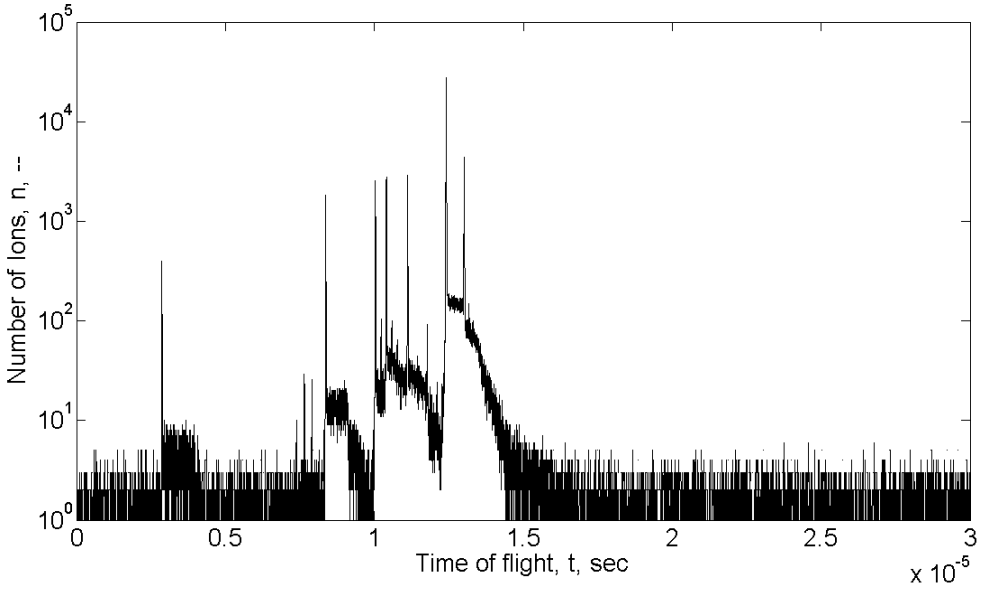

Figure 5.2. A mass spectrum acquired from a premixed-laminar flame experiment at the Advanced Light Source.

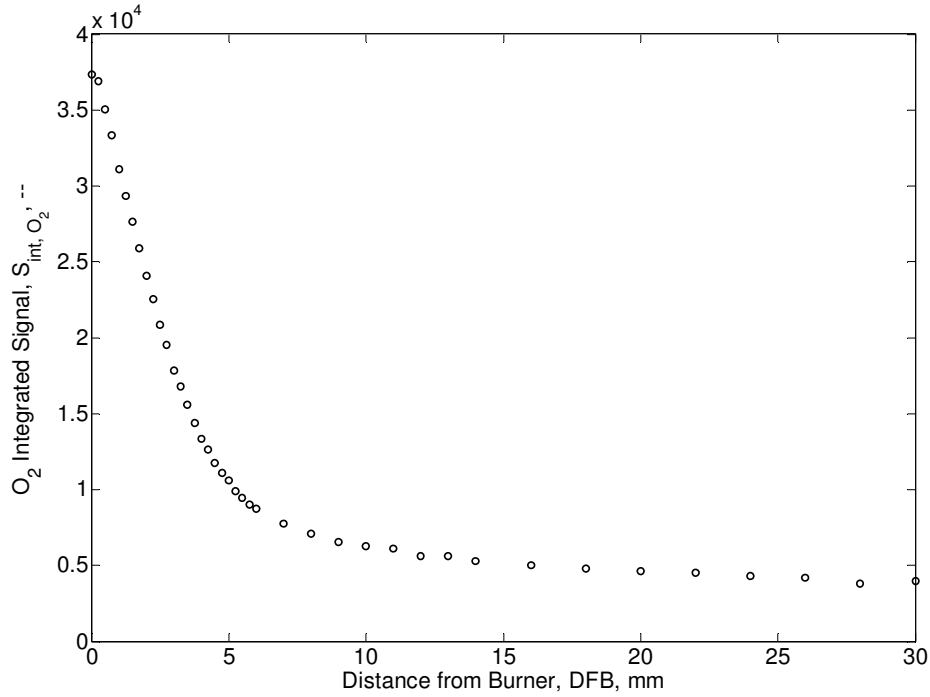

Figure 5.3. The integrated signal profile for O_2 over the distance from the burner.

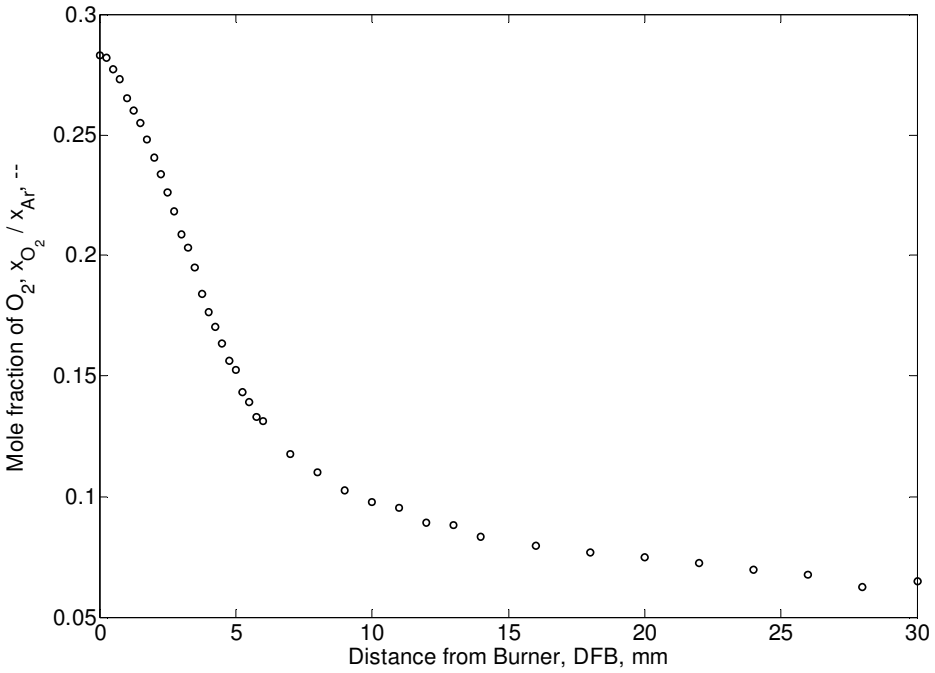

Figure 5.4. O_2 concentration profile computed from raw experimental data.

Traditionally the data is further analyzed to derive the species concentrations from the integrated signal profiles by the following equation.

$$\frac{x_i}{x_j} = \frac{S_i}{S_j} \cdot F_{i,j} \tag{5.1}$$

where S_i is the integrated signal of species i, x_i is the mole fraction of species i, and $F_{i,j}$ is the calibration factor for the ratio of species i over j. The calibration factor is determined from calibration experiments, computed from more fundamental quantities, or back calculated from mole balances. Detailed procedures for the mass-spectra experimental data analysis is given in previous studies [70,73,74]. A plot of the O_2 concentration derived from the integrated signal profile is given in Figure 5.4.

In this work predictions of the signals are made by transforming the model results to raw signal format by the Instrumental Model. This alternative approach is discussed in greater detail in section 5.3 where the Instrumental Model for this experiment is introduced.

5.1.2 Targets

The model was evaluated against a set of experimental *targets*, which are particular features of data selected for analysis [50]. Table 5.1 lists the chosen targets, specifying the species, photoionization energy, experimental target value, and estimated uncertainty bounds. The selected targets exhibited strong species signal ratios, which are integrated species signals normalized to the argon signal. The photoionization energy of the reference species, argon, is 16.2 eV. It should be noted that the convention used for specifying uncertainty bounds of targets, parameters, and prediction intervals is [*lower bound, upper bound*].

The chosen targets can be classified generally as three different types: peak value, peak location, and location of half-rise or half-decay. The peak value, denoted by PV, defines the peak value of the species signal ratio. The peak location, denoted by PL, defines the location of the peak species signal ratio. The location of half-rise or half-decay, denoted by HL and applied to monotonically increasing or decreasing species signal ratios, is the location at which ½ of the species signal ratio has risen or decayed.

Table 5.1. Experimental targets

Target Name	Species	Photoionization Energy (eV)	Experimental Value	Units	Uncertainty Bounds (% of nominal)
H2.PV	H_2	16.2	4.4×10^{-3}	*a*	[–10, 10]
H2.PL	H_2	16.2	0.432	cm	[–20, 10]
CH4.PV	CH_4	14.35	4.55×10^{-3}	*a*	[–10, 10]
CH4.PL	CH_4	14.35	0.170	cm	[–10, 10]
C2H2.HL	C_2H_2	16.2	0.292	cm	[–25, 10]
CO.PV	CO	14.35	1.120	*a*	[–10, 10]
CO.PL	CO	14.35	0.556	cm	[–10, 10]
O2.HL	O_2	16.2	0.415	cm	[–25, 10]
CO2.HL	CO_2	14.35	0.786	cm	[–25, 10]
H2O.T1	H_2O	16.2	1.86×10^{-2}	*a*	[–10, 10]
H2O.S0	H_2O	16.2	2.7×10^{-2}	*a*	[–10, 10]
H.HL	H	14.35	0.45	cm	[–25, 25]

a. Signal of species divided by signal of Ar; unitless.

Two additional targets, H2O.T1 and H2O.S0, have been selected for the purpose of determining the background H_2O mole fraction. H2O.T1 is defined as

$$\text{H2O.T1} = \frac{S_{\text{H}_2\text{O, 30 mm}} - S_{\text{H}_2\text{O, 0}}}{S_{\text{Ar, 0}}}, \tag{5.2}$$

where $S_{i,\,x}$ is the integrated signal of species i at distance x from the burner. H2O.S0 is defined as

$$\text{H2O.S0} = \frac{S_{\text{H}_2\text{O, 0}}}{S_{\text{Ar, 0}}}, \tag{5.3}$$

which is the species signal ratio of H_2O normalized to Ar at the burner surface.

5.2 Flame Model

5.2.1 Reaction Set

The reaction set used in this work is taken from the continuous efforts of Westmoreland and coworkers. The initial reaction set was assembled from the literature and theoretical calculations for ethylene and allene flame simulation [75]. The reaction set was further developed by improving the C_3-C_6 reaction subset, adding a cyclohexane subset [73,74], and more recently improving the simulation of fuel-rich 1-hexene and cyclohexane flames [68,76]. The entire reaction set is given in Appendix I.

5.2.2 Laminar Flame Simulations

Flame simulations were performed with CHEMKIN II subroutines [37] and the PREMIX [44] laminar flame code, incorporating multi-component transport and thermal diffusion [77]. Most reactions were considered reversible. The reverse rate coefficients were calculated from the forward rates and the chemical equilibrium constants. Most thermodynamic and transport parameters were obtained from the Burcat [34] or Sandia [35,77] databases. For some species not included in those databases, the method of Benson's group additivity [78] was used to estimate the thermodynamic data. Literature data and analogies to molecules of similar structure were used for transport parameters. A listing of the thermodynamic and transport properties is included in Appendix I.

5.3 Instrumental Model

The Instrumental Model was used in calculating experimental species signals from modeled species mole fractions. The Instrumental Model for the mass spectrometry data of the premixed flat flame is found by solving eq (5.1) for the integrated signal ratio. The Instrumental Model is given by

$$\frac{S_i}{S_j} = \frac{x_i}{x_j} \cdot F_{i,j}^{-1}, \tag{5.4}$$

where S_i is the integrated signal of species i, x_i is the mole fraction of species i, and $F_{i,j}$ is the calibration factor for the ratio of species i over j. Similar to the data analysis discussed in section 5.1.1, the calibration factors were determined from calibration measurements or extracted from the flame data using atom balance methods [70]. When calibration experiments and atom balance methods are impractical, the calibration factors can be estimated as

$$F_{i,j} = \frac{\sigma_i(E)}{\sigma_j(E)} \cdot \frac{MD_i}{MD_j}, \tag{5.5}$$

where $\sigma_i(E)$ is the photoionization cross section for species i at photon-energy E and MD_i is the mass discrimination factor for species i. The values for $F_{i,j}$, $\sigma_i(E)$, and MD_i used in this analysis are shown in Table 5.2. The uncertainty bounds for the calibration factors of eq (5.4) were determined from experimental calibration data and knowledge of the experimental data. The uncertainty bounds for the photoionization cross section and mass discrimination factors in eq (5.5) were estimated as ±15% of the values given by references [79-81] or measured from the current experiment, respectively.

The following targets use the calibration factor given in eq (5.4): H2.PV, CH4.PV, and CO.PV. The calibration factor defined in eq (5.5) is applied to H2O.T1 and H2O.S0. Targets defined in terms of distance from burner such as H2.PL, CH4.PL, CO.PL, C2H2.HL, O2.HL, CO2.HL, and H.HL do not require Instrumental Models since the signal profile and mole fraction profile have the same length scale.

Table 5.2. Instrumental Model parameters

Parameter Name	Photoionization Energy (eV)	Parameter Bounds	Source
$F_{H_2,Ar}$	16.2/16.2	[0.1499, 0.1566]	Calibration experiment
$F_{CH_4,CO2}$	14.35/14.35	[0.8938, 1.0434]	Calibration experiment
$F_{CO_2,\ Ar}$	14.35/16.2	[4.3542, 5.3218][a]	Extracted from atom balance
$F_{CO,\ Ar}$	14.35/16.2	[4.2019, 5.1357][a]	Extracted from atom balance
σ_{H_2O}	16.2	[12.2403, 16.5605][b]	Ref [79]
σ_{Ar}	16.2	[26.6440, 36.0478][b]	Ref [82]
MD_{H_2O}	–	[0.7953, 1.0760][b]	Calibration experiment
MD_{Ar}	–	[0.8466, 1.1454][b]	Calibration experiment

a. Relative uncertainty of 10%
b. Relative uncertainty of 15%

5.4 Dimensionality Reduction

Surrogate models, part of the Data Collaboration methodology, [1,12,50] were developed to approximate the detailed flame model responses. They were generated by sampling flame simulations over the reaction parameter space according to Latin-hypercube designs and fitting the results into second-order polynomials in the active variables as discussed in Chapter 2.

The entire reaction parameter space has a dimensionality of about 1000. To minimize the number of computer experiments that must be performed in this high-dimensional space, dimensionality reduction was performed in two steps: local-sensitivity analysis and active-subspace discovery.

5.4.1 Local-Sensitivity Analysis

In the first step of the analysis, the impact factors, products of corresponding sensitivity and uncertainty, were calculated to identify the active variables [8,50]. The calculation of the target sensitivity to each reaction model parameter from species sensitivities followed that of Goldenberg and Frenklach [48] discussed in section 2.5.1. In this step, active variables were identified by selecting parameters with the 20 largest impact factors for each of the 12 targets listed in Table 5.1and the 6 prediction features discussed later in section 5.8. The union of these parameters resulted in 50 active variables. Figure 5.5 shows the reactions with the 20 largest impact factors for the O2.HL target. Table 5.3 lists all of the active variables identified by this method, their rate coefficients, and associated uncertainty bounds. Uncertainty bounds of the active variables were obtained from either GRI Mech 3.0 [9] or were assumed to be a factor of 2 below and above the rate coefficient value reported in the reaction set. An additional variable, $x_{H_2O,in}$, which is discussed further in section 5.7 for the prediction of background H_2O, is added resulting in a total of 51 active variables.

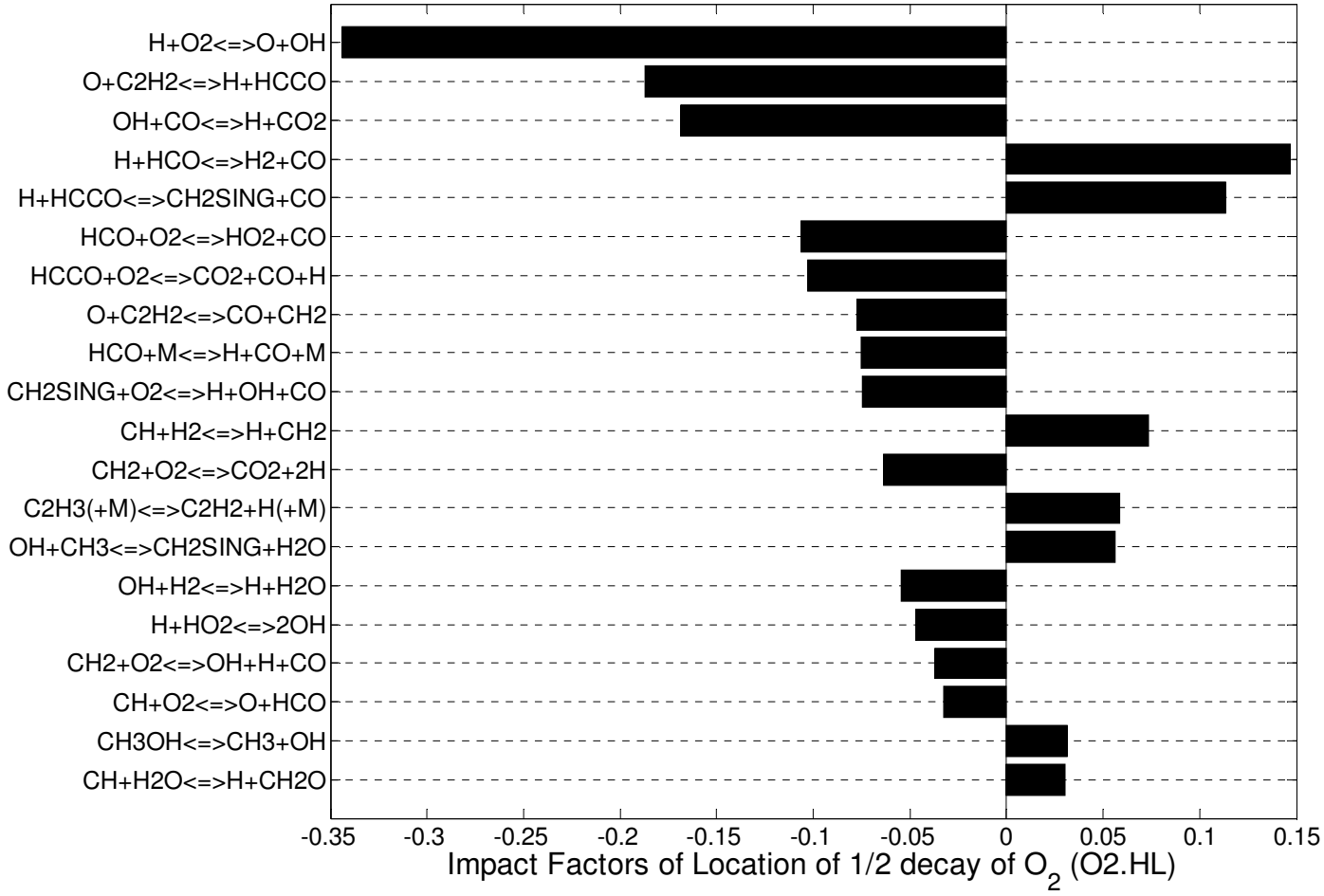

Figure 5.5. A plot of the reactions with the 20 largest impact factors for the location of ½ decay of O_2 target, O2.HL.

Table 5.3. List of active variables, reaction name, rate coefficient values, and uncertainty bounds.

Name	Reaction	Model Rate Coefficient Value	Uncertainty Bounds, factors relative to model value
X1	$O+H+M \rightarrow OH+M$	4.7100×10^{18}	[0.50, 2.00][b]
X2	$H+OH+M \rightarrow H_2O+M$	2.2100×10^{22}	[0.50, 2.00][a]
X3	$H_2O+O \rightarrow 2OH$	2.9700×10^{6}	[0.63, 1.60][a]
X4	$O+H_2 \rightarrow H+OH$	5.0800×10^{4}	[0.63, 1.60][a]
X5	$OH+H_2 \rightarrow H+H_2O$	2.1600×10^{8}	[0.77, 1.30][a]
X6	$H+O_2 \rightarrow O+OH$	2.0761×10^{16}	[0.87, 1.15][a]
X7	$H+HO_2 \rightarrow O_2+H_2$	1.6600×10^{13}	[0.31, 1.25][a]
X8	$H+HO_2 \rightarrow 2OH$	7.0800×10^{13}	[0.81, 3.23][a]
X9	$OH+HO_2 \rightarrow O_2+H_2O$	4.6400×10^{13}	[1.00, 4.00][a]
X10	$OH+CO \rightarrow H+CO_2$	4.1000×10^{4}	[0.83, 1.20][a]
X11	$O+HCO \rightarrow H+CO_2$	3.0000×10^{13}	[0.50, 2.00][b]
X12	$H+HCO \rightarrow H_2+CO$	7.3000×10^{13}	[0.33, 2.00][a]
X13	$OH+HCO \rightarrow H_2O+CO$	3.0000×10^{13}	[0.50, 2.00][b]
X14	$HCO+M \rightarrow H+CO+M$	1.8700×10^{17}	[0.50, 2.00][a]
X15	$HCO+O_2 \rightarrow HO_2+CO$	4.2200×10^{12}	[0.19, 1.69][a]
X16	$H+CH_2O \rightarrow HCO+H_2$	5.1800×10^{7}	[0.50, 2.00][a]
X17	$OH+CH_2O \rightarrow HCO+H_2O$	3.4300×10^{9}	[0.50, 2.00][a]
X18	$H+CH_2OH \rightarrow OH+CH_3$	9.6300×10^{13}	[0.40, 2.50][a]
X19	$CH_3OH \rightarrow CH_3+OH$	1.9000×10^{16}	[0.50, 2.00][b]
X20	$H+CH_4 \rightarrow CH_3+H_2$	6.6000×10^{8}	[0.67, 1.50][a]
X21	$OH+CH_4 \rightarrow CH_3+H_2O$	1.0000×10^{8}	[0.83, 1.20][a]
X22	$O+CH_3 \rightarrow H+CH_2O$	5.0600×10^{13}	[0.71, 1.40][a]
X23	$O+CH_3 \rightarrow H+H_2+CO$	3.3700×10^{13}	[0.71, 1.40][a]
X24	$OH+CH_3 \rightarrow CH_2(s)+H_2O$	6.4400×10^{17}	[0.33, 3.00][a]
X25	$CH_3+HCO \rightarrow CH_4+CO$	1.2100×10^{14}	[0.50, 2.00][b]
X26	$O+CH_2 \rightarrow H+HCO$	8.0000×10^{13}	[0.50, 2.00][b]

X27	$CH_2+O_2 \rightarrow OH+H+CO$	5.0000×10^{12}	[0.50, 2.00][a]
X28	$CH_2+O_2 \rightarrow CO_2+2H$	5.8000×10^{12}	[0.50, 2.00][a]
X29	$CH_2(s)+Ar \rightarrow CH_2+Ar$	9.0000×10^{12}	[0.71, 1.40][a]
X30	$CH_2(s)+CO_2 \rightarrow CO+CH_2O$	1.4000×10^{13}	[0.50, 2.00][b]
X31	$CH_2(s)+O_2 \rightarrow H+OH+CO$	2.8000×10^{13}	[0.63, 1.60][a]
X32	$CH_2(s)+O_2 \rightarrow CO+H_2O$	1.2000×10^{13}	[0.63, 1.60][a]
X33	$CH_2(s)+H_2 \rightarrow CH_3+H$	7.0000×10^{13}	[0.50, 2.00][a]
X34	$CH_2(s)+H_2O \rightarrow CH_2+H_2O$	3.0000×10^{13}	[0.33, 3.00][a]
X35	$CH+O_2 \rightarrow O+HCO$	6.7100×10^{13}	[0.79, 2.03][a]
X36	$CH+H_2 \rightarrow H+CH_2$	1.0800×10^{14}	[0.34, 2.70][a]
X37	$CH+H_2O \rightarrow H+CH_2O$	5.7100×10^{12}	[0.33, 3.00][a]
X38	$C_2H_4+CO \rightarrow C_2H_3+HCO$	1.5100×10^{14}	[0.50, 2.00][b]
X39	$C_2H_4+C_2H_2 \rightarrow 2C_2H_3$	2.4100×10^{13}	[0.50, 2.00][b]
X40	$C_2H_3 (+M) \rightarrow C_2H_2+H(+M)$	3.8600×10^{8}	[0.50, 2.00][b]
X41	$H+C_2H_3 \rightarrow H_2+C_2H_2$	9.6400×10^{13}	[0.50, 2.00][b]
X42	$C_2H_3+O_2 \rightarrow HCO+CH_2O$	5.4200×10^{12}	[0.40, 2.50][a]
X43	$C_2H_3+O_2 \rightarrow C_2H_3OO$	5.6100×10^{19}	[0.50, 2.00][b]
X44	$O+C_2H_2 \rightarrow H+HCCO$	1.3500×10^{7}	[0.50, 2.00][b]
X45	$O+C_2H_2 \rightarrow CO+CH_2$	6.9400×10^{6}	[0.50, 2.00][b]
X46	$C_2H_2+CH_2(s) \rightarrow C_3H_3+H$	3.4200×10^{15}	[0.50, 2.00][b]
X47	$O+HCCO \rightarrow H+2CO$	1.0000×10^{14}	[0.50, 2.00][b]
X48	$H+HCCO \rightarrow CH_2(s)+CO$	5.0000×10^{13}	[0.50, 2.00][b]
X49	$HCCO+O_2 \rightarrow CO_2+CO+H$	4.7800×10^{12}	[0.50, 2.00][b]
X50	$CH_3CHO \rightarrow CH_3+HCO$	9.5900×10^{14}	[0.50, 2.00][b]

a. Ref. [9]

b. Assumed uncertainty bounds.

5.4.2 Evaluation of Brute Force Sensitivity Analysis

The method of brute force sensitivity analysis, discussed in section 2.5.2, was compared to Taylor series approximation method, which was discussed in section 2.5.1. Sensitivity coefficients of 9 targets with respect to 14 active variables were calculated. Table 5.4 lists the sensitivity coefficients calculated by both the brute force method and from the Taylor series approximation method for the reaction coefficient of $H + O_2 \rightarrow O + OH$. The error in the Taylor series approximation varies from 0.18% to 17%. It was concluded that while the error in the approximation of the feature sensitivity may propagate to the surrogate model fit, the Taylor series approximation is acceptable for the evaluation of feature sensitivities.

Table 5.4. Sensitivity coefficients calculated by brute force and from the Taylor series approximation for 9 modeling features for the reaction $H + O_2 \rightarrow O + OH$.

	Brute Force	Taylor Series	Relative Error (%)
H2.PL	-0.0660	-0.0716	8.36
H2.PV	-0.0658	-0.0618	6.00
CH4.PL	0.0735	0.0835	13.70
CH4.PV	-0.0862	-0.1009	17.02
C2H2.HL	-0.1461	-0.1500	2.67
CO.PL	-0.0160	-0.0166	4.25
CO.PV	-0.1440	-0.1457	1.17
O2.HL	-0.1499	-0.1496	0.18
CO2.HL	-0.1394	-0.1408	0.94

5.4.3 Evaluation of Sensitivity to H_2O Diffusion Coefficient

Previous studies have shown that the sensitivity of transport properties is comparable to that of kinetic parameters [83,84]. The sensitivity of the response of the H2O.S0 feature to the Lennard-Jones potential well depth ε_{H_2O}. The diffusion coefficient depends on the Lennard-Jones potential well depth through the collision integral as described in Kee et al [77].

The sensitivity was calculated, by the brute force method, perturbing the input parameter ε_{H_2O}/k_B and evaluating the response of the feature H2O.S0 by

$$\frac{\Delta\left(\frac{x_{H_2O}}{x_{Ar}}\right)_{DFB=0}}{\Delta\frac{\varepsilon_{H_2O}}{k_B}} * \frac{\frac{\varepsilon_{H_2O}}{k_B}}{\left(\frac{x_{H_2O}}{x_{Ar}}\right)_{DFB=0}} \tag{5.9}$$

The original and perturbed values of the input and the response are given below in Table 5.5 along with the estimated sensitivity. The sensitivity to the Lennard-Jones potential well depth was an order of magnitude less than the sensitivity to the previously

chosen active parameters. It was concluded that the transport property of H_2O may be excluded from the active variable set.

Table 5.5. Values used in the computation of sensitivity of H2O.S0 to the Lennard-Jones potential well depth.

	ε_{H_2O}/k_B (K)	$\left(\frac{x_{H_2O}}{x_{Ar}}\right)_{DFB=0}$	Sensitivity
Nominal	572.4	0.079694	-0.0232
Perturbed	778.94	0.079028	

5.4.4 Active Subspace Discovery

In the second step, the parameter space was further reduced by active-subspace discovery [49], a method for identification of a lower-dimensional subspace discussed in section 2.6. The method of active-subspace discovery was adapted from Russi for application to the laminar flame. A surrogate model fit was determined for each of the 12 targets and 6 prediction features of the laminar flame. A single active-subspace dimension was determined such that the fitting error criterion for all targets and prediction features was satisfied. Differing from Russi, the gradients of each entry in the design matrix were computed simultaneously with the response, due to the long simulation times run on a dedicated cluster.

The procedure for each surrogate model requires detailed model responses $\boldsymbol{y}$ at each point of the design, design matrix $\mathbf{X}$, and gradient of the response $\mathbf{F}$. Detailed model responses were computed from a Latin hypercube sampling design of 32 computer experiments over the active variable space. The 51 active variables were transformed into factorial variables ranging from -1 to 1 and are given in the design matrix $\mathbf{X}$. At each design point the gradient $\mathbf{F}$ of the response was computed with respect to each active variable. The algorithm which was used to fit a surrogate model for each target or prediction feature over a range of singular values is given in Table 5.1. The fitting errors from the surrogate models of all targets and prediction features are examined to determine a single active-subspace dimension which satisfies the error criterion. The MATLAB code which executes this algorithm is included in Appendix J.

Singular value decomposition of the response gradient was performed as part of the method of active subspace discovery. A plot of the singular values for the target O2.HL is shown in Figure 5.6. The steep drop in the singular value as the number of singular vectors increases demonstrates that a lower dimension subspace can be used to approximate this target. Singular value plots for each target and prediction feature are given in Appendix K.

The dimension of the active subspace that accurately represents the full model was determined by iteratively increasing the singular values used to fit the approximating model. The surrogate model fit, mean fitting error, and maximum fitting error were computed and compiled for determination of the active-subspace dimension.

Table 5.6. Implementation of Active Subspace Discovery to Laminar Flame adapted from Russi [49].

Require: y **{response vector of experimental design}**
Require: X {design matrix}
Require: F {gradient of response with respect to active variables}
1: $n \leftarrow$ number of rows of design matrix (i.e. number of runs)
2: **for** i=1,…,n
3: $\mathbf{U}, \mathbf{\Sigma}, \mathbf{V} \leftarrow$ SVD of $\mathbf{F}$ {such that $\mathbf{F} = \mathbf{U\Sigma V}^T$}
4: $\mathbf{S} \leftarrow$ first i columns of $\mathbf{V}$
5: $\mathbf{z} \leftarrow \mathbf{S}^T\mathbf{X}$ {design matrix in low dimension}
6: $\mathbf{Q}_{\text{low dim},i} \leftarrow (\mathbf{z}^T\mathbf{z})^{-1}\mathbf{z}^T\boldsymbol{y}$ (such that $\hat{\boldsymbol{y}} = [1; \mathbf{z}]\mathbf{Q}_{\text{low dim},i}[1; \mathbf{z}]$)
7: $\hat{\boldsymbol{y}} \leftarrow [1; \mathbf{z}]\mathbf{Q}_{\text{low dim},i}[1; \mathbf{z}]$
8: $\mathbf{Q}_{\text{high dim},\,i} \leftarrow [1\ 0;\ 0\ \mathbf{S}]\ \mathbf{Q}_{\text{low dim},i}\ [1\ 0;\ 0\ \mathbf{S}^T]$
9: $\boldsymbol{\varepsilon}_{\text{avg},\,i} \leftarrow \text{mean}((\hat{\boldsymbol{y}} - \boldsymbol{y})/\boldsymbol{y}))$ {mean relative fitting error}
10: $\boldsymbol{\varepsilon}_{\text{max},\,i} \leftarrow \max((\hat{\boldsymbol{y}} - \boldsymbol{y})/\boldsymbol{y}))$ {maximum relative fitting error}
11: **end**
12: **return** $\mathbf{Q}_{\text{high dim},i}$, $\boldsymbol{\varepsilon}_{\text{avg},i}$, $\boldsymbol{\varepsilon}_{\text{max},i}$ for all i

A coefficient matrix $\mathbf{Q}_{\text{low dim}}$ in the low dimensional space was determined by a least squares fit to the detailed computer experiments. The surrogate model is given by

$$\hat{y} = \begin{bmatrix} 1 \\ \mathbf{S}^T\mathbf{X} \end{bmatrix}^T \mathbf{Q}_{\mathbf{low\ dim}} \begin{bmatrix} 1 \\ \mathbf{S}^T\mathbf{X} \end{bmatrix}. \tag{5.6}$$

The model is written with the coefficient matrix in active variable space as

$$\hat{y} = \begin{bmatrix} 1 \\ \mathbf{X} \end{bmatrix}^T \mathbf{Q}_{\mathbf{high\ dim}} \begin{bmatrix} 1 \\ \mathbf{X} \end{bmatrix}, \tag{5.7}$$

where

$$\mathbf{Q}_{\mathbf{high\ dim}} = \begin{bmatrix} 1 & 0 \\ 0 & \mathbf{S} \end{bmatrix} \mathbf{Q}_{\mathbf{low\ dim}} \begin{bmatrix} 1 & 0 \\ 0 & \mathbf{S}^T \end{bmatrix}. \tag{5.8}$$

In this work, a surrogate model is deemed to be acceptable when the maximum relative fitting error is below 15% and the average relative fitting error is below 5%. The fitting error was assessed with both in-design and out-of-design samples, where the out-of-design samples were randomly chosen points in the parameter space. Table 5.7 lists the relative average and maximum fitting errors for both in-sample and out-of-sample for the O2.HL target. It shows that a surrogate model in two dimensions is sufficient to approximate this target within specified error tolerances. It was found that an active subspace dimension of four was sufficient to build accurate surrogate models for all targets and prediction features. The fitting errors over an increasing number of singular values for each of the 12 targets and 6 prediction features are given in Appendix K.

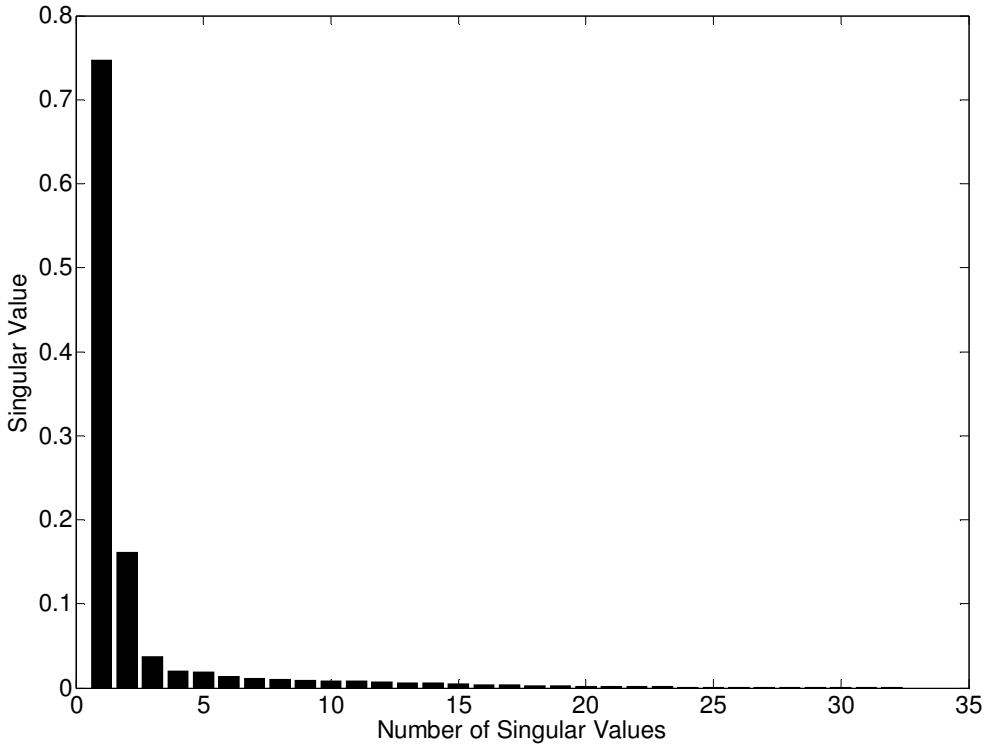

Figure 5.6. A plot of singular values of the O2.HL target.

Table 5.7. The relative average and maximum fitting errors in percentage of the surrogate model for O2.HL with increasing active subspace dimension.

Subspace Dimension	In-sample errors (%)		Out-of-sample errors (%)	
	Average	Maximum	Average	Maximum
1	2.96	11.28	2.63	7.04
2	0.52	1.77	0.74	2.23
3	0.48	1.40	0.69	2.68
4	0.39	1.26	0.79	2.20
5	0.17	0.58	0.57	1.45
6	0.04	0.16	0.93	2.43

It was found that further dimensionality reduction by active subspace discovery noticeably reduces the computational time for model building. For the system with 51 active variables and an active subspace dimension of 4, active subspace discovery reduced the computational time by a factor of 2.7. Based on this experience, for a system of 100 active variables and an active subspace dimension of 4, a rough estimate of the time reduction is about a factor of 10.

5.5 Data Collaboration

Data Collaboration was used to evaluate dataset consistency and make uncertainty-quantified predictions of the premixed laminar flame features. Figure 5.7 shows how the experiment, Instrumental Model, and surrogate model come together to create a dataset unit. The mass spectra counts, $S_{i,\text{obs}}$, are analyzed to integrated signals. The experimental targets are features of the integrated species signal profile, $S_{i,\text{calc}}$. The model results, $x_{i,\text{pred}}$, are transformed by the Instrumental Model to give a feature of the predicted signal profile, $S_{i,\text{pred}}$. The predicted signal is calculated from the surrogate model, Instrumental Model, and calibration data. The calibration parameters are the photoionization cross section, mass discrimination factor, and direct calibration factor, given by σ_i, MD_i, or $F_{i,j}$ respectively.

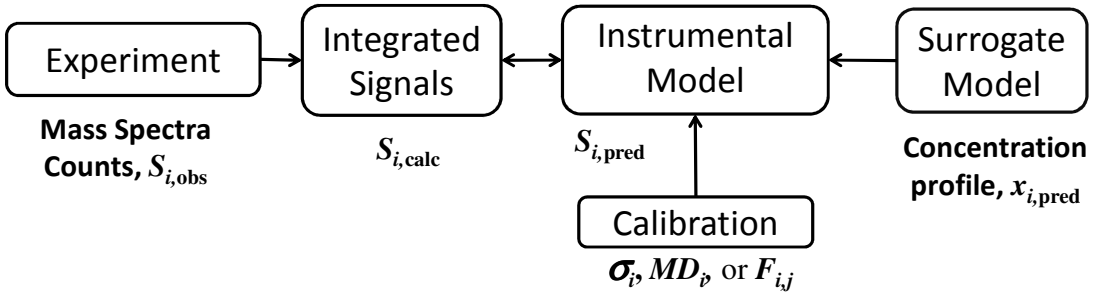

Figure 5.7. A schematic showing the data analysis approach of the premixed laminar flame with the Instrumental Model. Data Collaboration is used to determine dataset consistency of the dataset given by $S_{i,\text{calc}}$,with uncertainties, and $S_{i,\text{pred}}$ respectively.

5.5.1 Dataset Consistency

The consistency measure, introduced in section 2.2.2, was computed for the laminar flame dataset consisting of the experimental targets and uncertainty bounds listed in Table 5.1, and the corresponding surrogate models. The consistency measure was computed to be in the interval [0.1362, 0.2623], which indicates that the dataset is consistent. A screenshot of the Data Collaboration interface is shown in Figure 5.8. The left panel of this figure depicts the consistency measure bounds. The right panel displays the impact factors of the target and parameter bounds on the consistency measure [11]. The impact factors identify which targets and parameters contribute most to the consistency measure. The largest impact factor on the dataset consistency is the lower uncertainty bound of C2H2.HL target, meaning if one wanted to improve consistency, more information on the lower bound of C2H2.HL would have the greatest impact.

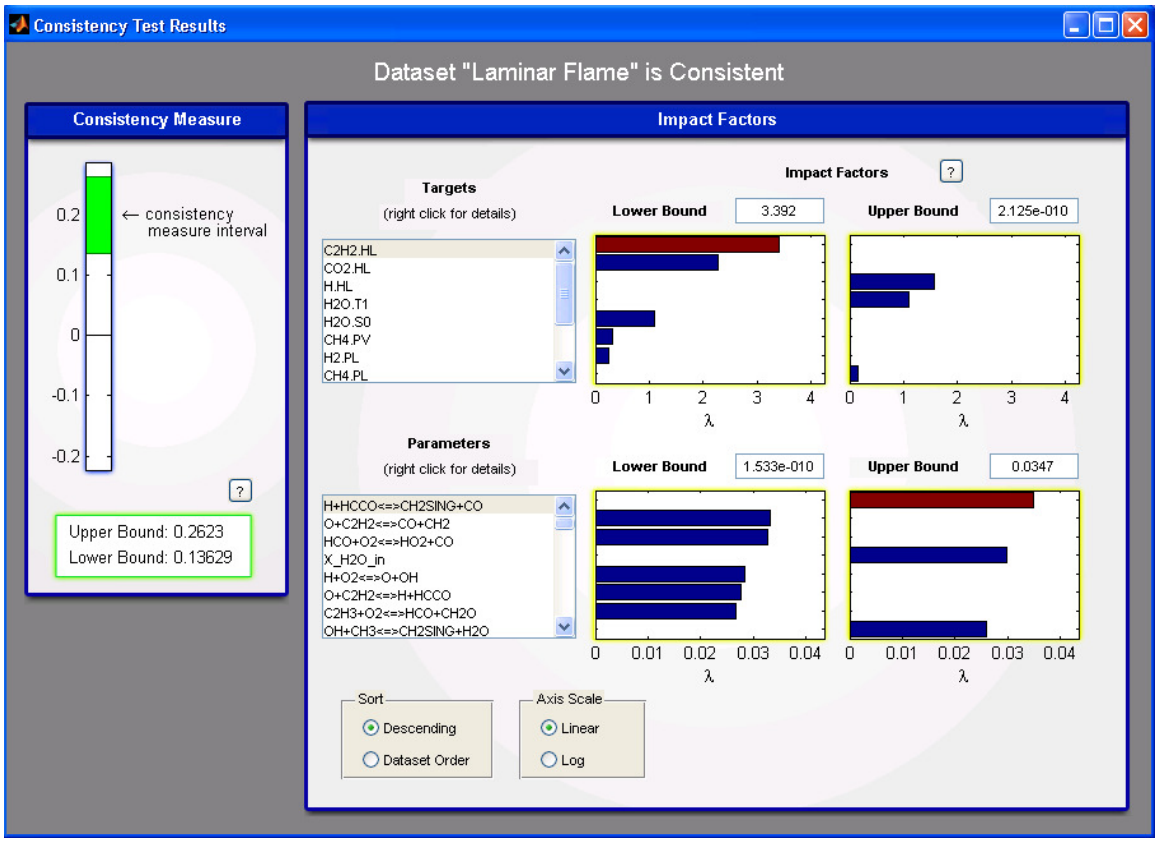

Figure 5.8. A snapshot of Data Collaboration interface of the PrIMe infrastructure. The premixed flat flame dataset has consistency measure bounds of [0.1362, 0.2623], thus is consistent.

5.6 Predictions

With dataset consistency established, the prediction intervals for O, OH, C_2H_3, and background H_2O mole fraction were determined.

5.7 Predicting Unmeasured Quantities – Background H_2O Mole Fraction

First, consider the objective of estimating the amount of background water vapor in the air using Data Collaboration. At any given point in a premixed laminar flat flame, the signal of H_2O results from 1) H_2O as a combustion product at that location, 2) H_2O transported to that point by convection or diffusion, or 3) background H_2O vapor which is initially present in the flame chamber.

The background water vapor is modeled as if it were a component of the inlet premixed gas mixture. The parameter $x_{H_2O,in}$ designates the mole fraction of H_2O in the inlet. From experimental considerations, as much as 50% of the water at the burner surface has been assumed to come from the background. The mole fraction of H_2O at the feed was estimated from calculating 0-50% of the experimentally determined mole fraction of water at the burner surface, resulting in $x_{H_2O,in}$ bounds of [0, 0.014778]. The prediction of background water was determined by repeatedly running Data Collaboration at trial lower bound values to identify the value which made the entire dataset consistent. The range of mole fraction of H_2O, $x_{H_2O,in}$, predicted in this manner for the given dataset is [0.002956, 0.014778]. In terms of percentage of water at the burner surface from the background, the prediction is [8.8, 44] %.

5.8 Predicting Weak-signal Properties – O, OH, C_2H_3

Surrogate models were developed for the prediction of the peak mole fractions and peak locations of O, OH, and C_2H_3. These species are difficult to measure in the flame due to weak and noisy signals. The intervals predicted for the O, OH, and C_2H_3 targets are listed in Table 5.8. The results using only the nominal parameter values are also shown for comparison. Figure 5.9 shows the prediction intervals for O.PV, the peak value of O, in the Data Collaboration interface. The prediction intervals are displayed on the left-hand side while the impact factors are displayed on the right-hand side. Similar to the consistency measure, the impact factors identify which targets and parameters contribute most to the prediction interval [13]. If one desires to improve the prediction interval of a model, reducing the uncertainty bounds of the targets and parameters with the highest impact factor would have the greatest effect.

Table 5.8. The predicted intervals for the O, OH, and C_2H_3 features. The result using the nominal parameter values is also shown.

Prediction Feature Names	Species	Outer Prediction Intervals	Result using Nominal Parameters	Unit
O.PV	O	[0.0273, 0.0429]	0.0373	*a*
O.PL	O	[1.8651, 2.2031]	1.9403	cm
OH.PV	OH	[0.0297, 0.0359]	0.0321	*a*
OH.PL	OH	[1.5963, 1.6749]	1.6069	cm
C2H3.PV	C_2H_3	[0.0086, 0.1148] × 10^{-3}	0.0451 × 10^{-3}	*a*
C2H3.PL	C_2H_3	[0.0060, 0.0390]	0.0136	cm

a. Mole fraction of the predicted species divided by the mole fraction of Ar; unitless.

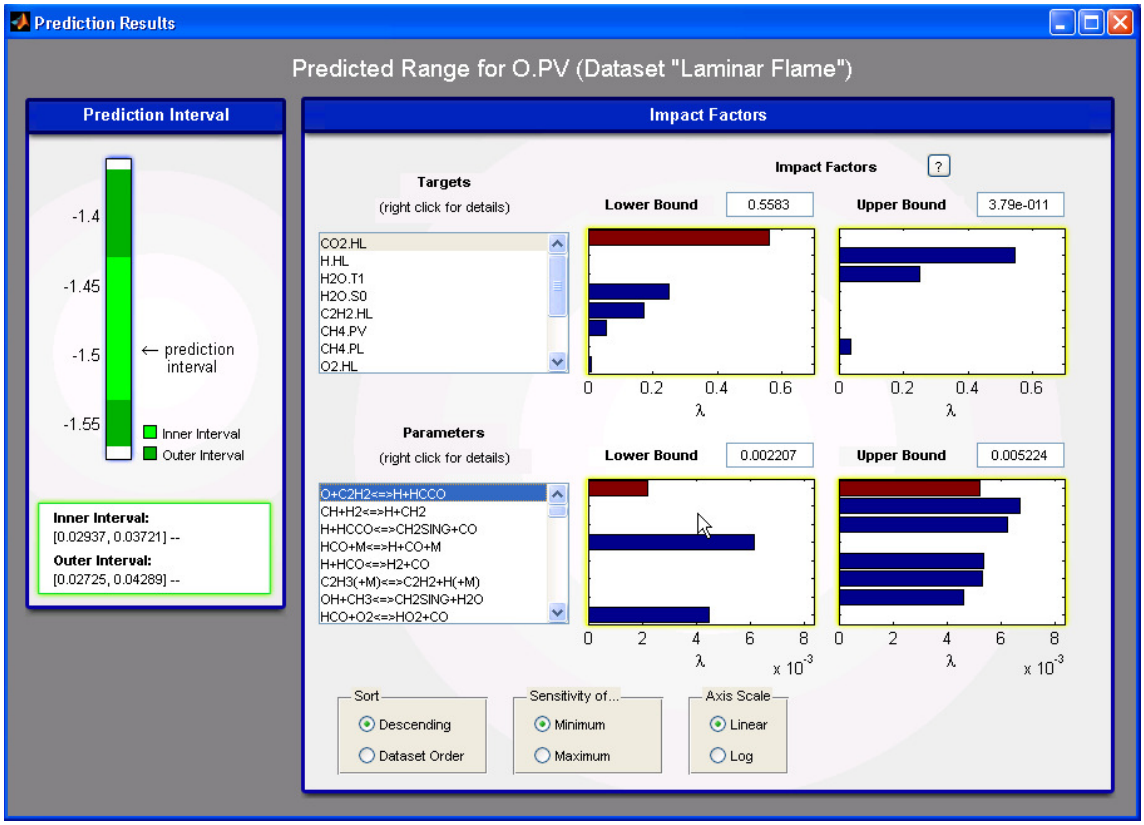

Figure 5.9. Prediction intervals for O.PV [0.0273, 0.0429] as shown in the Data Collaboration interface of the PrIMe infrastructure.

From Figure 5.9 it is seen that among all target and parameter uncertainties the lower bound of the CO2.HL target has the largest impact factor on the prediction interval for O.PV. This suggests that to improve the prediction of O.PV, better estimates of the lower bound of CO2.HL should be obtained. An analysis was performed, where the lower uncertainty bound of CO2.HL, shown in Table 5.1, was increased from -25% to -16%. The consistency measure decreased due to the tighter constraints from [0.1362, 0.2623] to [0.00, 0.15] indicating that the feasible set was decreased. As expected, the prediction bounds of O.PV, displayed in Table 5.8, were narrowed from [0.0273, 0.0429] to [0.029, 0.039]. The impact factor of the lower bound of CO2.HL remained the maximum of all targets and parameters. Further increases in the lower uncertainty bound of CO2.HL resulted in an inconclusive dataset consistency.

Conversely, the lower uncertainty bound of CO2.HL was decreased from -25% to -28%. The consistency measure increased from [0.1362, 0.2623] to [0.1660, 0.2892], demonstrating an easing of the constraints on the feasible set. The prediction interval of O.PV was slightly increased from [0.0273, 0.0429] to [0.0267, 0.0437]. At this decreased uncertainty bound of CO2.HL the impact factor of the H.HL target became the dominant impact factor.

It has been suggested by the experimenter [85] that the gas which is sampled by the instrument is not exactly at the tip of the sampling probe, but some small distance up stream. To reduce the uncertainty in the target value, an alternative approach would be to include the probe perturbation effect in the Instrumental Model.

5.9 Conclusions

The methodology of Instrumental Model and Data Collaboration enabled a rigorous comparison between model and data to quantify what is meant by “model predicts the data”. The model is shown to be quantifiably consistent with data, and hence can be further applied to predicting properties. As specific examples, prediction of an unmeasured property, background water vapor, was quantified and error bounds for weak-signal properties, O, OH, and C_2H_3, were computed. Bringing more data into the analysis can eliminate further assumptions and tighten model and prediction uncertainties. The impact factors produced by Data Collaboration suggest where the main effort for improving model and prediction uncertainties should be placed, which in the present case clearly suggest improving target uncertainties.

Chapter 6

Summary and Future Work

In this dissertation an approach leading to consistent treatment of experimental data for the building of predictive models, called the PrIMe Instrumental Model, was introduced. The Instrumental Model is a formalized approach to capturing the protocols and procedures of experimental data analysis. The Instrumental Model was applied to two sets of experimental data demonstrating its utility in the analysis of raw experimental data. In Chapter 1 a new approach to archival and analysis of raw experimental data was motivated. The supporting technologies and methods for the work in this dissertation were given in Chapter 2. The concept of the Instrumental Model was introduced in Chapter 3 with examples of how one encodes the data analysis procedure in XML. The Instrumental was applied to shock tube experimental data in Chapter 4. It was shown how a derived property, concentration, can be calculated on-the-fly from the raw experimental data with the Instrumental Model. In Chapter 5 the Instrumental Model was extended to a more complex experiment, a premixed-laminar flame measured with a photoionization mass spectrometer. The laminar flame dataset, including raw data and model predictions by the Instrumental Model, was determined to be consistent. Predictions of an unmeasured quantity and weak-signal properties were made.

In Chapter 4, it was shown how the archival of scientific data was improved by the proper treatment of experimental data by the Instrumental Model approach. The raw experimental data and data analysis procedure can be archived in a consistent manner. This feature of the Instrumental Model encourages scientific discovery by allowing one to make new interpretations of experimental data with the application of newly discovered physical theories.

In Chapter 5, it was demonstrated that the Instrumental Model assists in making predictions of raw experimental data. Furthermore, the combination of Instrumental Model and Data Collaboration make possible a quantitative evaluation of dataset consistency with raw experimental data. It was shown how predictions of unmeasured and weak-signal quantities can be made from knowledge of the raw experimental data, Instrumental Model, calibration data, and theoretical model.

To push the capabilities of the Instrumental Model further, a greater emphasis should be placed on integration with the web-based PrIMe Workflow Application. Creation, submission, and linking experimental data to an Instrumental Model should be made possible through the PrIMe Workflow Application.

Greater benefits of the Instrumental Model/Data Collaboration approach can be realized by including more data to create extensive datasets. Including data from

heterogeneous experiment types representing varied phenomena will lead to a more systematic approach to building improved predictive models.

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Appendix A.

Example Calculation of Feature Sensitivities from Normalized Species Sensitivities

For the laminar flame experiment, one important experimental feature is the peak value of the mass spectra signal ratio of H2 over Ar. The relationship between the species concentration and experimental integrated mass spectra signals is given by

$$\frac{S_{H_2}}{S_{Ar}} = \frac{x_{H_2}}{x_{Ar}} * {F_{H_2,Ar}}^{-1}, \tag{B.1}$$

where S_{H_2} is the integrated mass spectra signal for H2, S_{Ar} is the integrated mass spectra signal for Ar, and $F_{H_2,Ar}$ is the calibration factor from calibration data [65]. The experimental feature is defined as

$$C = \text{peak}\left(\frac{S_{H_2}}{S_{Ar}}\right) = \text{peak}\left(\frac{x_{H_2}}{x_{Ar}} * {F_{H_2,Ar}}^{-1}\right). \tag{B.2}$$

The perturbed concentrations $\tilde{x}_{H_2} and\ \tilde{x}_{Ar}$ are computed from concentrations, x_{H_2} and x_{Ar}, and sensitivities, $E_{H_2,j}$ and $E_{Ar,j}$,with a first order Taylor series [48] by perturbing each model parameter by $\Delta\theta_j$ as

$$\tilde{x}_{H_2,j} \approx x_{H_2} + E_{H_2,j}\Delta\theta_j \tag{B.3a}$$

and

$$\tilde{x}_{Ar,j} \approx x_{Ar} + E_{Ar,j}\Delta\theta_j. \tag{B.3b}$$

Since the Taylor series approximation is valid for small $\Delta\theta_j$ the value of $\Delta\theta_j$ was chosen to be $0.005\ \theta_j$. It was found that the feature sensitivities reach an asymptotic limit for values of $\Delta\theta_j/\theta_j < 0.01$.

A perturbed feature $\tilde{C}_\text{j}$ can be calculated from the perturbed mole fractions as

$$\tilde{C}_\text{j} = \text{peak}\left(\frac{\tilde{x}_{H_2}}{\tilde{x}_{Ar}} * {F_{H_2,Ar}}^{-1}\right). \tag{B.4}$$

The peak value is determined from a cubic splines interpolation over the discrete set of simulation responses. The Taylor series approximation is also used to compute the absolute feature sensitivity from the perturbed feature $\tilde{C}_\text{j}$ by

$$E_{C,j} = \left(\frac{\tilde{C}(k_j + \Delta k_j) - C}{\Delta k_j} \right). \tag{B.5}$$

Finally, the logarithmic sensitivity of the feature C, $E_{log_{C,j}}$, is calculated from the feature sensitivity by

$$E_{log_{C,j}} = \frac{\theta_j}{C} E_{C,j}. \tag{B.6}$$

Similarly, the sensitivity of the feature with respect to the calibration factors can be computed. The perturbed signal ratio can be calculated by

$$\frac{\widetilde{S_{H_2}}}{S_{Ar}} \approx \frac{S_{H_2}}{S_{Ar}} + \frac{\partial \left(\frac{S_{H_2}}{S_{Ar}} \right)}{\partial F} \Delta F, \tag{B.7}$$

where

$$\frac{\partial \left(\frac{S_{H_2}}{S_{Ar}} \right)}{\partial F} = -\frac{x_{H_2}}{x_{Ar}} * {F_{H_2,Ar}}^{-2}. \tag{B.8}$$

The perturbed feature is calculated by

$$\tilde{C}_{\mathrm{F}} = \mathrm{peak}\left(\frac{\widetilde{S_{H_2}}}{S_{Ar}} \right). \tag{B.9}$$

The sensitivity and logarithmic sensitivity of the feature with respect to the calibration factor is calculated from

$$E_{C,F} = \left(\frac{\tilde{C}(F + \Delta F) - C}{\Delta F} \right) \tag{B.10}$$

and

$$E_{log_{C,F}} = \frac{F}{C} E_{C,F}. \tag{B.11}$$

Appendix B.

PrIMe Instrumental Model XML Schema

```
<?xml version="1.0" encoding="UTF-8"?>
<xs:schema xmlns="http://purl.org/NET/prime/"
targetNamespace="http://purl.org/NET/prime/" xmlns:xs="http://www.w3.org/2001/XMLSchema"
xmlns:m="http://www.w3.org/1998/Math/MathML"  elementFormDefault="qualified">
    <xs:import namespace="http://www.w3.org/1998/Math/MathML"
schemaLocation="http://www.w3.org/Math/XMLSchema/mathml2/mathml2.xsd"/>

  <xs:annotation id="ID">
    <xs:documentation xml:lang="en">PrIMe Instrumental Model XML
schema</xs:documentation>
  </xs:annotation>

  <xs:annotation id="copyright">
    <xs:documentation xml:lang="en">primekinetics.org 2008-2009</xs:documentation>
  </xs:annotation>

  <xs:annotation id="createdBy">
    <xs:documentation xml:lang="en">Devin R. Yeates, University of California at
Berkeley, 9 Sept 2008</xs:documentation>
  </xs:annotation>

  <xs:annotation id="authoredBy">
    <xs:documentation xml:lang="en">Michael Frenklach, University of California at
Berkeley</xs:documentation>
    <xs:documentation xml:lang="en">Devin R. Yeates, University of California at
Berkeley</xs:documentation>
  </xs:annotation>

  <xs:annotation id="lastEditedBy">
    <xs:documentation xml:lang="en">Xiaoqing You, University of California at Berkeley,
16 Sept 2010</xs:documentation>
  </xs:annotation>

  <xs:element name="instrumentalModel">
    <xs:complexType>
      <xs:sequence>
        <xs:element name="copyright" type="xs:string" minOccurs="0" maxOccurs="1" />
        <xs:element name="content" type="xs:string" minOccurs="0" maxOccurs="unbounded"
/>
        <xs:element name="preferredKey" type="preferredKeyType" minOccurs="0"
maxOccurs="unbounded" />
        <xs:element name="bibliographyLink" type="bibliographyLinkType" minOccurs="0"
maxOccurs="unbounded" />
        <xs:element name="keyword" type="xs:string" minOccurs="0" maxOccurs="unbounded"
/>
        <xs:element name="property" type="propertyType" minOccurs="0"
maxOccurs="unbounded" />
        <xs:element name="variable" type="variableType" minOccurs="0"
maxOccurs="unbounded" />
        <xs:element name="instrumentalModelExpression"
type="instrumentalModelExpressionType" minOccurs="0" maxOccurs="1" />
        <xs:element name="additionalDataItem" type="additionalDataItemType" minOccurs="0"
maxOccurs="unbounded" />
      </xs:sequence>
      <xs:attribute name="primeID" type="primeInstrumentalModelIDType" use="required" />
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  </xs:element>
```

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        <xs:element name="value" type="xs:string" minOccurs="0" maxOccurs="1" />
        <xs:element name="uncertainty" type="uncertaintyType" minOccurs="0" maxOccurs="2"
/>
        <xs:element name="component" type="componentType" minOccurs="0"
maxOccurs="unbounded" />
        <xs:element name="speciesLink" type="speciesLinkType" minOccurs="0"
maxOccurs="unbounded" />
    </xs:sequence>
    <xs:attribute name="id" type="xs:string" use="optional" />
    <xs:attribute name="label" type="xs:string" use="optional" />
    <xs:attribute name="name" type="xs:string" use="required" />
    <xs:attribute name="units" type="xs:string" use="optional" />
    <xs:attribute name="description" type="xs:string" use="optional" />
  </xs:complexType>

  <xs:complexType name="componentType">
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        <xs:element name="speciesLink" type="speciesLinkType" minOccurs="1" maxOccurs="1"
/>
        <xs:element name="amount" type="amountType" minOccurs="0" maxOccurs="1" />
        <xs:element name="uncertainty" type="uncertaintyType" minOccurs="0" maxOccurs="2"
/>
    </xs:sequence>
  </xs:complexType>

  <xs:complexType name="amountType">
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            <xs:attribute name="units" type="xs:string" use="required" />
        </xs:extension>
    </xs:simpleContent>
  </xs:complexType>

  <xs:complexType name="uncertaintyType">
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            <xs:attribute name="kind" type="xs:string" use="required" />
            <xs:attribute name="transformation" type="xs:string" use="required" />
        </xs:extension>
    </xs:simpleContent>
  </xs:complexType>

  <xs:complexType name="speciesLinkType">
    <xs:attribute name="preferredKey" type="xs:string" use="required" />
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  </xs:complexType>


  <xs:complexType name="variableType">
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        <xs:element name="expression" type="expressionType" minOccurs="0" maxOccurs="1" />
    </xs:sequence>
    <xs:attribute name="id" type="xs:string" use="required" />
    <xs:attribute name="type" type="variableTypeType" use="optional" />
  </xs:complexType>

    <xs:simpleType name="variableTypeType">
    <xs:restriction base="xs:string">
      <xs:enumeration value="vector" />
      <xs:enumeration value="matrix" />
    </xs:restriction>
  </xs:simpleType>

  <xs:complexType name="instrumentalModelExpressionType">
    <xs:sequence>
        <xs:element ref="m:math"/>
    </xs:sequence>
```

```
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    <xs:attribute name="implicit" type="implicitType" use="required" />
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  <xs:complexType name="expressionType">
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            <xs:attribute name="group" type="xs:string" use="optional"/>
        </xs:extension>
    </xs:simpleContent>
  </xs:complexType>

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      <xs:pattern value="im\d{8}" />
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  <xs:simpleType name="primeSpeciesIDType">
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  <xs:simpleType name="implicitType">
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  <xs:complexType name="additionalDataItemType">
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        <xs:attribute name="description" type="xs:string" use="optional" />
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    </xs:simpleContent>
  </xs:complexType>

  <xs:simpleType name="primeBiblioIDType">
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    </xs:restriction>
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  <xs:simpleType name="itemTypeTypes">
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      <xs:enumeration value="file" />
      <xs:enumeration value="text" />
      <xs:enumeration value="MATLAB function" />
    </xs:restriction>
  </xs:simpleType>
</xs:schema>
```

Appendix C.

PrIMe Experiment XML Schema

```
<?xml version="1.0" encoding="UTF-8"?>

<xs:schema xmlns="http://purl.org/NET/prime/"
           targetNamespace="http://purl.org/NET/prime/"
           xmlns:xs="http://www.w3.org/2001/XMLSchema"
           elementFormDefault="qualified">

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      <xs:documentation xml:lang="en">PrIMe Experiments XML schema</xs:documentation>
   </xs:annotation>

   <xs:annotation id="copyright">
      <xs:documentation xml:lang="en"> ©primekinetics.org 2005-2009</xs:documentation>
   </xs:annotation>

   <xs:annotation id="createdBy">
      <xs:documentation xml:lang="en">Zoran M. Djurisic, University of California at
Berkeley, 20 Jan 2005</xs:documentation>
   </xs:annotation>

   <xs:annotation id="authoredBy">
      <xs:documentation xml:lang="en">Michael Frenklach, University of California at
Berkeley</xs:documentation>
      <xs:documentation xml:lang="en">Zoran M. Djurisic, University of California at
Berkeley</xs:documentation>
      <xs:documentation xml:lang="en">Devin R. Yeates, University of California at
Berkeley</xs:documentation>
   </xs:annotation>


   <xs:annotation id="lastEditedBy">
      <xs:documentation xml:lang="en">Michael Frenklach, University of California at
Berkeley, 28 February 2011</xs:documentation>
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            <xs:element name="content"            type="contentType"
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            <xs:element name="preferredKey"       type="preferredKeyType"
minOccurs="0" maxOccurs="unbounded" />
            <xs:element name="bibliographyLink"   type="bibliographyLinkType"
minOccurs="1" maxOccurs="unbounded" />
            <xs:element name="apparatus"          type="apparatusType"
minOccurs="1" maxOccurs="1"         />
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```

```
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minOccurs="1" maxOccurs="unbounded" />
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minOccurs="0" maxOccurs="unbounded" />
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            <xs:attribute name="bibliography" type="primeBiblioIDType" use="optional"/>
         </xs:extension>
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   </xs:complexType>

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      <xs:simpleContent>
         <xs:extension base="xs:string">
            <xs:attribute name="type"  type="xs:string" use="optional"/>
            <xs:attribute name="group" type="xs:string" use="optional"/>
         </xs:extension>
      </xs:simpleContent>
   </xs:complexType>

   <xs:complexType name="bibliographyLinkType">
      <xs:attribute name="preferredKey" type="xs:string"         use="required"/>
      <xs:attribute name="primeID"      type="primeBiblioIDType" use="required"/>
   </xs:complexType>

   <xs:complexType name="apparatusType">
      <xs:sequence>
         <xs:element name="kind"     type="kindType"     minOccurs="1" maxOccurs="1" />
         <xs:element name="mode"     type="modeType"     minOccurs="0"
maxOccurs="unbounded" />
         <xs:element name="property" type="propertyType" minOccurs="0"
maxOccurs="unbounded" />
      </xs:sequence>
   </xs:complexType>

   <xs:simpleType name="kindType">
      <xs:restriction base="xs:string">
         <xs:enumeration value="flame"/>
         <xs:enumeration value="flow reactor"/>
         <xs:enumeration value="rapid compression machine"/>
         <xs:enumeration value="shock tube"/>
         <xs:enumeration value="spherical bomb"/>
         <xs:enumeration value="stirred reactor"/>
      </xs:restriction>
   </xs:simpleType>

   <xs:simpleType name="modeType">
      <xs:restriction base="xs:string">
         <xs:enumeration value="laminar"/>
         <xs:enumeration value="turbulent"/>
         <xs:enumeration value="premixed"/>
         <xs:enumeration value="opposed jet"/>
         <xs:enumeration value="incident shock"/>
         <xs:enumeration value="reflected shock"/>
         <xs:enumeration value="burner-stabilized"/>
```

```
         <xs:enumeration value="stagnation"/>
         <xs:enumeration value="twin flat"/>
         <xs:enumeration value="curved"/>
         <xs:enumeration value="tubular"/>
         <xs:enumeration value="porous plate"/>
         <xs:enumeration value="counterflow"/>
         <xs:enumeration value="spherical"/>
         <xs:enumeration value="dynamic"/>
         <xs:enumeration value="steady"/>
      </xs:restriction>
   </xs:simpleType>

   <xs:complexType name="commonPropertiesType">
      <xs:sequence>
         <xs:element name="property" type="propertyType" minOccurs="1"
maxOccurs="unbounded" />
      </xs:sequence>
   </xs:complexType>

   <xs:complexType name="propertyType">
      <xs:sequence>
         <xs:element name="value"       type="xs:string"       minOccurs="0"
maxOccurs="1" />
         <xs:element name="uncertainty" type="uncertaintyType" minOccurs="0"
maxOccurs="2" />
         <xs:element name="component"   type="componentType"   minOccurs="0"
maxOccurs="unbounded" />
         <xs:element name="speciesLink" type="speciesLinkType" minOccurs="0"
maxOccurs="unbounded" />
        <xs:element name="derivedProperty"   type="derivedPropertyType"    minOccurs="0"
maxOccurs="unbounded" />
      </xs:sequence>
      <xs:attribute name="id"                      type="xs:string"
use="optional"/>
      <xs:attribute name="label"                   type="xs:string"
use="optional"/>
      <xs:attribute name="name"                    type="propertyNameType"
use="required"/>
      <xs:attribute name="units"                   type="propertyUnitsType"
use="optional"/>
      <xs:attribute name="description"             type="xs:string"
use="optional"/>
      <xs:attribute name="derivedPropertyExists" type="xs:string"  use="optional"/>
   </xs:complexType>

   <xs:simpleType name="propertyNameType">
      <xs:restriction base="xs:string">
         <xs:enumeration value="distance"/>
         <xs:enumeration value="diameter"/>
         <xs:enumeration value="length"/>
         <xs:enumeration value="volume"/>
         <xs:enumeration value="pressure"/>
         <xs:enumeration value="temperature"/>
         <xs:enumeration value="concentration"/>
         <xs:enumeration value="composition"/>
         <xs:enumeration value="density"/>
         <xs:enumeration value="flow rate"/>
         <xs:enumeration value="speed"/>
         <xs:enumeration value="flame speed"/>
         <xs:enumeration value="time"/>
         <xs:enumeration value="residence time"/>
         <xs:enumeration value="ignition delay"/>
```

```
      <xs:enumeration value="material"/>
      <xs:enumeration value="initial composition"/>
      <xs:enumeration value="sensitivity" />
      <xs:enumeration value="voltage" />
      <xs:enumeration value="equivalence ratio" />
      <xs:enumeration value="parameter" />
      <xs:enumeration value="number" />
      <xs:enumeration value="current" />
      <xs:enumeration value="energy" />
      <xs:enumeration value="area" />
      <xs:enumeration value="light" />
   </xs:restriction>
</xs:simpleType>

 <xs:simpleType name="propertyUnitsType">
    <xs:restriction base="xs:string">
        <xs:enumeration value="µ"/>
        <xs:enumeration value="µm"/>
        <xs:enumeration value="nm"/>
        <xs:enumeration value="mm"/>
        <xs:enumeration value="cm"/>
        <xs:enumeration value="m"/>
        <xs:enumeration value="Mbarn"/>
        <xs:enumeration value="cm³"/>
        <xs:enumeration value="dm³"/>
        <xs:enumeration value="L"/>
        <xs:enumeration value="m³"/>
        <xs:enumeration value="Pa"/>
        <xs:enumeration value="bar"/>
        <xs:enumeration value="atm"/>
        <xs:enumeration value="Torr"/>
        <xs:enumeration value="K"/>
        <xs:enumeration value="°F"/>
        <xs:enumeration value="°C"/>
        <xs:enumeration value="mol/cm³"/>
        <xs:enumeration value="mol/dm³"/>
        <xs:enumeration value="mol/m³"/>
        <xs:enumeration value="molecule/cm³"/>
        <xs:enumeration value="molecule/dm³"/>
        <xs:enumeration value="molecule/m³"/>
        <xs:enumeration value="1/cm³"/>
        <xs:enumeration value="1/dm³"/>
        <xs:enumeration value="1/m³"/>
        <xs:enumeration value="arbitrary"/>
        <xs:enumeration value="mole fraction"/>
        <xs:enumeration value="volume fraction"/>
        <xs:enumeration value="mass fraction"/>
        <xs:enumeration value="ppm"/>
        <xs:enumeration value="g/cm³"/>
        <xs:enumeration value="kg/m³"/>
        <xs:enumeration value="g/(cm² s)"/>
        <xs:enumeration value="kg/(m² s)"/>
        <xs:enumeration value="mol/(m² s)"/>
        <xs:enumeration value="dm³/min"/>
        <xs:enumeration value="slm"/>
        <xs:enumeration value="g/s"/>
        <xs:enumeration value="m/s"/>
        <xs:enumeration value="cm/s"/>
        <xs:enumeration value="hr"/>
        <xs:enumeration value="min"/>
        <xs:enumeration value="s"/>
        <xs:enumeration value="ms"/>
```

```
            <xs:enumeration value="µs"/>
            <xs:enumeration value="ns"/>
            <xs:enumeration value="ps"/>
            <xs:enumeration value="fs"/>
            <xs:enumeration value="mV"/>
            <xs:enumeration value="mV/psi"/>
            <xs:enumeration value="cm^-1*atm^-1"/>
            <xs:enumeration value="nA"/>
            <xs:enumeration value="eV"/>
            <xs:enumeration value="unitless"/>
            <xs:enumeration value="dimensionless"/>
            <xs:enumeration value=""/>
         </xs:restriction>
     </xs:simpleType>

   <xs:complexType name="componentType">
      <xs:sequence>
         <xs:element name="speciesLink" type="speciesLinkType" minOccurs="1"
maxOccurs="1" />
         <xs:element name="amount"      type="amountType"      minOccurs="0"
maxOccurs="1" />
         <xs:element name="uncertainty" type="uncertaintyType" minOccurs="0"
maxOccurs="2" />
      </xs:sequence>
   </xs:complexType>

   <xs:complexType name="uncertaintyType">
      <xs:simpleContent>
         <xs:extension base="xs:double">
            <xs:attribute name="bound"          type="xs:string" use="required"/>
            <xs:attribute name="kind"           type="xs:string" use="required"/>
            <xs:attribute name="transformation" type="xs:string" use="required"/>
         </xs:extension>
      </xs:simpleContent>
   </xs:complexType>

   <xs:complexType name="speciesLinkType">
      <xs:attribute name="preferredKey" type="xs:string"          use="required"/>
      <xs:attribute name="primeID"      type="primeSpeciesIDType" use="required"/>
      <xs:attribute name="method"     type="speciesLinkMethod"      use="optional"/>
   </xs:complexType>


   <xs:complexType name="amountType">
      <xs:simpleContent>
         <xs:extension base="xs:double">
            <xs:attribute name="units" type="xs:string" use="required" />
         </xs:extension>
      </xs:simpleContent>
   </xs:complexType>

   <xs:complexType name="dataGroupType">
      <xs:sequence>
         <xs:element name="dataGroupLink"           type="dataGroupLinkType"
    minOccurs="0" maxOccurs="1" />
         <xs:element name="property"                type="propertyType"
    minOccurs="2" maxOccurs="unbounded" />
         <xs:element name="dataPoint"               type="dataPointType"
    minOccurs="0" maxOccurs="unbounded"/>
      </xs:sequence>
      <xs:attribute name="id"    type="xs:string" use="required"/>
      <xs:attribute name="label" type="xs:string" use="optional"/>
```

```
      <xs:attribute name="dataPointForm" type="dataType" use="optional"/>
   </xs:complexType>

   <xs:simpleType name="dataType">
       <xs:restriction base="xs:string">
           <xs:enumeration value = "XML" />
           <xs:enumeration value = "HDF5" />
           <xs:enumeration value = "CDF" />
       </xs:restriction>
    </xs:simpleType>

    <xs:simpleType name="speciesLinkMethod">
       <xs:restriction base="xs:string">
           <xs:enumeration value = "relativeAtomicMass" />
           <xs:enumeration value = "isotopeAbundance" />
       </xs:restriction>
    </xs:simpleType>

   <xs:complexType name="dataGroupLinkType">
      <xs:attribute name="dataGroupID" type="xs:string" use="required"/>
      <xs:attribute name="dataPointID" type="xs:string" use="required"/>
   </xs:complexType>

   <xs:complexType name="derivedPropertyType">
     <xs:sequence>
       <xs:element name="feature" type="featureType" minOccurs="0" maxOccurs="unbounded"
/>
     </xs:sequence>
     <xs:attribute name="id"      type="xs:string" use="optional"/>
     <xs:attribute name="label"       type="xs:string"         use="optional"/>
     <xs:attribute name="name"        type="propertyNameType"  use="required"/>
     <xs:attribute name="units"       type="propertyUnitsType" use="optional"/>
     <xs:attribute name="description" type="xs:string"         use="optional"/>
   </xs:complexType>

   <xs:complexType name="featureType">
      <xs:sequence>
         <xs:element name="fraction"  type="xs:string" minOccurs="0" maxOccurs="1"/>
         <xs:element name="indicator"  type="variableType" minOccurs="1"
maxOccurs="unbounded"/>
         <xs:element name="observable" type="variableType" minOccurs="1"
maxOccurs="unbounded"/>
      </xs:sequence>
      <xs:attribute name="id"   type="xs:string"       use="required"/>
      <xs:attribute name="type"  use="required">
       <xs:simpleType>
         <xs:restriction base="xs:token">
           <xs:enumeration value="instrumentalModel"/>
         </xs:restriction>
       </xs:simpleType>
     </xs:attribute>
     <xs:attribute name="primeID" type="primeInstrumentalModelIDType" use="optional" />
   </xs:complexType>

   <xs:complexType name="variableType">
      <xs:sequence>
       <xs:choice>
            <xs:element name="value" type="valueType" minOccurs="0" maxOccurs="1"/>
            <xs:element name="valueLink" type="valueLinkType" minOccurs="0"
maxOccurs="1"/>
            <xs:element name="dataAttributeLink" type="dataAttributeLinkType"
minOccurs="0" maxOccurs="1"/>
```

```
            <xs:element name="speciesLink" type="speciesLinkType" minOccurs="0"
maxOccurs="1"/>
            <xs:element name="propertyLink" type="propertyLinkType" minOccurs="0"
maxOccurs="unbounded"/>
            <xs:element name="feature" type="featureType" minOccurs="0" maxOccurs="1"/>
        </xs:choice>
      </xs:sequence>
      <xs:attribute name="id"                        type="xs:string" use="required"/>
      <xs:attribute name="featureID"                 type="xs:string" use="optional"/>
      <xs:attribute name="variableID"                type="xs:string" use="optional"/>
      <xs:attribute name="transformation"            type="xs:string" use="optional"/>
   </xs:complexType>

   <xs:complexType name="valueType">
      <xs:simpleContent>
         <xs:extension base="xs:double"/>
      </xs:simpleContent>
   </xs:complexType>

   <xs:complexType name="valueLinkType">
      <xs:simpleContent>
         <xs:extension base="xs:string">
            <xs:attribute name="experimentPrimeID"  type="primeExperimentIDType"
use="required"/>
            <xs:attribute name="dataGroupID"        type="xs:string"
use="required"/>
            <xs:attribute name="dataPointID"         type="xs:string"
use="required"/>
            <xs:attribute name="propertyID"       type="xs:string"
use="required"/>
         </xs:extension>
      </xs:simpleContent>
   </xs:complexType>

   <xs:complexType name="dataAttributeLinkType">
     <xs:attribute name="id" type="xs:string" use="required"/>
     <xs:attri?ute name="primeID" type="primeDataAttributeIDType" use="required"/>
   </xs:complexType>

   <xs:complexType name="propertyLinkType">
       <xs:simpleContent>
           <xs:extension base="xs:string">
               <xs:attribute name="id" type="xs:string" use="optional" />
               <xs:attribute name="experimentPrimeID" type="primeExperimentIDType"
use="optional" />
               <xs:attribute name="dataGroupID" type="xs:string" use="optional" />
               <xs:attribute name="propertyID" type="xs:string" use="required" />
               <xs:attribute name="propertyName" type="xs:string" use="optional" />
               <xs:attribute name="componentPrimeID" type="primeSpeciesIDType"
use="optional" />
           </xs:extension>
       </xs:simpleContent>
   </xs:complexType>

   <xs:complexType name="dataPointType">
      <xs:sequence>
         <xs:element name="x1" type="xType" minOccurs="1" maxOccurs="1" />
         <xs:element name="x2" type="xType" minOccurs="1" maxOccurs="1" />
         <xs:element name="x3" type="xType" minOccurs="0" maxOccurs="1" />
         <xs:element name="x4" type="xType" minOccurs="0" maxOccurs="1" />
         <xs:element name="x5" type="xType" minOccurs="0" maxOccurs="1" />
         <xs:element name="x6" type="xType" minOccurs="0" maxOccurs="1" />
```

```
         <xs:element name="x7" type="xType" minOccurs="0" maxOccurs="1" />
         <xs:element name="x8" type="xType" minOccurs="0" maxOccurs="1" />
         <xs:element name="x9" type="xType" minOccurs="0" maxOccurs="1" />
        <xs:element name="x10" type="xType" minOccurs="0" maxOccurs="1" />
        <xs:element name="x11" type="xType" minOccurs="0" maxOccurs="1" />
      </xs:sequence>
      <xs:attribute name="id" type="xs:string" use="optional"/>
   </xs:complexType>

   <xs:complexType name="xType" mixed="true">
      <xs:sequence>
         <xs:element name="uncertainty"  type="uncertaintyType"  minOccurs="0"
maxOccurs="2" />
      </xs:sequence>
   </xs:complexType>

   <xs:simpleType name="primeExperimentIDType">
      <xs:restriction base="xs:string">
         <xs:pattern value="x\d{8}"/>
      </xs:restriction>
   </xs:simpleType>

   <xs:simpleType name="primeBiblioIDType">
      <xs:restriction base="xs:string">
         <xs:pattern value="b\d{8}"/>
      </xs:restriction>
   </xs:simpleType>

   <xs:simpleType name="primeSpeciesIDType">
      <xs:restriction base="xs:string">
         <xs:pattern value="s\d{8}"/>
      </xs:restriction>
   </xs:simpleType>

   <xs:simpleType name="primeInstrumentalModelIDType">
      <xs:restriction base="xs:string">
         <xs:pattern value="im\d{8}"/>
      </xs:restriction>
   </xs:simpleType>

   <xs:simpleType name="primeDataAttributeIDType">
      <xs:restriction base="xs:string">
         <xs:pattern value="a\d{8}"/>
      </xs:restriction>
   </xs:simpleType>

   <xs:complexType name="attributableString">
      <xs:simpleContent>
         <xs:extension base="xs:string">
            <xs:attribute name="source" type="xs:string" use="optional"/>
         </xs:extension>
      </xs:simpleContent>
   </xs:complexType>

   <xs:complexType name="additionalDataItemType">
      <xs:simpleContent>
         <xs:extension base="xs:string">
            <xs:attribute name="itemType"    type="itemTypeTypes" use="required"/>
            <xs:attribute name="description" type="xs:string"     use="optional"/>
            <xs:attribute name="MIME"        type="xs:string"     use="optional"/>
         </xs:extension>
      </xs:simpleContent>
```

```
   </xs:complexType>

   <xs:simpleType name="itemTypeTypes">
      <xs:restriction base="xs:string">
         <xs:enumeration value="URI"/>
         <xs:enumeration value="file"/>
         <xs:enumeration value="text"/>
      </xs:restriction>
   </xs:simpleType>
</xs:schema>
```

Appendix D.

PrIMe Instrumental Model XML record of the shock tube data analysis.

```
<?xml version="1.0" encoding="UTF-8"?>
<instrumentalModel xsi:schemaLocation="http://purl.org/NET/prime/
http://warehouse.primekinetics.org/schema/instrumentalModel.xsd
http://www.w3.org/1998/Math/MathML http://www.w3.org/Math/XMLSchema/mathml2/mathml2.xsd"
primeID="im00000001" xmlns="http://purl.org/NET/prime/"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xmlns:m="http://www.w3.org/1998/Math/MathML" >
    <copyright>primekinetics.org 2008</copyright>
    <preferredKey group="prime">Beer's Law for the P(10) 1->2 transition of
CO</preferredKey>
    <keyword>laser absorption</keyword>
    <property description="Planck constant" name="parameter" units="erg*s" id="h">
        <value>6.6262e-27</value>
    </property>
    <property description="Speed of light" name="speed" units="cm/s" id="c_light">
        <value>2.997e10</value>
    </property>
    <property description="Boltzmann constant" name="parameter" units="erg*K^-1" id="kb">
        <value>1.3807e-16</value>
    </property>
    <property description="Frequency of transition" name="frequency" units="cm^-1"
id="wvo">
        <value>2077.138</value>
    </property>
    <property description="Energy difference between the ground state and the vibrational
state va" name="energy" units="cm^-1" id="Delta_E^va_0">
        <value>2143.3</value>
    </property>
    <property description="Energy difference between vibrational states va and va+1"
name="energy" units="cm^-1" id="Delta_E^va+1_va">
        <value>2116.7</value>
    </property>
    <property description="CO rotational constants for vibrational state va"
name="parameter" units="cm^-1" id="B_va">
        <value>1.905</value>
    </property>
    <property description="CO rotational constants for vibrational state va+1"
name="parameter" units="cm^-1" id="B_va+1">
        <value>1.888</value>
    </property>
    <property description="Rotational quantum number" name="parameter" units="unitless"
id="Ja">
        <value>10</value>
    </property>
    <property description="Dipole moment matrix elements" name="parameter" units="debye^2"
id="R_CO^2">
        <value>2.28e-2</value>
    </property>
    <property description="Reference Temperature" name="temperature" units="K" id="Tref">
```

```
        <value>298</value>
    </property>
    <property description="Ideal gas constant" name="parameter" units="atm*m^3*mol^-1*K^-
1" id="R">
        <value>8.205e-5</value>
    </property>
    <variable id="C" />
    <variable id="V_inf" />
    <variable id="V" />
    <variable id="V_0" />
    <variable id="L" />
    <variable id="T" />
    <variable id="C_tot" />
    <variable id="gamma" />
    <variable id="P" >
        <expression type="MathML">
            <m:math>
                <m:apply>
                    <m:times/>
                    <m:ci>R</m:ci>
                    <m:ci>T</m:ci>
                    <m:ci>C_tot</m:ci>
                </m:apply>
            </m:math>
        </expression>
    </variable>
    <variable id="n">
        <expression type="MathML">
            <m:math>
                <m:apply>
                    <m:plus/>
                    <m:apply>
                        <m:times/>
                        <m:cn>0.71</m:cn>
                        <m:apply>
                            <m:divide/>
                            <m:apply>
                                <m:times/>
                                <m:apply>
                                    <m:minus/>
                                    <m:ci>T</m:ci>
                                    <m:cn>1300</m:cn>
                                </m:apply>
                                <m:apply>
                                    <m:minus/>
                                    <m:ci>T</m:ci>
                                    <m:cn>2000</m:cn>
                                </m:apply>
                                <m:apply>
                                    <m:minus/>
                                    <m:ci>T</m:ci>
                                    <m:cn>2700</m:cn>
                                </m:apply>
                                <m:apply>
                                    <m:minus/>
                                    <m:ci>T</m:ci>
                                    <m:cn>3500</m:cn>
                                </m:apply>
                            </m:apply>
                            <m:cn>3.078e12</m:cn>
                        </m:apply>
                    </m:apply>
```

```
<m:apply>
    <m:times/>
    <m:cn>0.69</m:cn>
    <m:apply>
        <m:divide/>
        <m:apply>
            <m:times/>
            <m:apply>
                <m:minus/>
                <m:ci>T</m:ci>
                <m:cn>800</m:cn>
            </m:apply>
            <m:apply>
                <m:minus/>
                <m:ci>T</m:ci>
                <m:cn>2000</m:cn>
            </m:apply>
            <m:apply>
                <m:minus/>
                <m:ci>T</m:ci>
                <m:cn>2700</m:cn>
            </m:apply>
            <m:apply>
                <m:minus/>
                <m:ci>T</m:ci>
                <m:cn>3500</m:cn>
            </m:apply>
        </m:apply>
        <m:cn>-1.078e12</m:cn>
    </m:apply>
</m:apply>
<m:apply>
    <m:times/>
    <m:cn>0.68</m:cn>
    <m:apply>
        <m:divide/>
        <m:apply>
            <m:times/>
            <m:apply>
                <m:minus/>
                <m:ci>T</m:ci>
                <m:cn>800</m:cn>
            </m:apply>
            <m:apply>
                <m:minus/>
                <m:ci>T</m:ci>
                <m:cn>1300</m:cn>
            </m:apply>
            <m:apply>
                <m:minus/>
                <m:ci>T</m:ci>
                <m:cn>2700</m:cn>
            </m:apply>
            <m:apply>
                <m:minus/>
                <m:ci>T</m:ci>
                <m:cn>3500</m:cn>
            </m:apply>
        </m:apply>
        <m:cn>8.82e11</m:cn>
    </m:apply>
</m:apply>
```

```
<m:apply>
    <m:times/>
    <m:cn>0.67</m:cn>
    <m:apply>
        <m:divide/>
        <m:apply>
            <m:times/>
            <m:apply>
                <m:minus/>
                <m:ci>T</m:ci>
                <m:cn>800</m:cn>
            </m:apply>
            <m:apply>
                <m:minus/>
                <m:ci>T</m:ci>
                <m:cn>1300</m:cn>
            </m:apply>
            <m:apply>
                <m:minus/>
                <m:ci>T</m:ci>
                <m:cn>2000</m:cn>
            </m:apply>
            <m:apply>
                <m:minus/>
                <m:ci>T</m:ci>
                <m:cn>3500</m:cn>
            </m:apply>
        </m:apply>
        <m:cn>-1.4896e12</m:cn>
    </m:apply>
</m:apply>
<m:apply>
    <m:times/>
    <m:cn>0.66</m:cn>
    <m:apply>
        <m:divide/>
        <m:apply>
            <m:times/>
            <m:apply>
                <m:minus/>
                <m:ci>T</m:ci>
                <m:cn>800</m:cn>
            </m:apply>
            <m:apply>
                <m:minus/>
                <m:ci>T</m:ci>
                <m:cn>1300</m:cn>
            </m:apply>
            <m:apply>
                <m:minus/>
                <m:ci>T</m:ci>
                <m:cn>2000</m:cn>
            </m:apply>
            <m:apply>
                <m:minus/>
                <m:ci>T</m:ci>
                <m:cn>2700</m:cn>
            </m:apply>
        </m:apply>
        <m:cn>7.128e12</m:cn>
    </m:apply>
</m:apply>
```

```
            </m:apply>
        </m:math>
    </expression>
</variable>
<variable id="erfc(a)" >
    <expression type="MathML">
        <m:math>
            <m:apply>
                <m:minus/>
                <m:cn>1</m:cn>
                <m:apply>
                    <m:times/>
                    <m:apply>
                        <m:divide/>
                        <m:cn>2</m:cn>
                        <m:apply>
                            <m:root/>
                            <m:pi/>
                        </m:apply>
                    </m:apply>
                    <m:apply>
                        <m:int/>
                        <m:bvar><m:ci>u</m:ci></m:bvar>
                        <m:lowlimit><m:cn>0</m:cn></m:lowlimit>
                        <m:uplimit><m:ci>a</m:ci></m:uplimit>
                        <m:apply>
                            <m:exp/>
                            <m:apply>
                                <m:power/>
                                <m:apply>
                                    <m:times/>
                                    <m:cn>-1</m:cn>
                                    <m:ci>u</m:ci>
                                </m:apply>
                                <m:cn>2</m:cn>
                            </m:apply>
                        </m:apply>
                    </m:apply>
                </m:apply>
            </m:apply>
        </m:math>
    </expression>
</variable>
<variable id="delta_nu_c" >
    <expression type="MathML">
        <m:math>
            <m:apply>
                <m:times/>
                <m:ci>gamma</m:ci>
                <m:ci>P</m:ci>
                <m:apply>
                    <m:power/>
                    <m:apply>
                        <m:divide/>
                        <m:ci>Tref</m:ci>
                        <m:ci>T</m:ci>
                    </m:apply>
                    <m:ci>n</m:ci>
                </m:apply>
            </m:apply>
        </m:math>
    </expression>
```

```
</variable>
<variable id="delta_nu_d" >
    <expression type="MathML">
        <m:math>
            <m:apply>
                <m:times/>
                <m:ci>wvo</m:ci>
                <m:apply>
                    <m:root/>
                    <m:apply>
                        <m:divide/>
                        <m:apply>
                            <m:times/>
                            <m:cn>2</m:cn>
                            <m:apply>
                                <m:ln/>
                                <m:cn>2</m:cn>
                            </m:apply>
                            <m:ci>kb</m:ci>
                            <m:ci>T</m:ci>
                        </m:apply>
                        <m:apply>
                            <m:times/>
                            <m:ci>m</m:ci>
                            <m:apply>
                                <m:power/>
                                <m:ci>c_light</m:ci>
                                <m:cn>2</m:cn>
                            </m:apply>
                        </m:apply>
                    </m:apply>
                </m:apply>
            </m:apply>
        </m:math>
    </expression>
</variable>
<variable id="a" >
    <expression type="MathML">
        <m:math>
            <m:apply>
                <m:times/>
                <m:apply>
                    <m:divide/>
                    <m:ci>delta_nu_c</m:ci>
                    <m:ci>delta_nu_d</m:ci>
                </m:apply>
                <m:apply>
                    <m:root/>
                    <m:apply>
                        <m:ln/>
                        <m:cn>2</m:cn>
                    </m:apply>
                </m:apply>
            </m:apply>
        </m:math>
    </expression>
</variable>
<variable id="Q_CO">
    <expression type="MathML">
        <m:math>
            <m:apply>
                <m:divide/>
```

```
                <m:apply>
                    <m:exp/>
                    <m:apply>
                        <m:divide/>
                        <m:apply>
                            <m:times/>
                            <m:cn>-1</m:cn>
                            <m:ci>h</m:ci>
                            <m:ci>wvo</m:ci>
                        </m:apply>
                        <m:apply>
                            <m:times/>
                            <m:cn>2</m:cn>
                            <m:ci>kb</m:ci>
                            <m:ci>T</m:ci>
                        </m:apply>
                    </m:apply>
                </m:apply>
                <m:apply>
                    <m:minus/>
                    <m:cn>1</m:cn>
                    <m:apply>
                        <m:exp/>
                        <m:apply>
                            <m:divide/>
                            <m:apply>
                                <m:times/>
                                <m:cn>-1</m:cn>
                                    <m:ci>h</m:ci>
                                <m:ci>wvo</m:ci>
                            </m:apply>
                            <m:apply>
                                <m:times/>
                                <m:ci>kb</m:ci>
                                <m:ci>T</m:ci>
                            </m:apply>
                        </m:apply>
                    </m:apply>
                </m:apply>
            </m:apply>
        </m:math>
    </expression>
</variable>
<variable id="voigt" >
    <expression type="MathML">
        <m:math>
            <m:apply>
                <m:times/>
                <m:apply>
                    <m:divide/>
                    <m:cn>1</m:cn>
                    <m:ci>delta_nu_d</m:ci>
                </m:apply>
                <m:apply>
                    <m:root/>
                    <m:apply>
                        <m:divide/>
                        <m:apply>
                            <m:ln/>
                            <m:cn>2</m:cn>
                        </m:apply>
                        <m:pi/>
```

```
                    </m:apply>
                </m:apply>
                <m:apply>
                    <m:exp/>
                    <m:apply>
                        <m:power/>
                        <m:ci>a</m:ci>
                        <m:cn>2</m:cn>
                    </m:apply>
                </m:apply>
                <m:ci>erfc(a)</m:ci>
            </m:apply>
        </m:math>
    </expression>
</variable>
<variable id="epsilon" >
    <expression type="MathML">
        <m:math>
            <m:apply>
                <m:times/>
                <m:apply>
                    <m:divide/>
                    <m:apply>
                        <m:times/>
                        <m:cn>8</m:cn>
                        <m:apply>
                            <m:power/>
                            <m:pi/>
                            <m:cn>3</m:cn>
                        </m:apply>
                    </m:apply>
                    <m:apply>
                        <m:times/>
                        <m:cn>3</m:cn>
                        <m:ci>h</m:ci>
                        <m:ci>c_light</m:ci>
                    </m:apply>
                </m:apply>
                    <m:ci>wvo</m:ci>
                <m:apply>
                    <m:divide/>
                    <m:apply>
                        <m:exp/>
                        <m:apply>
                            <m:divide/>
                            <m:apply>
                                <m:times/>
                                <m:cn>-1</m:cn>
                                <m:ci>Delta_E^v''_0</m:ci>
                            </m:apply>
                            <m:apply>
                                <m:times/>
                                <m:ci>kb</m:ci>
                                <m:ci>T</m:ci>
                            </m:apply>
                        </m:apply>
                    </m:apply>
                    <m:ci>Q_CO</m:ci>
                </m:apply>
                <m:apply>
                    <m:minus/>
                    <m:apply>
```

```
    <m:times/>
    <m:apply>
        <m:divide/>
        <m:apply>
            <m:times/>
            <m:ci>h</m:ci>
            <m:ci>c_light</m:ci>
            <m:ci>B_v''</m:ci>
        </m:apply>
        <m:apply>
            <m:times/>
            <m:ci>kb</m:ci>
            <m:ci>T</m:ci>
        </m:apply>
    </m:apply>
    <m:apply>
        <m:exp/>
        <m:apply>
            <m:divide/>
            <m:apply>
                <m:times/>
                <m:cn>-1</m:cn>
                <m:ci>B_v''</m:ci>
                <m:ci>J''</m:ci>
                <m:apply>
                    <m:plus/>
                    <m:ci>J''</m:ci>
                    <m:cn>1</m:cn>
                </m:apply>
                <m:ci>h</m:ci>
                <m:ci>c_light</m:ci>
            </m:apply>
            <m:apply>
                <m:times/>
                <m:ci>kb</m:ci>
                <m:ci>T</m:ci>
            </m:apply>
        </m:apply>
    </m:apply>
</m:apply>
<m:apply>
    <m:times/>
    <m:apply>
        <m:divide/>
        <m:apply>
            <m:times/>
            <m:ci>h</m:ci>
            <m:ci>c_light</m:ci>
            <m:ci>B_v''+1</m:ci>
        </m:apply>
        <m:apply>
            <m:times/>
            <m:ci>kb</m:ci>
            <m:ci>T</m:ci>
        </m:apply>
    </m:apply>
    <m:apply>
        <m:exp/>
        <m:apply>
            <m:divide/>
            <m:apply>
                <m:times/>
```

```
                                    <m:cn>-1</m:cn>
                                    <m:apply>
                                        <m:plus/>
                                        <m:ci>Delta_E^v''+1_v''</m:ci>
                                        <m:apply>
                                            <m:times/>
                                            <m:ci>B_v''+1</m:ci>
                                            <m:ci>J''</m:ci>
                                            <m:apply>
                                                   <m:minus/>
                                                   <m:ci>J''</m:ci>
                                                   <m:cn>1</m:cn>
                                            </m:apply>
                                            <m:ci>h</m:ci>
                                            <m:ci>c_light</m:ci>
                                        </m:apply>
                                    </m:apply>
                                </m:apply>
                                <m:apply>
                                    <m:times/>
                                    <m:ci>kb</m:ci>
                                    <m:ci>T</m:ci>
                                </m:apply>
                            </m:apply>
                        </m:apply>
                    </m:apply>
                </m:apply>
                <m:ci>R_CO^2</m:ci>
                <m:ci>J''</m:ci>
                <m:ci>voigt</m:ci>
            </m:apply>
        </m:math>
    </expression>
</variable>
<variable id="LHS" >
    <expression type="MathML">
        <m:math>
            <m:apply>
                <m:times/>
                <m:cn>-1</m:cn>
                <m:ci>epsilon</m:ci>
                <m:ci>L</m:ci>
                <m:ci>C</m:ci>
            </m:apply>
        </m:math>
    </expression>
</variable>
<variable id="RHS">
    <expression type="MathML">
        <m:math>
            <m:apply>
                <m:ln />
                <m:apply>
                    <m:divide/>
                    <m:apply>
                        <m:minus />
                        <m:ci>V_inf</m:ci>
                        <m:ci>V</m:ci>
                    </m:apply>
                    <m:apply>
                        <m:minus />
                        <m:ci>V_inf</m:ci>
```

```
                        <m:ci>V_0</m:ci>
                    </m:apply>
                </m:apply>
            </m:apply>
        </m:math>
    </expression>
</variable>
<instrumentalModelExpression type="MathML" implicit="true">
    <m:math>
        <m:apply>
            <m:minus />
            <m:ci>LHS</m:ci>
            <m:ci>RHS</m:ci>
        </m:apply>
    </m:math>
</instrumentalModelExpression>
<additionalDataItem MIME=" " itemType="MATLAB function" description="MATLAB code of
instrumental model">BeerLawCO.m</additionalDataItem>
<additionalDataItem MIME=" " itemType="text" description="instrumental model
description">
Beer-Lambert Law for the P(10) 1->2 transition of CO describing molecular absorption of
light in terms of transient, incident, and reference volatages.
</additionalDataItem>
<additionalDataItem MIME=" " itemType="latex" description="LaTeX string of molar
absorptivity">$$\varepsilon_{\rm{CO}} = \frac{8\pi^3}{3hc} \nu_0 \frac{e^{\frac{- \Delta
E^{\nu^{\prime \prime}}_0}{k_{\rm{B}} T}}}{Q_{\rm{CO}}} \left( \frac{h c B_{\nu^{\prime
\prime}}}{k_{\rm{B}} T} e^{\frac{-B_{\nu^{\prime \prime}} J^{\prime \prime} (J^{\prime
\prime}+1)hc}{k_{\rm{B}} T}} - \frac{hcB_{\nu^{\prime \prime}+1}}{k_{\rm{B}} T}
e^{\frac{-(\Delta E^{\nu^{\prime \prime}+1}_{\nu^{\prime \prime}}+B_{\nu^{\prime
\prime}+1} J^{\prime \prime} (J^{\prime \prime}-1)hc)}{k_{\rm{B}} T}} \right) \times
\left(|R_{\rm{CO}}|^2 J^{\prime \prime} \right) f(\nu_0) $$</additionalDataItem>
<additionalDataItem MIME=" " itemType="latex" description="LaTeX string of Beer-
Lambert Law">$$\frac{I}{I_0} = \frac{V_\infty-V}{V_\infty-V_0} = e^{-
\varepsilon_{\rm{CO}}[\rm{CO}]L}$$</additionalDataItem>
</instrumentalModel>
```

Appendix E.

PrIMe Experiment XML record of the shock tube experiment

```
<?xml version="1.0" encoding="utf-8"?>
<experiment xmlns="http://purl.org/NET/prime/" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" primeID="x00000012"
xsi:schemaLocation="http://purl.org/NET/prime/ http://warehouse.primekinetics.org/schema/experiment.xsd">
    <copyright>primekinetics.org 2009</copyright>
    <bibliographyLink preferredKey="Eiteneer et al., 1998" primeID="b00011422"/>
    <bibliographyLink preferredKey="Eiteneer, 2000" primeID="b00014778"/>
    <apparatus>
        <kind>shock tube</kind>
        <mode>reflected shock</mode>
        <property description="Internal shock tube diameter" id="D_internal" label="D_internal" name="diameter" units="cm">
            <value>8.26</value>
        </property>
        <property description="Shock tube wall material" label="wall_material" name="material" units="">
            <value>stainless steel</value>
        </property>
        <property description="Driver section length" label="l_driver" name="length" units="m">
            <value>1.5</value>
        </property>
        <property description="Driven section length" label="l_driven" name="length" units="m">
            <value>4.9</value>
        </property>
        <property description="tube wall thickness" label="t_tube_wall" name="length" units="cm">
            <value>0.32</value>
        </property>
        <property description="Overall Time constant of CO Detection System" label="tau" name="time" units="µs">
            <value>0.6</value>
        </property>
        <property description="Piezoelectric pressure transducer rise time" label="tau_rise_pressure_transducer" name="time"
units="µs">
            <value>2</value>
        </property>
```

```
    <property description="Piezoelectric pressure transducer sensitivity" name="sensitivity" units="mV/psi">
        <value>4.95</value>
    </property>
</apparatus>
<commonProperties>
    <property description="Reference transmitted voltage" id="V_0" label="V_0" name="voltage" units="mV">
        <value>-3090</value>
    </property>
    <property description="Incident voltage" id="V_inf" label="V_inf" name="voltage" units="mV">
        <value>2000</value>
    </property>
    <property description="Post Shock Temperature" id="T_5" label="T_5" name="temperature" units="K">
        <value>1784</value>
        <uncertainty bound="plusminus" kind="relative" transformation="1">0.0035</uncertainty>
    </property>
    <property description="Total mixture density" id="C_tot" label="C_5" name="concentration" units="mol/m³">
        <value>15.76</value>
        <uncertainty bound="plusminus" kind="relative" transformation="1">0.0044</uncertainty>
    </property>
    <property description="Initial Temperature" label="T_1" name="temperature" units="°C">
        <value>25</value>
    </property>
    <property description="Initial Pressure" id="P_initial" label="P_1" name="pressure" units="Torr">
        <value>43.4</value>
    </property>
    <property name="initial composition">
        <component>
            <speciesLink preferredKey="CH2O" primeID="s00009076"/>
            <amount units="volume fraction">0.014743</amount>
            <uncertainty bound="plusminus" kind="relative" transformation="1">0.01</uncertainty>
        </component>
        <component>
            <speciesLink preferredKey="O2" primeID="s00010295"/>
            <amount units="volume fraction">0.002465</amount>
            <uncertainty bound="plusminus" kind="relative" transformation="1">0.01</uncertainty>
        </component>
        <component>
            <speciesLink preferredKey="Ar" primeID="s00000049"/>
            <amount units="volume fraction">0.982792</amount>
            <uncertainty bound="plusminus" kind="relative" transformation="1">0.01</uncertainty>
        </component>
```

```
        </property>
    </commonProperties>
    <dataGroup id="dg1" label="CO profile">
        <property id="x1" name="time" units="µs" label="t" description="time" />
        <property id="x2" name="concentration" units="unitless" label="[CO]/[CO]max" description="CO concentration, relative to maximum
CO concentration">
            <speciesLink preferredKey="CO" primeID="s00009358" />
        </property>
        <dataPoint id="dp1">
            <x1>30.7</x1>
            <x2>0.5</x2>
        </dataPoint>
    </dataGroup>
    <dataGroup dataPointForm="HDF5" id="dg2" label="Experimental run 33">
        <dataGroupLink dataGroupID="" dataPointID=""/>
        <property description="time" id="x1" label="t" name="time" units="µs"/>
        <property derivedPropertyExists="true" description="Transient Voltage" id="x2" label="V" name="voltage" units="mV">
            <derivedProperty description="CO concentration" id="CO" label="[CO]" name="concentration" units="mol/m³">
                <feature id="C_CO" primeID="im00000001" type="instrumentalModel">
                    <indicator id="V_inf" transformation="1" variableID="V_inf">
                        <propertyLink propertyID="V_inf"/>
                    </indicator>
                    <indicator id="V" transformation="1" variableID="V">
                        <propertyLink dataGroupID="dg2" propertyID="x2"/>
                    </indicator>
                    <indicator id="V_0" transformation="1" variableID="V_0">
                        <propertyLink propertyID="V_0"/>
                    </indicator>
                    <indicator id="gamma" transformation="1" variableID="gamma">
                        <dataAttributeLink id="gammaCalibration" primeID="a00000078"/>
                    </indicator>
                    <indicator id="L" transformation="1" variableID="L">
                        <propertyLink propertyID="D_internal"/>
                    </indicator>
                    <indicator id="C_tot" transformation="1" variableID="C_tot">
                        <propertyLink propertyID="C_tot"/>
                    </indicator>
                    <indicator id="T" transformation="1" variableID="T">
                        <propertyLink propertyID="T_5"/>
                    </indicator>
                    <observable id="C" variableID="C"/>
```

```
                </feature>
            </derivedProperty>
        </property>
    </dataGroup>
    <additionalDataItem MIME=" " description="experiment description" itemType="text">
        Shock tube experiment measuring voltages from CH2O/Argon.
    </additionalDataItem>
    <additionalDataItem MIME=" " description="experiment comment" itemType="text">
        The post-shock temperature and concentration were corrected to values after complete decomposition of trioxane.
    </additionalDataItem>
</experiment>
```

Appendix F.

PrIMe Target Data Attribute XML record of shock tube target

```
<?xml version="1.0" encoding="utf-8" standalone="no" ?>
<dataAttribute xmlns="http://purl.org/NET/prime/" xmlns:xsi="http://www.w3.org/2001/XMLSchema-
instance" type="target" primeID="a00000044" xsi:schemaLocation="http://purl.org/NET/prime/
http://warehouse.primekinetics.org/schema/dataAttribute.xsd">
    <copyright>©primekinetics.org 2007</copyright>
    <origin type="primeID">b00014718</origin>
    <preferredKey group="prime">GRI-Mech 3.0 - BCO.T1</preferredKey>
    <propertyLink dataGroupID="dg2" experimentPrimeID="x00000010" id="t" propertyID="x1"/>
    <propertyLink dataGroupID="dg2" experimentPrimeID="x00000010" id="[CO]" propertyID="x2" derivedProperty="true"
derivedPropertyID="CO"/>
    <feature id="t([CO]peak/2)" type="timeToFractionalPeakValue">
        <fraction>0.5</fraction>
        <indicator id="t" propertyID="t" transformation="1"/>
        <observable id="[CO]" propertyID="[CO]" transformation="1"/>
    </feature>
    <dataAttributeValue type="actual">
        <indicator featureID="t([CO]peak/2)" id="[CO]" propertyID="[CO]" transformation="1"/>
        <observable featureID="t([CO]peak/2)" id="t" propertyID="t" transformation="1">
            <property name="time" units="µs" label="t([CO]peak/2)" description="time to half CO peak concentration">
                <valueLink dataGroupID="dg1" dataPointID="dp1" experimentPrimeID="x00000010" propertyID="x1"/>
            </property>
            <bounds kind="relative" source="b00014796">
                <upper id="ub">1.1</upper>
                <lower id="lb">0.9</lower>
            </bounds>
        </observable>
    </dataAttributeValue>
    <additionalDataItem MIME=" " description="Data Attribute description" itemType="text">
Time to half maximum [CO] during CH2O decomposition at 2124 K, 1.17 atm
    </additionalDataItem>
</dataAttribute>
```

Appendix G.

TargetViewer code

```
function dataAttributeViewer(daPrimeID)
%dataAttributeViewer(dataAttributePrimeID)
%The dataAttributeViewer displays the selected dataAttribute and plots it
%in relation to the underlying experiment.
%
% Copyright 2009 primekinetics.org
% Created by: Devin R. Yeates, University of California at Berkeley, 30 January 2009.
% Last edited by: Devin R. Yeates, University of California at Berkeley, 25 February 2009.

%% Data Attribute instantiation
connObj = primeConnection('get','primeGuest');
[daPath, statusMsg] = primeID2path(connObj, daPrimeID);
if ~isempty(statusMsg)
    display(statusMsg)
end

%dataAttribute class:  Instantiate dataAttribute object from chosen dataAttribute primeID
dataAttributeObj = primeDataAttribute(connObj, daPath);
daPreferredKey = get(dataAttributeObj,'preferredKey');
daValue = getDataAttribute(dataAttributeObj);
daValue.daValue = daValue.daValue + 370;  %Correction for delay applies only to a44.

%% Experiment instantiation

daData = [];
daProps = [];
```

```
%Get experimentPrimeID and create a DOM Node of the dataGroup
expPrimeID = get(dataAttributeObj, 'propertyLink._experimentPrimeID');
dgID = get(dataAttributeObj, 'propertyLink._dataGroupID');
propertyID = get(dataAttributeObj, 'propertyLink._propertyID');
n_exp = length(expPrimeID);

for ii = 1:n_exp
    [expPath, statusMsg] = primeID2path(connObj, expPrimeID{ii});

    if ~isempty(statusMsg)
        display(statusMsg)
    end

    %Create Experiment object
    expObj(ii) = primeExperiment(connObj, expPath);


    %dataGroup class:  Instantiate dataGroup object from experiment object.
    dGroupID = get(expObj(ii),'dataGroup._id');
    ind = find(strcmp(dGroupID,dgID) == 1);

    %% Data Group Instantiation
    dg(ii) = get(expObj(ii),'dataGroup',ind);

    %get dataPoints related to propertyLink
    dgProps = get(dg(ii),'properties');
    dgPropsID = {dgProps.id};

    %find index of dataPoints relating to propertyLink propertyID
    propInd = find(strcmp(dgPropsID,propertyID{ii}));
    allDataPoints = get(dg(ii),'dataPoints');
    dataPoints = [allDataPoints(:,propInd).value]';

    daProps = [daProps dg(ii).properties(propInd)];
    daData = [daData dataPoints];
```

```
%if derivedPropertyExists="true":
%GUI:  create instrumental model tab in GUI

%% Instrumental Model Instantiation
derivedPropNode = getDerivedPropertyNode(dg(ii));
derivedProperties = getDerivedProperties(dg(ii));

if ~isempty(derivedProperties)

    n_derivedProps = length(derivedProperties);

    for jj = 1:n_derivedProps

        [imPath, statusMsg] = primeID2path(connObj, derivedProperties(jj).primeID);

        if ~isempty(statusMsg)
            display(statusMsg)
        end
        %instantiate instrumental model
        im(jj) = primeInstrumentalModel(connObj,imPath);
    end

end

%% Interface from Instrumental Model to Calculation Code
%Go into derivedPropertyNode and Identify variableID's and propertyID's
if ~isempty(derivedProperties)
    featureNode = derivedPropNode.item(0).getElementsByTagName('feature');
    indicatorNodes = featureNode.item(0).getElementsByTagName('indicator');
    indicatorLength = indicatorNodes.getLength();
    for kk = 1:indicatorLength
        variableIDs(kk) = indicatorNodes.item(kk-1).getAttribute('variableID');
        propertyIDs(kk) = indicatorNodes.item(kk-1).getAttribute('propertyID');
    end

    %Find propertyIDs and assign values
```

```
n = length(variableIDs);
foundPropertyInd = zeros(1,n);
values = cell(n,1);

commPropID = get(expObj(ii),'commonProperties.property._id');
commProp = get(expObj(ii),'commonProperties.property');
n_commProp = length(commPropID);
commPropChar = cell2struct(commProp,'value',n_commProp);

appPropID = get(expObj(ii),'apparatus.property._id');
appProp = get(expObj(ii),'apparatus.property');
n_appProp = length(appPropID);
appPropChar = cell2struct(appProp,'value',n_appProp);

n_dgProp = length(dgPropsID);
for kk=1:n
    for jj = 1:n_commProp  %Search common properties
        if strcmp(propertyIDs(kk),commPropID(jj))
            commPropNum = str2num(commPropChar(jj).value);
            values{kk} = commPropNum(1);
            foundPropertyInd(kk) = 1;
        end
    end
    for jj = 1:n_appProp  %Search apparatus properties
        if strcmp(propertyIDs(kk),appPropID(jj))
            appPropNum = str2num(appPropChar(jj).value);
            values{kk} = appPropNum(1);
            foundPropertyInd(kk) = 1;
        end
    end
    for jj = 1:n_dgProp   %Search DataGroup properties
        if strcmp(propertyIDs(kk),dgPropsID{jj})
            dgPropNum = get(dg(ii),'dataPoints');
            values{kk} = [dgPropNum(:,jj).value]';
            foundPropertyInd(kk) = 1;
        end
```

```
            end
        end


        %Otherwise look for dataAttributeLink
        daIndex = find(foundPropertyInd == 0);
        %[r_daIndex,n_daIndex] = size(daIndex);

        daLink = indicatorNodes.item(daIndex-1).getElementsByTagName('dataAttributeLink');

        n_daLink = daLink.getLength();
        for kk = 1:n_daLink
            daLinkPrimeID_j = daLink.item(kk-1).getAttribute('primeID');
            daLinkPrimeID = char(daLinkPrimeID_j);
            [daLinkPath, statusMsg] = primeID2path(connObj, daLinkPrimeID);

            if ~isempty(statusMsg)
                display(statusMsg)
            end

            %Instantiate calibration dataAttribute
            featureDataAttribute(kk) = primeDataAttribute(connObj, daLinkPath);
            calDaValue = getDataAttribute(featureDataAttribute(kk));
            values{daIndex(kk)} = calDaValue.daValue;
            calDaValueDesc =
get(featureDataAttribute,'dataAttributeValue.observable.property._description');
        end
    end
end

%% GUI

if ~isempty(derivedProperties)
    enable_att = 'on';
else
    enable_att = 'off';
```

```
end

plotWindow = figure('Tag',         'theFigure',       ...
    'Name',       ['Target Viewer - ' daPreferredKey{:} ], ...
    'NumberTitle', 'off',                             ...
    'MenuBar',     'figure',                          ...
    'Toolbar',     'figure',                          ...
    'WindowStyle', 'normal');

setappdata(plotWindow, 'daData', daData);
setappdata(plotWindow, 'daProps', daProps);
setappdata(plotWindow, 'imVars', values);
setappdata(plotWindow, 'derivedProperties', derivedProperties);
setappdata(plotWindow, 'daValue', daValue);

menu.im = uimenu('Label', 'Instrumental Model');
menu.im_view = uimenu('Parent', menu.im, 'Label', 'View Instrumental Model Properties',...
    'Enable',enable_att,'Callback', {@figure_imProperties,im});

%% GUI Controls Panel
controlsPanel = uipanel('Parent',plotWindow, 'BorderType', 'beveledin', ...
    'Units', 'normalized', 'Position', [0.0 0.0 0.3 1.0]);

control.im_checkbox = uicontrol('Parent', controlsPanel,'tag', 'im_checkbox',...
    'Style', 'checkbox', 'Units', 'normalized', 'Enable', enable_att, ...
    'Position', [0.1 0.85 0.1 0.1],'Callback', {@plotDerivedProperty, plotWindow});
control.im_checkbox_label = uicontrol('Parent', controlsPanel, 'tag', 'im_checkbox_label',...
    'Style', 'text', 'String', 'Plot Using Instrumental Model', 'Units', 'normalized',...
    'HorizontalAlignment','left', 'Position', [0.22 0.825 0.75 0.1]);

control.target_checkbox = uicontrol('Parent', controlsPanel,'tag', 'target_checkbox',...
    'Style', 'checkbox', 'Units', 'normalized', 'Position', [0.1 0.75 0.1
0.1],'Callback',{@plotTargetValue, plotWindow});
control.target_checkbox_label = uicontrol('Parent', controlsPanel, 'tag', 'target_checkbox_label',...
    'Style', 'text', 'String', 'Plot Modeling Target Value', 'Units', 'normalized',...
    'HorizontalAlignment','left', 'Position', [0.22 0.725 0.7 0.1]);
```

```
control.calibrationvalue_label = uicontrol('Parent', controlsPanel, 'tag', 'calibrationvalue_label',...
    'Style', 'text', 'String', 'Calibrated Value', 'FontWeight', 'bold', 'Units', 'normalized',...
    'HorizontalAlignment','center', 'Position', [0.1 0.615 0.8 0.1]);
control.calibrationvalue_description = uicontrol('Parent', controlsPanel, 'tag',
'calibrationvalue_label',...
    'Style', 'text', 'String', calDaValueDesc{:}, 'Units', 'normalized',...
    'HorizontalAlignment','center', 'Position', [0.1 0.56 0.80 0.1]);
control.calibrationvalue_edit = uicontrol('Parent', controlsPanel,'tag', 'calibrationvalue_edit',...
    'Style', 'edit', 'String', calDaValue.daValue, 'Units', 'normalized',...
    'Enable', enable_att, 'Position', [0.2 0.51 0.6 0.05],'Callback',{@newCalibrationValue, plotWindow});
control.calibrationvalue_override = uicontrol('Parent', controlsPanel, 'tag',
'calibrationvalue_override',...
    'Style', 'pushbutton', 'String', 'Override Value', 'Units', 'normalized',...
    'Enable', enable_att , 'Position', [0.2 0.45 0.6 0.05],'Callback', {@plotDerivedProperty, plotWindow});

%% GUI Plot Panel
plotPanel = uipanel('Parent',plotWindow, 'bordertype', 'none', 'BackgroundColor', 'white', 'BorderType',
'beveledin', ...
    'Units', 'normalized', 'Position', [0.3 0.0 0.7 1.0]);
setappdata(plotWindow, 'plotPanel', plotPanel);

a = axes('parent',plotPanel);

%% Plot Experimental Data in original format

plotData('', '', plotWindow,plotPanel);

end

function figure_imProperties(hObj, eventdata, im)
%Show instrumental model properties in a separate figure

imPreferredKey = get(im,'preferredKey');

imWindow = figure('Tag',         'Instrumental Model',                              ...
```

```
    'Name',       ['Instrumental Model Details - ' imPreferredKey{:} ], ...
    'NumberTitle', 'off',                                    ...
    'MenuBar',     'none',                                ...
    'Toolbar',     'none',                                ...
    'WindowStyle', 'normal');

nProps = length(get(im,'property'));
imPropID = get(im,'property._id');
imPropValue = get(im,'property');
imPropUnits = get(im,'property._units');
imPropDesc = get(im,'property._description');

height = 300;
for ii = 1:nProps
        textHandle(ii) = uicontrol(imWindow,'Style','text',...
        'String', [imPropID{ii} ' = ' imPropValue{ii} '  ' imPropUnits{ii} ' -- ' imPropDesc{ii}],...
        'HorizontalAlignment', 'left', 'Position', [10 height 550 20]);
    height = height - 20;
end

end

function plotData(hObj, eventdata,plotWindow,plotPanel)
daData = getappdata(plotWindow, 'daData');
daProps = getappdata(plotWindow, 'daProps');

xData = daData(:,1);
yData = daData(:,2);

plot(xData,yData)

xlabel([daProps(1).description ' , ' daProps(1).label ' , ' daProps(1).units])
ylabel([daProps(2).description ' , ' daProps(2).label ' , ' daProps(2).units])

end
```

```
function plotDerivedProperty(hObj, eventdata,plotWindow,plotPanel)
daData = getappdata(plotWindow, 'daData');
daProps = getappdata(plotWindow, 'daProps');
values = getappdata(plotWindow, 'imVars');
derivedProperties = getappdata(plotWindow, 'derivedProperties');

derivedPropertyValues = BeerLawCO(values{1},values{2},values{3},values{4},values{5},values{6},values{7});

if (get(hObj,'Value') == get(hObj,'Max'))  % Checkbox is checked-take approriate action
    yData = derivedPropertyValues;
else  % Checkbox is not checked-take approriate action
    yData = daData(:,2);
end

xData = daData(:,1);

plot(xData,yData);

xlabel([daProps(1).description ' , ' daProps(1).label ' , ' daProps(1).units]);

if (get(hObj,'Value') == get(hObj,'Max'))  % Checkbox is checked-take approriate action
    ylabel([derivedProperties.description ' , ' derivedProperties.label ' , ' derivedProperties.units])
else  % Checkbox is not checked-take approriate action
    ylabel([daProps(2).description ' , ' daProps(2).label ' , ' daProps(2).units])
end
end

function newCalibrationValue(hObj, eventdata, plotWindow, controlsPanel)

values = getappdata(plotWindow, 'imVars');

user_value = str2double(get(hObj,'String'));
if isnan(user_value)
    errordlg('You must enter a numeric value','Bad Input','modal')
    return
end
```

```
values{4} = user_value;
setappdata(plotWindow, 'imVars', values);
end

function plotTargetValue(hObj, eventdata, plotWindow, controlsPanel)

daValue = getappdata(plotWindow, 'daValue');
%a = axes('parent',plotPanel);
ylimits = get(gca,'YLim');

if (get(hObj,'Value') == get(hObj,'Max'))  % Checkbox is checked-take approriate action
    hold on;

    x = [daValue.daValue,daValue.daValue];
    y = [-1e5,1e5];

    plot(x,y,'r-','LineWidth',2);

    set(gca,'YLim', ylimits);
    hold off;
else  % Checkbox is not checked-take approriate action
    plotDerivedProperty('','',plotWindow,'')
end

end
```

Appendix H.

PrimeInstrumentalModel Class Software

```
function y = primeInstrumentalModel(varargin)
% function y = primeInstrumentalModel(varargin)
%
% Constructor for class primeInstrumentalModel
%
% instrumentalModelObj = primeInstrumentalModel()   returns an empty primeInstrumentalModel object
% instrumentalModel                                 displays basic instrumentalModel information
% instrumentalModelObj = primeInstrumentalModel(connObj,filePath)  creates a primeInstrumentalModel object
from
%                                                   the contents of the
%                                                   specified XML file
% instrumentalModelObj = primeInstrumentalModel(connObj,propertyNode)  creates a primeInstrumentalModel
object from
%                                                   the contents of the
%                                                   specified dataGroup
%                                                   property node
%                   filepath is relative to the WebDAV Root.
%                   connObj is the primeConnection object

if nargin==0 % no arguments on input.  Create empty instrumental model object
    y = local_initInstrumentalModel;
    return
end

switch class(varargin{1})
    case 'primeInstrumentalModel'   % first input argument is primeInstrumentalModel object
        y = varargin{1};
        if length(varargin) > 1
```

```
            set(y,varargin{:});
        end
    case 'org.apache.xerces.dom.DeferredDocumentImpl'
        y.node = varargin{1};
        y.primeid = '';
        y.key = '';
        y = class(y, 'primeInstrumentalModel');
    otherwise % at least one input argument, the first not an instrumentalModel or connection object
        y = primeInstrumentalModel;
        set(y, varargin{:});
end

function im = local_initInstrumentalModel
% initializes a new member of class primeInstrumentalModel
im.node = '';
im.primeid = '';
im.key = '';
im = class(im,'primeInstrumentalModel');
return



function y = computeInstrumentalModel(imObj,values)

%get function handle
addDataItems = get(imObj,'additionalDataItems');
ind = strcmp({addDataItems.type},'MATLAB function');
[path,name] = fileparts(addDataItems(ind).contents);
fh = str2func(name);

%Compute feature property values

y = fh(values{:});


function y = getLatexExpression(instrumentalModel)
```

```
%GETLATEXEPRESSION(instrumentalModel)
%
%GETLATEXEXPRESSION returns the latex expression(s) of an instrumental model
%in a cell array

addData = get(instrumentalModel,'additionalDataItems');
ind = strcmp({addData.type},'latex');
y = {};
for ii = 1:length(addData)
    if (ind(ii) == 1)
        y = [y addData(ii).contents];
    end
end



function y = get(varargin)
% function y = GET(instrumentalModelObj, field, option)
%
% Returns the contents of the specified field
%
% instrumentalModelObj - primeInstrumentalModel object. Its node contains the contents of a PrIMe
instrumentalModel XML file
% field     - xml node, attribute or their predefined aggregate to return
% option    - specifies the index of the node whose contents is to be
%             retrieved. If the index is not specified, the contents of
%             all the elements of a given name is returned

if nargin > 0
    instrumentalModel = varargin{1};
end

if nargin == 1                                  % return the list of fields
    y = listFields(instrumentalModel.node);
    y = ['node'; y; 'data'];
    return
end
```

```
if nargin > 1
    field = varargin{2};
    if ~isa(field,'char')               % wrong type for the "field" argument
        error('character string expected as the second argument')
    end
end

switch field
    case {'node', 'data'}
        y = instrumentalModel.(field);
    case {'primeID', 'getPrimeID'}
        y = getPrimeID(instrumentalModel.node);
    case {'preferredKey', 'getPreferredKey'}
        y = getPreferredKey(instrumentalModel.node);
    case {'bibliography', 'getBibliography'}
        y = getBibliography(instrumentalModel.node);
    case {'additionalDataItem', 'getAdditionalDataItem', 'additionalDataItems', 'getAdditionalDataItems'}
        y = getAdditionalDataItems(instrumentalModel.node);
    case {'latex','expression','expressions','latex expression'}
        y = getLatexExpression(instrumentalModel);
    otherwise
        y = getField(instrumentalModel.node, field);
end


function set(instrumentalModelObj, varargin)
% function SET(instrumentalModelObj, field, value, option)
%
% Sets the field of primeInstrumentalModel object to a requested value
%
% instrumentalModelObj - primeInstrumentalModel object. Its node contains the contents of a PrIMe
instrumentalModel XML file
% field     - field to set
% value     - value to set the field to
% option    - optional parameter;
%             - index, in case instrumentalModelObj.node DOM object contains several nodes with the same
name
```

```
%             - string, containing the old content to be replaced; used to
%               identify the node or attribute whose contents should be changed

   if nargin == 1           % no field requested. Display the list of available fields
      y = listFields(instrumentalModelObj);
      disp(['node'; y; 'data']);
      return
   end

   if ~iscell(varargin{1})
      LOCAL_setField(instrumentalModelObj, varargin);
   else
      for i = 1:length(varargin)
         LOCAL_setField(instrumentalModelObj, varargin{i});
      end
   end
   assignin('caller', inputname(1), instrumentalModelObj);
```



```
function LOCAL_setField(c,record)
% sets a single node or attribute of DOM object contained in primeInstrumentalModel.node
   switch record{1}
      case fieldnames(struct(c))
         c.(record{1}) = record{2};
      otherwise
         LOCAL_setDataField(c, record{:});
   end
   assignin('caller', inputname(1), c);



function LOCAL_setDataField(c,field,value)
% sets a data field
   data.key = field;
   data.rec = value;
```

```
   c.data = mmap(c.data, 'add', data);
   assignin('caller', inputname(1), c);


function y = toString(varargin)
% instrumentalModelString = toString(instrumentalModelObj)
% instrumentalModelString = toString(instrumentalModelObj, form)
%
% instrumentalModelObj - primeInstrumentalModel object with a node - contents of a PrIMe instrumentalModel
XML file
% form      - string; 'short' or 'full'; if not specified, short is used as the default

   instrumentalModelObj = varargin{1};
   preferredKey = get(instrumentalModelObj,'preferredKey');
   y = char(preferredKey);


function display(instrumentalModel)
% function display(instrumentalModelObj)
%
% instrumentalModelObj - primeInstrumentalModel object;
%             instrumentalModel.node contains the contents of the PrIMe instrumentalModel XML file

   if isempty(instrumentalModel.node)
      disp('PrIMe instrumentalModel object: empty')
   else
      get(instrumentalModel,'preferredKey')
   end
```

Appendix I.

Reaction Set, Thermodynamic Properties, Transport Properties, and Flame Code Input File.

```
!=============================================================================================
ELEMENTS
H           ! 1.00797
C           ! 12.0112
O           ! 15.9994
AR          ! 39.9480
END
!
!=============================================================================================
SPECIES
H           ! H atom                                  1.00797
H2          ! molecular hydrogen                      2.01594
CH          ! methylidene, doublet                    13.0191
CH2         ! methylene, triplet B(1)                 14.0271
CH2SING     ! methylene, singlet A(1)                 14.0271
CH3         ! methyl radical, doublet                 15.0351
O           ! O atom, triplet p state                 15.9994
CH4         ! methane                                 16.0430
OH          ! hydroxyl radical                        17.0074
H2O         ! water vapor                             18.0153
C2H         ! ethynyl                                 25.0303
C2H2        ! acetylene / ethyne                      26.0382
H2CC        ! vinylidene                              26.0382
C2H3        ! vinyl / ethenyl                         27.0462
CO          ! carbon monoxide                         28.0106
C2H4        ! ethylene / ethene                       28.0542
```

```
HCO         ! formyl radical, doublet                29.0185
C2H5        ! ethyl                                  29.0622
CH2O        ! formaldehyde / methanal                30.0265
C2H6        ! ethane                                 30.0701
CH2OH       ! hydroxymethyl radical                  31.0345
CH3O        ! methoxy radical                        31.0345
CH3OH       ! methanol                               32.0424
O2          ! molecular oxygen                       31.9988
HO2         ! hydroperoxyl                           33.0068
H2O2        ! hydrogen peroxide                      34.0147
C3H2        ! propargylene, HCCCH                    38.0494
C3H3        ! propargyl, CH2CCH                      39.0574
AR          ! argon                                  39.948
AC3H4       ! allene / propadiene                    40.0653
PC3H4       ! methylacetylene / propyne              40.0653
HCCO        ! ketyl, ketenyl                         41.0297
AC3H5       ! allyl, resonant CH2=CH-CH2.            41.0733
TC3H5       ! propen-2-yl / CH2=C.-CH3               41.0733
SC3H5       ! propenyl (E and Z) / .CH=CH-CH3        41.0733
CH2CO       ! ketene                                 42.0376
C3H6        ! propylene / propene                    42.0813
CH3CO       ! acetyl                                 43.0456
CH2CHO      ! vinoxy / formylmethyl                  43.0456
nC3H7       ! n-propyl / .CH2-CH2-CH3                43.0892
iC3H7       ! isopropyl / CH3-CH.-CH3                43.0892
C2H4O       ! oxirane, cy(-CH2CH2O-)                 44.0536
CH3CHO      ! acetaldehyde                           44.0536
C3H8        ! propane                                44.0972
CO2         ! carbon dioxide                         44.0100
C2H5O       ! ethoxy, CH3-CH2-O.                     45.0616
C4H2        ! diacetylene, but-1,3-diyne             50.0605
iC4H3       ! .CH=C=C=CH2 / HCC-C.=CH2               51.0685
nC4H3       ! .CH=CH-CCH, but-1-en-3-ynyl            51.0685
C4H4        ! vinyl acetylene, but-3-enyne           52.0765
n-C4H5      ! but-1,3-dienyl                         53.0845
i-C4H5      ! but-1,3-dien-2-yl / methylpropargyl    53.0845
iiC4H6      ! 1,2-butadiene, but-1,2-diene           54.0924
iiiC4H6     ! 1,3-butadiene, but-1,3-diene           54.0924
```

```
C2H3CO      ! propenoyl, 1-oxoprop-2-enyl             55.0568
C4H7        ! .CH2-CH2-CH=CH2, but-3-enyl             55.1004
C2H3CHO     ! acrolein, 2-propenal                    56.0647
IC4H8       ! 1-butene / CH2=CH-CH2-CH3               56.1084
C2H3CH2O    ! allyloxy, CH2=CH-CH2O.                  57.0727
nC4H9       ! n-butyl, .CH2CH2CH2CH3                  57.1143
C2H3OO      ! vinylperoxyl                            59.0450
C2H5OO      ! ethylperoxyl                            61.0610
C5H5        ! cyclopentadienyl                        65.0932
C5H6        ! cyclopentadiene                         66.1011
C6H2        ! 1,3,5-hexatriyne (triacetylene)         74.0801
C6H3        ! hexadiynenyl                            75.0881
l-C6H4      ! CH2=CH-CC-CCH                           76.0960
c-C6H4      ! benzyne                                 76.0960
n-C6H5      ! HCC-CH=CH-CH=CH.                        77.1039
i-C6H5      ! 1,3-hexadiene-5-yne-2-yl                77.1039
A1          ! phenyl                                  77.1039
A           ! benzene                                 78.1118
FC6H6       ! fulvene                                 78.1118
l-C6H6      ! 1,3-hexadiene-5-yne                     78.1118
CYC6H7      ! cyclohexa-2,4-dienyl (allylic)          79.1198
n-C6H7      ! 1,3,5-hexatrienyl                       79.1198
i-C6H7      ! HCC-CH=CH-CH=CH2                        79.1198
C5H4O       ! 2,4-cyclopentadien-1-one                80.0847
CY13C6H8    ! cyclohexa-1,3-diene                     80.1277
C6H8        ! 1,3,5-hexatriene                        80.1277
C5H5O       ! cyclopenta-3-en-1-on-2-yl               81.0926
C6H9        ! 3,5-hexadienyl                          81.1357
CYC6H9      ! cyclohexenyl                            81.1357
C5H4OH      ! 2,4-Cyclopentadien-1-ol                 82.1005
CYC6H10     ! cyclohexene                             82.1436
C6H10       ! 1,5-hexadiene                           82.1436
CYC6H11     ! cyclohexyl                              83.1515
C6H11-12    ! 1-hexen-2-yl / hex-1-en-2-yl            83.1515
C6H11-13    ! 1-hexen-3-yl / hex-1-en-3-yl            83.1515
C6H11-14    ! 1-hexen-4-yl / hex-1-en-4-yl            83.1515
C6H11-15    ! 1-hexen-5-yl / hex-1-en-5-yl            83.1515
C6H11       ! C6H11-16, 1-hexen-6-yl / hex-5-enyl     83.1515
```

```
CYC6H12     ! cyclohexane                                84.1595
hexene1     ! 1-hexene, CH2=CHCH2CH2CH2CH3               84.1595
hex1yl      ! 1-hexyl, .CH2CH2CH2CH2CH2CH3               85.1674
hex2yl      ! 2-hexyl,  CH3-CH.-CH2CH2CH2CH3             85.1674
hex3yl      ! 3-hexyl,  CH3CH2-CH.-CH2CH2CH3             85.1674
C6H4CH3     ! methylphenyl                               91.1305
C6H5CH2     ! benzyl                                     91.1305
C6H5CH3     ! toluene                                    92.1384
C6H5O       ! phenoxyl (C6H5-O.)                         93.1033
C6H5OH      ! phenol                                     94.1112
C6H4CCH     ! ethynylphenyl                              101.1251
C6H5CCH     ! phenylacetylene, ethynylbenzene            102.1331
C6H5CHCH    ! beta-styryl                                103.1411
C6H5CHCH2   ! styrene                                    104.1491
C6H5CO      ! phenylformyl                               105.1139
C6H5CH2CH2  ! phenylethyl radical                        105.1571
C6H5CHO     ! benzaldehyde                               106.1219
C6H5CH2CH3  ! ethylbenzene                               106.1650
OC6H4CH3    ! methylphenoxy                              107.1299
C6H5CH2O    ! benzyloxy                                  107.1299
C6H5OCH2    ! methylenephenylether                       107.1299
C6H4O2      ! benzoquinone                               108.0948
C6H5OCH3    ! methylphenylether                          108.1378
HOC6H4CH3   ! cresol                                     108.1378
C6H5CH2OH   ! benzyl alcohol                             108.1378
C6H5CH2OO   ! benzylperoxy                               123.1292
C6H5C6H5    ! biphenyl                                   154.2078
BiBenzyl    ! bibenzyl C6H5CH2CH2C6H5                    182.2677
!
END
!
!=============================================================================================
REACTIONS
!
!--------H2/O2 chemistry---------
2O+M=O2+M                               6.16E+15  -0.50        0.  !  (1) TSA/HAM 86
  H2O/12.0/ H2/2.5/ AR/0.0/
2O+AR=O2+AR                             1.89E+13   0.00    -1790.  !  (1) TSA/HAM 86
```

```
O+H+M=OH+M                                4.71E+18  -1.00        0.  !  (1) TSA/HAM 86
  H2O/12.0/ H2/2.5/ AR/0.75/
H2+M=2H+M                                 4.58E+19  -1.40   104380.  !  (1) TSA/HAM 86
  H2O/12.0/ H2/2.5/ AR/0.05/
H2+AR=2H+AR                               5.84E+18  -1.10   104380.  !  (1) TSA/HAM 86
H+OH+M=H2O+M                              2.21E+22  -2.00        0.  ! (45) Baulch 92
  H2O/12.0/ H2/2.5/ AR/0/
H+OH+AR=H2O+AR                            8.41E+21  -2.00        0.  !  (1) TSA/HAM 86
H2O2(+M)=2OH(+M)                          2.95E+14   0.00    48400.  !  (2) BRO/COB 87
  LOW                                    /1.20E+17   0.00    45500./ !  (3) Warnatz 84
  H2O/12.00/ H2/2.5/ AR/0.16/
H2O+O=OH+OH                               2.97E+06   2.02    13400.  !  (4) Sutherland 91
O+H2=H+OH                                 5.08E+04   2.67     6290.  !  (5) Sutherland 86
OH+H2=H+H2O                               2.16E+08   1.51     3430.  !  (6) Michael/Sutherland 88
H+O2(+M)=HO2(+M)                          1.48E+12   0.60        0.  !  (7) Cobos 85
  LOW                                    /3.50E+16  -0.41    -1120./ !  (8) Mueller 99
  H2O/12.0/ H2/2.5/ AR/0.05/
H+O2=O+OH                                 4.489E+08  1.257   16191.  !  (9) Miller/Pilling 05
  DUPLICATE
H+O2=O+OH                                 2.076E+16 -0.673   16191.  !  (9) Miller/Pilling 05
  DUPLICATE
O+HO2=OH+O2                               3.25E+13   0.00        0.  ! (10) Baulch 94
H+HO2=O2+H2                               1.66E+13   0.00      820.  !  (8) Mueller 99
H+HO2=2OH                                 7.08E+13   0.00      300.  !  (8) Mueller 99
OH+HO2=O2+H2O                             4.64E+13   0.00     -500.  ! (11) GRI 1.2
2HO2=O2+H2O2                              1.30E+11   0.00    -1630.  ! (12) HIP/TRO 90
  DUPLICATE
2HO2=O2+H2O2                              4.20E+14   0.00    11980.  ! (12) HIP/TRO 90
  DUPLICATE
O+H2O2=OH+HO2                             9.55E+06   2.00     3970.  !  (1) TSA/HAM 86
H+H2O2=HO2+H2                             4.82E+13   0.00     7950.  !  (1) TSA/HAM 86
H+H2O2=OH+H2O                             2.41E+13   0.00     3970.  !  (1) TSA/HAM 86
OH+H2O2=HO2+H2O                           1.00E+12   0.00        0.  ! (13) HIP/TRO 92
  DUPLICATE
OH+H2O2=HO2+H2O                           5.80E+14   0.00     9560.  ! (13) HIP/TRO 92
  DUPLICATE
!---------CO/CO2 chemistry------------
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O+CO(+M)=CO2(+M)                          1.80E+10    0.00      2385.  !  (1) TSA/HAM 86
  LOW                                    /6.02E+14    0.00      3000./
  H2/2./ O2/6./ H2O/6./ CH4/2./ CO/1.5/ CO2/3.5/ C2H6/3.0/ AR/0.5/
O2+CO=O+CO2                               2.50E+12    0.00     47800.  !  (3) Warnatz 84
H2+CO(+M)=CH2O(+M)                        4.30E+07    1.50     79600.  ! (14) GRI-Mech 1.2
  LOW                                    /5.07E+27   -3.42     84350./
  TROE /0.932 197 1540 10300/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
OH+CO=H+CO2                               4.10E+04    2.11     -1578.  ! (15) Carriere 04
HO2+CO=OH+CO2                             1.50E+14    0.00     23600.  ! (16) Baulch 76
O+HCO=OH+CO                               3.00E+13    0.00         0.  !  (1) TSA/HAM 86
O+HCO=H+CO2                               3.00E+13    0.00         0.  !  (1) TSA/HAM 86
H+HCO(+M)=CH2O(+M)                        1.09E+12    0.48      -260.  ! (17) Eiteneer 98
  LOW                                    /2.47E+24   -2.57       425./
  TROE /0.7824 271 2755 6570/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
H+HCO=H2+CO                               7.30E+13    0.00         0.  ! (18) TIMONEN 87a
OH+HCO=H2O+CO                             3.00E+13    0.00         0.  !  (1) TSA/HAM 86
HCO+M=H+CO+M                              1.87E+17   -1.00     17000.  ! (19) TIMONEN 87b
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
HCO+O2=HO2+CO                             4.22E+12    0.00         0.  ! (20) TIMONEN 88
HCO+HO2=CO2+OH+H                          3.00E+13    0.00         0.  !  (1) TSA/HAM 86
!
!---------CHxO chemistry------------
!
O+CH2O=OH+HCO                             1.81E+13    0.00      3078.  !  (1) TSA/HAM 86
O2+CH2O=HO2+HCO                           2.05E+13    0.00     38920.  !  (1) TSA/HAM 86
H+CH2O=HCO+H2                             5.18E+7     1.66      1834.  ! (21) Hochgreb 92
H+CH2O(+M)=CH2OH(+M)                      5.40E+11    0.45      3600.  ! (22) GRI 3.0
  LOW                                    /1.27E+32   -4.82      6530./
  TROE /0.7187 103 1291 4160/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/
H+CH2O(+M)=CH3O(+M)                       5.40E+11    0.45      2600.  ! (14) GRI-Mech 1.2
  LOW                                    /2.20E+30   -4.80      5560./
  TROE /0.758 94 1555 4200/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/
OH+CH2O=HCO+H2O                           3.43E+09    1.18      -447.  !  (1) TSA/HAM 86
HO2+CH2O=HCO+H2O2                         1.47E+13    0.00     15200.  ! (21) Hochgreb 92
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O+CH2OH=OH+CH2O                    4.20E+13    0.00         0.  ! (23) Tsang 87
H+CH2OH=H2+CH2O                    6.00E+12    0.00         0.  ! (23) Tsang 87
H+CH2OH=OH+CH3                     9.63E+13    0.00         0.  !  (1) TSA/HAM 86
OH+CH2OH=H2O+CH2O                  2.40E+13    0.00         0.  ! (23) Tsang 87
CH2OH+O2=HO2+CH2O                  2.41E+14    0.00      5017.  ! (24) Grotheer 88
  DUPLICATE
CH2OH+O2=HO2+CH2O                  1.51E+15   -1.00         0.  ! (24) Grotheer 88
  DUPLICATE
CH2OH+HO2=CH2O+H2O2                1.20E+13    0.00         0.  ! (23) Tsang 87
CH2OH+HCO=CH3OH+CO                 1.20E+14    0.00         0.  ! (23) Tsang 87
CH2OH+HCO=CH2O+CH2O                1.80E+14    0.00         0.  ! (23) Tsang 87
2CH2OH=CH3OH+CH2O                  3.00E+12    0.00         0.  ! (23) Tsang 87
CH2OH+CH3O=CH3OH+CH2O              2.40E+13    0.00         0.  ! (23) Tsang 87
O+CH3O=OH+CH2O                     6.00E+12    0.00         0.  !  (1) TSA/HAM 86
H+CH3O=H2+CH2O                     2.00E+13    0.00         0.  !  (3) Warnatz 84
H+CH3O=OH+CH3                      3.20E+13    0.00         0.  ! (14) GRI-Mech 1.2
OH+CH3O=H2O+CH2O                   1.80E+13    0.00         0.  ! (23) Tsang 87
CH3O+O2=HO2+CH2O                   9.03E+13    0.00     11980.  ! (26) Wantuck 87
  DUPLICATE
CH3O+O2=HO2+CH2O                   2.20E+10    0.00      1748.  ! (26) Wantuck 87
  DUPLICATE
CH3O+HO2=CH2O+H2O2                 3.00E+11    0.00         0.  ! (23) Tsang 87
CH3O+CO=CH3+CO2                    1.57E+13    0.00     11800.  ! (23) Tsang 87
CH3O+HCO=CH3OH+CO                  9.00E+13    0.00         0.  ! (23) Tsang 87
2CH3O=CH3OH+CH2O                   6.00E+13    0.00         0.  ! (23) Tsang 87
O+CH3OH=OH+CH2OH                   3.88E+05    2.50      3080.  ! (23) Tsang 87
H+CH3OH=CH2OH+H2                   1.44E+13    0.00      6095.  ! (25) Held 98
H+CH3OH=CH3O+H2                    3.60E+12    0.00      6095.  ! (25) Held 98
OH+CH3OH=CH2OH+H2O                 7.10E+06    1.80      -596.  ! (27) Bott 91
OH+CH3OH=CH3O+H2O                  1.00E+06    2.10       496.5 ! (27) Bott 91
CH3+CH3OH=CH2OH+CH4                3.19E+01    3.17      7172.  ! (23) Tsang 87
O2+CH3OH=CH2OH+HO2                 2.05E+13    0.00     44900.  ! (23) Tsang 87
HCO+CH3OH=CH2OH+CH2O               9.63E+03    2.90     13110.  ! (23) Tsang 87
HO2+CH3OH=CH2OH+H2O2               3.98E+13    0.00     19400.  ! (28) Cathonnet 82
CH3O+CH3OH=CH2OH+CH3OH             3.00E+11    0.00      4060.  ! (23) Tsang 87
CH3OH=CH3+OH                       1.90E+16    0.00     91800.  ! (23) Tsang 87
CH3OH(+M)=CH2OH+H(+M)              2.69E+16   -0.08     98940.  ! (25) Held 98
  LOW                             /2.34E+40   -6.33    103100./
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  TROE /0.773 693 5333 /
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
!
!---------CH4 (CHx) chemistry------------
!
O+CH4=OH+CH3                            1.02E+09   1.50       8600.  !  (1) TSA/HAM 86
H+CH4=CH3+H2                            6.60E+08   1.62      10840.  ! (22) GRI 3.0
OH+CH4=CH3+H2O                          1.00E+08   1.60       3120.  ! (30) Cohen 91
CH+CH4=H+C2H4                           6.00E+13   0.00          0.  ! (31) Butler 80
CH2SING+CH4=2CH3                        1.60E+13   0.00       -570.  ! (22) GRI 3.0
CH2+CH4=2CH3                            2.46E+06   2.00       8270.  ! (32) Bohland 85
O+CH3=H+CH2O                            5.06E+13   0.00          0.  ! (22) GRI 3.0
O+CH3=H+H2+CO                           3.37E+13   0.00          0.  ! (22) GRI 3.0
H+CH3(+M)=CH4(+M)                       1.39E+16  -0.53        536.  ! (22) GRI 3.0
  LOW                                  /2.62E+33  -4.76       2440. /
  TROE /0.783 74 2941 6964/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
OH+CH3=CH2+H2O                          5.60E+07   1.60       5420.  ! (22) GRI 3.0
OH+CH3=CH2SING+H2O                      6.44E+17  -1.34       1417.  ! (22) GRI 3.0
HO2+CH3=O2+CH4                          1.00E+12   0.00          0.  ! (33) Reid 84
HO2+CH3=OH+CH3O                         2.00E+13   0.00          0.  !  (1) TSA/HAM 86
CH+CH3=H+C2H3                           3.00E+13   0.00          0.  ! (34) Miller 89
CH2SING+CH3=H+C2H4                      1.20E+13   0.00       -570.  ! (14) GRI-Mech 1.2
CH3+O2=O+CH3O                           3.56E+13   0.00      30480.  ! (22) GRI 3.0
CH3+O2=OH+CH2O                          2.31E+12   0.00      20315.  ! (22) GRI 3.0
CH3+H2O2=HO2+CH4                        2.45E+04   2.47       5180.  ! (22) GRI 3.0
2CH3(+M)=C2H6(+M)                       6.77E+16  -1.18        654.  ! (22) GRI 3.0
  LOW                                  /3.40E+41  -7.03       2763./
  TROE /0.619 73.2 1180 9999/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
2CH3=H+C2H5                             6.84E+12   0.10      10600.  ! (22) GRI 3.0
CH3+HCO=CH4+CO                          1.21E+14   0.00          0.  !  (1) TSA/HAM 86
CH3+CH2O=HCO+CH4                        3.32E+03   2.81       5860.  ! (22) GRI 3.0
CH2+CH3=H+C2H4                          4.00E+13   0.00          0.  !  (3) Warnatz 84
O+CH2=H+HCO                             8.00E+13   0.00          0.  ! (35) Herron 88
O+CH2SING=H2+CO                         1.50E+13   0.00          0.  !  (1) TSA/HAM 86
O+CH2SING=H+HCO                         1.50E+13   0.00          0.  !  (1) TSA/HAM 86
H+CH2(+M)=CH3(+M)                       6.00E+14   0.00          0.  ! (22) GRI 3.0
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  LOW                                /1.04E+26  -2.76       1600./
  TROE /0.562 91 5836 8552/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
H+CH2SING=CH+H2                       3.00E+13   0.00          0.  !  (1) TSA/HAM 86
OH+CH2=H+CH2O                         2.00E+13   0.00          0.  !  (1) TSA/HAM 86
OH+CH2=CH+H2O                         1.13E+07   2.00       3000.  !  (1) TSA/HAM 86
OH+CH2SING=H+CH2O                     3.00E+13   0.00          0.  !  (1) TSA/HAM 86
HO2+CH2=OH+CH2O                       2.00E+13   0.00          0.  !  (1) TSA/HAM 86
CH+CH2=H+C2H2                         4.00E+13   0.00          0.  ! (36) Braun 81
CH2+O2=OH+H+CO                        5.00E+12   0.00       1500.  ! (37) Vinckier 79
CH2+O2=CO2+2H                         5.80E+12   0.00       1500.  ! (37) Vinckier 79
CH2+O2=O+CH2O                         2.40E+12   0.00       1500.  ! (37) Vinckier 79
CH2+H2=H+CH3                          5.00E+05   2.00       7230.  ! (22) GRI 3.0
2CH2=H2+C2H2                          1.60E+15   0.00      11944.  ! (38) Bauerle 95
2CH2=H+H+C2H2                         2.00E+14   0.00      10989.  ! (38) Bauerle 95
CH2SING+CO=CH2+CO                     9.00E+12   0.00          0.  ! (22) GRI 3.0
CH2SING+AR=CH2+AR                     9.00E+12   0.00        600.  ! (22) GRI 3.0
CH2SING+CO2=CH2+CO2                   7.00E+12   0.00          0.  ! (39) Koch 90
CH2SING+CO2=CO+CH2O                   1.40E+13   0.00          0.  ! (39) Koch 90
CH2+CO(+M)=CH2CO(+M)                  8.10E+11   0.50       4510.  ! (22) GRI 3.0
  LOW                                /2.69E+33  -5.11       7095./
  TROE /0.5907 275 1226 5185/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.00/ C2H6/3.00/
CH2SING+O2=H+OH+CO                    2.80E+13   0.00          0.  ! (40) Langford 83
CH2SING+O2=CO+H2O                     1.20E+13   0.00          0.  ! (40) Langford 83
CH2SING+H2=CH3+H                      7.00E+13   0.00          0.  ! (22) GRI 3.0
CH2SING+H2O(+M)=CH3OH(+M)             4.82E+17  -1.16       1145.  ! (22) GRI 3.0
  LOW                                /1.88E+38  -6.36       5040./
  TROE /0.6027 208 3922 10180/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/
CH2SING+H2O=CH2+H2O                   3.00E+13   0.00          0.  ! (41) Hack 88
CH2SING+H2O=H2+CH2O                   6.82E+10   0.25       -935.  ! (22) GRI 3.0
O+CH=H+CO                             5.70E+13   0.00          0.  ! (42) MESSING 80
OH+CH=H+HCO                           3.00E+13   0.00          0.  ! (43) Glarborg 86
CH+O2=O+HCO                           6.71E+13   0.00          0.  ! (22) GRI 3.0
CH+H2=H+CH2                           1.08E+14   0.00       3110.  ! (22) GRI 3.0
CH+H2O=H+CH2O                         5.71E+12   0.00       -755.  ! (10) Baulch 94
CH+CO(+M)=HCCO(+M)                    5.00E+13   0.00          0.  ! (14) GRI-Mech 1.2
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  LOW                               /2.69E+28  -3.74       1936./
  TROE /0.5757 237 1652 5069/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
CH+CO2=HCO+CO                        1.90E+14   0.00      15792.  ! (44) Markus 96
CH+CH2O=H+CH2CO                      9.46E+13   0.00       -515.  ! (45) Baulch 92
CH+HCCO=CO+C2H2                      5.00E+13   0.00          0.  ! (34) Miller 89
!
!---------C2H6 chemistry------------
!
O+C2H6=OH+C2H5                       3.00E+07   2.00       5115.  ! (46) Miller 92
H+C2H6=C2H5+H2                       5.40E+02   3.50       5210.  ! (46) Miller 92
OH+C2H6=C2H5+H2O                     7.26E+06   2.00        864.  ! (45) Baulch 92
CH3+C2H6=C2H5+CH4                    5.50E-01   4.00       8300.  ! (46) Miller 92
CH2SING+C2H6=CH3+C2H5                4.00E+13   0.00       -550.  ! (47) Wegener 90
C2H6+O2=C2H5+HO2                     4.04E+13   0.00      50872.  !  (1) TSA/HAM 86
C2H6+CH2OH=CH3OH+C2H5                1.99E+02   3.00      13976.  ! (23) Tsang 87
C2H6+CH3O=CH3OH+C2H5                 2.41E+11   0.00       7094.  !  (1) TSA/HAM 86
C2H6+C2H=C2H2+C2H5                   3.61E+12   0.00          0.  !  (1) TSA/HAM 86
C2H6+C2H3=C2H4+C2H5                  6.01E+02   3.30      10502.  !  (1) TSA/HAM 86
C2H6+CH3CO=CH3CHO+C2H5               1.81E+4    2.75      17527.  !  (1) TSA/HAM 86
C2H6+HCO=CH2O+C2H5                   4.70E+04   2.72      18235.  !  (1) TSA/HAM 86
!
!---------C2H5 chemistry------------
!
O+C2H5=CH3+CH2O                      2.24E+13   0.00          0.  ! (22) GRI 3.0
O+C2H5=H+CH3CHO                      1.10E+14   0.00          0.  ! (22) GRI 3.0
H+C2H5=H2+C2H4                       2.00E+12   0.00          0.  ! (22) GRI 3.0
H+C2H5(+M)=C2H6(+M)                  5.21E+17  -0.99       1580.  ! (22) GRI 3.0
  LOW                               /1.99E+41  -7.080      6685./
  TROE /0.8422 125 2219 6882/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
C2H5+O2=HO2+C2H4                     1.92E+07   1.02      -2035.  ! (48) Miller 00
C2H5+HO2=C2H5O+OH                    3.00E+13   0.00          0.  ! (49) Bozzelli 90
C2H5+HO2=C2H4+H2O2                   3.01E+11   0.00          0.  !  (1) TSA/HAM 86
C2H5+OH=C2H4+H2O                     2.41E+13   0.00          0.  !  (1) TSA/HAM 86
C2H5+CH3=CH4+C2H4                    1.13E+12  -0.50          0.  !  (1) TSA/HAM 86
CH3+C2H5(+M)=C3H8(+M)                9.60E+14  -0.50          0.  ! (50) Qin/Wan 00
  LOW                               /6.80E+61  -13.42      6000./
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  TROE /1.00 1000 1433.9 5328.8/
C2H5+CH2OH=C2H4+CH3OH                  2.41E+12   0.00          0.  ! (23) Tsang 87
C2H5+CH2OH=C2H6+CH2O                   2.41E+12   0.00          0.  ! (23) Tsang 87
C2H5+CH3O=C2H6+CH2O                    2.41E+13   0.00          0.  !  (1) TSA/HAM 86
C2H5+C2H=C2H2+C2H4                     1.81E+12   0.00          0.  !  (1) TSA/HAM 86
CH2+C2H5=C2H4+CH3                      1.81E+13   0.00          0.  !  (1) TSA/HAM 86
CH2SING+C2H5=C2H4+CH3                  9.00E+12   0.00          0.  !  (1) TSA/HAM 86
C2H5+CH2SING=C3H6+H                    9.00E+12   0.00          0.  !  (1) TSA/HAM 86
C2H5+H2O2=C2H6+HO2                     8.73E+09   0.00        974.  !  (1) TSA/HAM 86
!
!---------C2H4 chemistry------------
!
H+C2H4(+M)=C2H5(+M)                    5.40E+11   0.45       1820.  ! (22) GRI 3.0
  LOW                                 /6.00E+41  -7.62       6970./
  TROE /0.9753 210 984 4374/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
H+C2H4=C2H3+H2                         1.12E+07   2.12      13366.  ! (51) Bhargava 98
OH+C2H4=C2H3+H2O                       5.53E+05   2.31       2900.  ! (51) Bhargava 98
CH3+C2H4=C2H3+CH4                      2.27E+05   2.00       9200.  ! (22) GRI 3.0
CH3+C2H4(+M)<=>nC3H7(+M)               2.55E+06   1.600      5700.  ! (52) Tsang 88
  LOW                                 /3.00E+63  -14.6       18170./
  TROE /0.1894 277. 8748. 7891./
  H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/0.70/
C2H4(+M)=H2+C2H2(+M)                   8.00E+12   0.44       88770. ! (22) GRI 3.0
  LOW                                 /1.58E+51  -9.30       97800./
  TROE /0.7345 180 1035 5417/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
C2H4+CH2SING=C3H6                      9.03E+13   0.00          0.  !  (1) TSA/HAM 86
C2H4+HO2=C2H4O+OH                      6.03E+09   0.00       7949.  !  (1) TSA/HAM 86
C2H4+O=H+CH2CHO                        7.33E+07   1.60       1260.  ! (53) Westmoreland PC
C2H4+O=CH3+HCO                         1.13E+08   1.60       1020.  ! (53) Westmoreland PC
C2H4+O=C2H3+OH                         2.15E+06   2.55      11900.  ! (53) Westmoreland PC
C2H4+O2=C2H3+HO2                       4.22E+13   0.00      60800.  ! (54) Wang 97
C2H4+CO=C2H3+HCO                       1.51E+14   0.00      90616.  !  (1) TSA/HAM 86
C2H4+C2H=C4H4+H                        1.21E+13   0.00          0.  !  (1) TSA/HAM 86
C2H4+C2H2=C2H3+C2H3                    2.41E+13   0.00      68360.  !  (1) TSA/HAM 86
C2H4+C2H4=C2H5+C2H3                    4.82E+14   0.00      71539.  !  (1) TSA/HAM 86
!
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!---------C2H3 chemistry------------
!
H+C2H3(+M)=C2H4(+M)                     6.08E+12    0.27       280.  ! (22) GRI 3.0
  LOW                                  /1.40E+30   -3.86      3320./
  TROE /0.782 207.5 2663 6095/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
C2H3(+M)=C2H2+H(+M)                     3.86E+08    1.62     37058.  ! (55) Knyazev 96
  LOW                                  /2.56E27    -3.40     35789.7/
  TROE /0.2134 36.643 7794.56 4007.66/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
H+C2H3=H2+C2H2                          9.64E+13    0.00         0.  !  (1) TSA/HAM 86
OH+C2H3=H2O+C2H2                        5.00E+12    0.00         0.  ! (56) Lutz 88
C2H3+O2=HCO+CH2O                        5.42E+12    0.00         0.  ! (15) Carriere 04 20Torr
C2H3+HO2=OH+CH2CO+H                     3.01E+13    0.00         0.  !  (1) TSA/HAM 86
C2H3+CH3=C2H2+CH4                       3.92E+11    0.00         0.  !  (1) TSA/HAM 86
C2H3+O=CH2CO+H                          3.00E+13    0.00         0.  ! (57) Heinemann 86
C2H3+O2=C2H2+HO2                        1.34E+06    1.61      -383.  ! (58) Mebel96
  DUPLICATE
C2H3+O2=C2H2+HO2                        1.37E+02    3.37      3663.  ! (53) Westmoreland PC
  DUPLICATE
C2H3+O2=C2H3OO                          5.61E+19   -3.30       165.4 ! (15) Carriere 04 20Torr
C2H3OO+H=CH2CHO+OH                      1.00E+14    0.00         0.  ! (15) Carriere 04 20Torr
C2H3OO+CH2=CH2CHO+CH2O                  2.00E+13    0.00         0.  ! (15) Carriere 04 20Torr
C2H3OO+OH=CH2CHO+HO2                    2.00E+13    0.00         0.  ! (15) Carriere 04 20Torr
C2H3OO+O=CH2CHO+O2                      2.00E+13    0.00         0.  ! (15) Carriere 04 20Torr
C2H3+O2=O+CH2CHO                        1.31E+01    3.55      2311.5 ! (15) Carriere 04 20Torr
C2H3+CH2OH=C2H4+CH2O                    3.01E+13    0.00         0.  !  (1) TSA/HAM 86
C2H3+CH3O=C2H4+CH2O                     2.41E+13    0.00         0.  !  (1) TSA/HAM 86
C2H3+CH3OH=C2H4+CH3O                    1.44E+01    3.10      6935.  !  (1) TSA/HAM 86
C2H3+CH3OH=C2H4+CH2OH                   3.19E+01    3.20      7172.  !  (1) TSA/HAM 86
C2H3+CO=C2H3CO                          1.51E+11    0.00      4809.  !  (1) TSA/HAM 86
C2H3+C2H=C4H4                           1.00E+14    0.00         0.  ! (59) Duran 88
C2H3+C2H=C2H2+C2H2                      9.64E+11    0.00         0.  !  (1) TSA/HAM 86
C2H3+CH3CO=C2H3CO+CH3                   1.81E+13    0.00         0.  !  (1) TSA/HAM 86
C2H5+C2H3=AC3H5+CH3                     8.00E+25   -3.46     11775.  !  (1) TSA/HAM 86 0.1 atm
C2H3+C2H5(+M)=IC4H8(+M)                 1.50E+13    0.00         0.  ! (60) Wang/Laskin 99
  LOW                                  /1.55E+56  -11.79      8984.5/
  TROE /0.198 2277.9 60000 5723.2/
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C2H3+C2H5=C2H2+C2H6                     4.82E+11    0.00         0.  !  (1) TSA/HAM 86
C2H3+CH2SING=C2H2+CH3                   1.81E+13    0.00         0.  !  (1) TSA/HAM 86
C2H3+CH2=C2H2+CH3                       1.81E+13    0.00         0.  !  (1) TSA/HAM 86
C2H3+H2O2=C2H4+HO2                      1.21E+10    0.00      -596.  !  (1) TSA/HAM 86
C2H3+CH2O=C2H4+HCO                      5.43E+03    2.81      5862.  !  (1) TSA/HAM 86
C2H3+CH2=AC3H4+H                        3.00E+13    0.00         0.  ! (61) Pauwels 95
C2H3+C2H3=i-C4H5+H                      1.50E+30   -4.95     13000.  ! (54) Wang 97 20Torr
C2H3+C2H3=n-C4H5+H                      1.10E+24   -3.28     12400.  ! (54) Wang 97 20Torr
!
!--------------------C2H2 chemistry------------
!
!-----------------------------------------H2CC chemistry-----------------------------------------
H2CC+C2H2(+M)=C4H4(+M)                  3.50E+05    2.055  -2400.    !(141) Laskin/Wang 00
  LOW                                  /1.40E+60  -12.599   7417./
  TROE /0.98 56. 580. 4164./
  H2/2.0/ CH4/2.0/ H2O/6.0/ C2H2/3.0/ CO/1.5/ C2H4/3.0/ C2H6/3.0/ CO2/2.0/
H2CC=C2H2                               1.0E+7      0.00       0.    !JAM(10/02) Miller Est
H2CC+C2H4=iiiC4H6                       1.0E+12     0.00       0.    !(141) Laskin/Wang 00
H2CC+O2=CH2+CO2                         1.00E+13    0.00       0.    !(141) Laskin/Wang 00
H2CC+H=C2H2+H                           1.00E+14    0.00       0.    !(141) Laskin/Wang 00
H2CC+OH=CH2CO+H                         2.00E+13    0.00       0.    !(141) Laskin/Wang 00
!-------------------------------------------------------------------------------------------------
!
O+C2H2=H+HCCO                           1.35E+07    2.00      1900.  ! (22) GRI 3.0
O+C2H2=OH+C2H                           4.60E+19   -1.41     28950.  ! (22) GRI 3.0
O+C2H2=CO+CH2                           6.94E+06    2.00      1900.  ! (22) GRI 3.0
OH+C2H2=H+CH2CO                         2.18E-04    4.50     -1000.  ! (62) Miller 86
OH+C2H2=C2H+H2O                         3.37E+07    2.00     14000.  ! (62) Miller 86
OH+C2H2=CH3+CO                          4.83E-04    4.00     -2000.  ! (62) Miller 86
C2H2+CH=C3H2+H                          1.10E+13    0.00         0.  ! (63) Warnatz 82
C2H2+CH2=C3H3+H                         1.20E+13    0.000     6620.  ! (64) Bohland 88
C2H2+CH3=C2H+CH4                        1.81E+11    0.00     17289.  !  (1) TSA/HAM 86
C2H2+O2=2HCO                            1.00E+12    0.00     28000.  ! (65) Hidaka 96
C2H2+CH2OH=C2H3+CH2O                    7.23E+11    0.00      9004.  ! (23) Tsang 87
C2H2+CO=C2H+HCO                         4.82E+14    0.00    106713.  !  (1) TSA/HAM 86
C2H2+C2H=C4H2+H                         3.00E+13    0.00         0.  ! (10) Baulch94 uncertainty 3.16
C2H2+C2H(+M)=nC4H3(+M)                  8.30E+10    0.90      -363.  ! (60) Wang/Laskin 99
  LOW                                  /1.24E+31   -4.72      1871./
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  TROE /1.0 100. 5613. 13387./
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ C2H2/2.5/ C2H4/2.5/
C2H2+C2H(+M)=iC4H3(+M)                 8.30E+10    0.90      -363.0 ! (60) Wang/Laskin 99
  LOW                                 /1.24E+31   -4.72      1871./
  TROE /1.0 100. 5613. 13387./
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ C2H2/2.5/ C2H4/2.5/
C2H3+C2H2=C4H4+H                       5.00E+14   -0.71      6700.  ! (54) Wang 97 20Torr
C2H2+CH2SING=C3H3+H                    3.42E15    -0.624     -230.7 ! (66) Hansen/Miller 08
C2H2+CH2SING=CH2+C2H2                  8.55E14    -0.624     -230.7 ! (66) Hansen/Miller 08
HCCO+C2H2=C3H3+CO                      1.00E+11    0.00      3000.  ! (46) Miller 92
C2H2+C2H3=n-C4H5                       1.10E+32   -7.33      6200.  ! (54) Wang 97 20Torr
C2H2+C2H3=i-C4H5                       2.10E+36   -8.78      9100.  ! (54) Wang 97 20Torr
!
!--------------------C2H chemistry------------
!
O+C2H=CH+CO                            1.00E+13    0.00         0.  !  (3) Warnatz84
H+C2H(+M)=C2H2(+M)                     1.000E+17  -1.00         0.  ! (22) GRI3.0
  LOW                                 /3.750E+33  -4.80      1900./
  TROE /0.6464 132 1315 5566/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
OH+C2H=H+HCCO                          2.00E+13    0.00         0.  ! (67) Frenklach 92
C2H+O2=HCO+CO                          1.00E+13    0.00      -775.  ! (22) GRI 3.0
C2H+H2=H+C2H2                          5.68E+10    0.90      1993.  ! (68) Farhat 93
C2H+HO2=HCCO+OH                        1.81E+13    0.00         0.  !  (1) TSA/HAM 86
C2H+CH3=C3H3+H                         2.41E+13    0.00         0.  !  (1) TSA/HAM 86
C2H+O2=HCCO+O                          6.03E+11    0.00         0.  !  (1) TSA/HAM 86
C2H+CH2OH=C2H2+CH2O                    3.61E+13    0.00         0.  !  (1) TSA/HAM 86
C2H+CH2OH=C3H3+OH                      1.21E+13    0.00         0.  !  (1) TSA/HAM 86
C2H+CH3OH=C2H2+CH2OH                   6.03E+12    0.00         0.  !  (1) TSA/HAM 86
C2H+CH3O=CH2O+C2H2                     2.41E+13    0.00         0.  !  (1) TSA/HAM 86
C2H+CH3OH=C2H2+CH3O                    1.21E+12    0.00         0.  ! (23) Tsang 87
C2H+CH2=CH+C2H2                        1.81E+13    0.00         0.  !  (1) TSA/HAM 86
C2H+CH2SING=C2H2+CH                    1.81E+13    0.00         0.  !  (1) TSA/HAM 86
!
!-----------------C2HxOy chemistry-----------------
!
O+HCCO=H+2CO                           1.00E+14    0.00         0.  ! (69) Frank 88
H+HCCO=CH2SING+CO                      5.00E13     0.00         0.  !  (3) Warnatz 84
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CH2+HCCO=C2H3+CO                        3.00E+13    0.00         0.  ! (62) Miller86
HCCO+O2=CO2+CO+H                        4.78E+12   -0.14      1150.  ! (70) Klippenstain 02
HCCO+O2=CO+CO+OH                        1.91E+11   -0.02      1023.  ! (70) Klippenstain 02
2HCCO=2CO+C2H2                          1.00E+13    0.00         0.  ! (34) Miller 89
HCCO+CH3=C2H4+CO                        5.00E+13    0.00         0.  ! (54) Wang 97
O+CH2CO=OH+HCCO                         1.00E+13    0.00      8000.  ! (34) Miller 89
O+CH2CO=CH2+CO2                         1.75E+12    0.00      1350.  ! (71) Cvetanovic 87
H+CH2CO=HCCO+H2                         5.00E+13    0.00      8000.  ! (34) Miller 89
H+CH2CO=CH3+CO                          3.28E+10    0.85      2839.  ! (72) Hranislavljevic 98
H+CH2CO(+M)=CH2CHO(+M)                  4.86E+11    0.42     -1755.  ! (22) GRI 3.0
  LOW                                  /1.01E+42   -7.63      3854./
  TROE /0.465 201 1773 5333.0/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
OH+CH2CO=HCCO+H2O                       7.50E+12    0.00      2000.  ! (34) Miller 89
CH2CO+OH=CH2OH+CO                       1.00E+13    0.00         0.  ! (45) Baulch 92
CH3CO+M=CH3+CO+M                        8.74E+42   -8.62     22410.  !  (1) TSA/HAM 86
CH2CHO+H=CH3CHO                         6.40E35    -7.60      5215.  ! (73) Hennessy 94
CH2CHO+H=CH3+HCO                        4.99E14    -0.32       912.  ! (73) Hennessy 94
CH2CHO+O=CH2O+HCO                       5.00E13     0.00         0.  ! (73) Hennessy 94
CH2CHO+OH=H2O+CH2CO                     1.20E+13    0.00         0.  ! (22) GRI 3.0
CH2CHO+OH=HCO+CH2OH                     3.01E+13    0.00         0.  ! (22) GRI 3.0
CH2CHO+O2=CH2CO+HO2                     1.57E11     0.00         0.  ! (45) Baulch 92
CH3CHO=CH3+HCO                          9.59E+14    0.00     74180.  ! (74) Dagaut 95
CH3CHO+O2=CH3CO+HO2                     2.00E+13    0.50     42200.  ! (10) Baulch 94
CH3CHO+H=CH2CHO+H2                      4.10E+09    1.16      2405.  ! (10) Baulch 94
CH3CHO+OH=CH3CO+H2O                     2.35E+10    0.73     -1113.  ! (10) Baulch 94
CH3CHO+O=CH2CHO+OH                      5.85E+12    0.00      1808.  ! (10) Baulch 94
CH3CHO+HO2=CH3CO+H2O2                   1.70E+12    0.00     10700.  ! (75) Colket 77
CH3CHO+CH3=CH3CO+CH4                    1.70E+12    0.00      8440.  ! (76) Wilk 89
CH3CHO+HCO=CH3CO+CH2O                   7.80E+13    0.00      8440.  ! (74) Dagaut 95
C2H5+O2=C2H5OO                          2.24E+10    0.77      -568.  ! (77) Wagner 90
C2H5OO+HO2=C2H5O+OH+O2                  1.75E+10    0.00     -3275.  ! (78) Fischer 00
C2H5O=CH3+CH2O                          1.00E+15    0.00     21523.  ! (79) Heicklen 88
C2H5O=CH3CHO+H                          2.00E+14    0.00     23215.  ! (79) Heicklen 88
C2H5O+O2=CH3CHO+HO2                     6.03E+10    0.00      1643.  ! (45) Baulch 92
C2H4O+O2=CH2CHO+HO2                     4.00E+13    0.00     61500.  ! (80) Dagaut 96
C2H4O+H=CH2CHO+H2                       2.00E13     0.00      8300.  ! (81) Lifshitz 83
C2H4O+H=C2H3+H2O                        5.00E+09    0.00      5000.  ! (81) Lifshitz 83
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C2H4O+H=C2H4+OH                     9.51E+10    0.00      5000.  ! (81) Lifshitz 83
C2H4O+OH=CH2CHO+H2O                 4.79E+13    0.00      5955.  ! (76) Wilk 89
C2H4O+O=CH2CHO+OH                   1.91E+12    0.00      5250.  ! (82) Bogan 78
C2H4O+HO2=CH2CHO+H2O2               4.00E+12    0.00     17000.  ! (80) Dagaut 96
C2H4O=CH3CHO                        6.00E+13    0.00     57167.  ! (80) Dagaut 96
C2H4O=CH3+HCO                       4.90E+13    0.00     57167.  ! (80) Dagaut 96
C2H4O=CH4+CO                        1.21E+13    0.00     57167.  ! (80) Dagaut 96
!
!---------C3H8 chemistry------------
!
C3H8+H=nC3H7+H2                     1.30E+06    2.54      6756.  ! (52) Tsang 88
C3H8+H=iC3H7+H2                     1.30E+06    2.40      4471.  ! (52) Tsang 88
C3H8+O=nC3H7+OH                     1.90E+05    2.68      3716.  ! (52) Tsang 88
C3H8+O=iC3H7+OH                     4.76E+04    2.71      2106.  ! (52) Tsang 88
C3H8+OH=iC3H7+H2O                   1.40E+03    2.80      -310.  ! (52) Tsang 88
C3H8+OH=nC3H7+H2O                   1.37E+03    2.70       580.  ! (52) Tsang 88
C3H8+O2=nC3H7+HO2                   3.97E+13    0.00     50872.  ! (52) Tsang 88
C3H8+O2=iC3H7+HO2                   3.97E+13    0.00     47693.  ! (52) Tsang 88
C3H8+HO2=nC3H7+H2O2                 4.76E+04    2.55     16494.  ! (52) Tsang 88
C3H8+HO2=iC3H7+H2O2                 9.64E+03    2.60     13910.  ! (52) Tsang 88
C3H8+CH3=nC3H7+CH4                  9.04E-01    3.65      7154.  ! (52) Tsang 88
C3H8+CH3=iC3H7+CH4                  1.51E+00    3.46      5481.  ! (52) Tsang 88
C3H8+CH2OH=nC3H7+CH3OH              1.99E+02    2.95      3976.  ! (52) Tsang 88
C3H8+CH3O=nC3H7+CH3OH               4.34E+11    0.00      6458.  ! (52) Tsang 88
C3H8+CH2SING=nC3H7+CH3              9.04E-01    3.65      7154.  ! (52) Tsang 88
C3H8+C2H3=nC3H7+C2H4                6.03E+02    3.30     10502.  ! (52) Tsang 88
C3H8+C2H=nC3H7+C2H2                 3.61E+12    0.00         0.  ! (52) Tsang 88
C3H8+C2H5=nC3H7+C2H6                9.04E-02    3.65      9141.  ! (52) Tsang 88
C3H8+HCO=nC3H7+CH2O                 2.05E+05    2.50     18431.  ! (52) Tsang 88
C3H8+iC3H7=nC3H7+C3H8               8.40E-03    4.20      8716.  ! (52) Tsang 88
C3H8+CH3CO=nC3H7+CH3CHO             4.22E+04    2.60     17658.  ! (52) Tsang 88
C3H8+CH2=nC3H7+CH3                  9.03E-01    3.65      7154.  ! (52) Tsang 88
C3H8+CH2OH=iC3H7+CH3OH              6.03E+01    2.95     11989.  ! (52) Tsang 88
C3H8+CH3O=iC3H7+CH3OH               1.45E+11    0.00      4571.  ! (52) Tsang 88
C3H8+CH2SING=iC3H7+CH3              1.51E+00    3.46      7472.  ! (52) Tsang 88
C3H8+C2H3=iC3H7+C2H4                1.02E+03    3.10      8829.  ! (52) Tsang 88
C3H8+C2H=iC3H7+C2H2                 1.21E+12    0.00         0.  ! (52) Tsang 88
C3H8+C2H5=iC3H7+C2H6                1.21E+00    3.46      7468.  ! (52) Tsang 88
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C3H8+HCO=iC3H7+CH2O                    1.08E+07    1.90     17006.  ! (52) Tsang 88
C3H8+CH3CO=iC3H7+CH3CHO                5.30E+06    2.00     16241.  ! (52) Tsang 88
C3H8+CH2=iC3H7+CH3                     1.51E+00    3.46      7472.  ! (52) Tsang 88
!
!---------C3H7 chemistry------------
!
nC3H7+H=C3H6+H2                        1.81E+12    0.00        0.   ! (52) Tsang 88
nC3H7+H(+M)=C3H8(+M)                   3.60E+13    0.00        0.   ! (52) Tsang 88
  LOW                                 /3.01E+58   -9.32    5833.6/
  TROE /0.498 1314 1314 50000/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/ 0.7/
nC3H7+H = C2H5+CH3                     3.40E+18   -1.33    5386.    ! (52) Tsang 88 0.1 atm
nC3H7+O=C2H5+CH2O                      9.60E+13    0.00       0.    ! (52) Tsang 88
nC3H7+O2=C3H6+HO2                      9.04E+10    0.00       0.    ! (52) Tsang 88
nC3H7+HO2=C2H5+OH+CH2O                 2.41E+13    0.00       0.    ! (52) Tsang 88
nC3H7+OH=C3H6+H2O                      2.41E+13    0.00       0.    ! (52) Tsang 88
nC3H7+CH3=CH4+C3H6                     1.14E+13   -0.32       0.    ! (52) Tsang 88
nC3H7+C2H5=C3H6+C2H6                   1.45E+12    0.00       0.    ! (52) Tsang 88
nC3H7+C2H5=C3H8+C2H4                   1.15E+12    0.00       0.    ! (52) Tsang 88
nC3H7+C2H3=C3H8+C2H2                   1.21E+12    0.00       0.    ! (52) Tsang 88
nC3H7+C2H2=AC3H5+C2H4                  7.23E11     0.00    9004.    ! (52) Tsang 88
nC3H7+C2H=C3H3+C2H5                    1.21E+13    0.00       0.    ! (52) Tsang 88
nC3H7+C2H=C3H6+C2H2                    6.03E+12    0.00       0.    ! (52) Tsang 88
nC3H7+iC3H7=C3H8+C3H6                  5.13E+13   -0.35       0.    ! (52) Tsang 88
nC3H7+HCO=CO+C3H8                      6.03E+13    0.00       0.    ! (52) Tsang 88
nC3H7+CH3O=C3H8+CH2O                   2.41E+13    0.00       0.    ! (52) Tsang 88
nC3H7+CH2SING=C2H5+C2H4                2.58E+13    0.00       0.    ! (52) Tsang 88
nC3H7+CH2SING=C3H6+CH3                 1.03E+13    0.00       0.    ! (52) Tsang 88
nC3H7+CH2=C2H4+C2H5                    1.81E+13    0.00       0.    ! (52) Tsang 88
nC3H7+CH2=C3H6+CH3                     1.81E+12    0.00       0.    ! (52) Tsang 88
nC3H7+CH2OH=C3H6+CH3OH                 4.82E+11    0.00       0.    ! (52) Tsang 88
iC3H7=CH3+C2H4                         1.00E+14    0.00   45000.    ! (83) Dagaut 92
iC3H7+H=C3H6+H2                        3.61E+12    0.00       0.    ! (52) Tsang 88
iC3H7+H(+M)=C3H8(+M)                   2.40E+13    0.00       0.    ! (52) Tsang 88
  LOW                                 /1.70E+58   -12.08   11263.7/
  TROE /0.649 1213.1 1213.1 13369.7/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
iC3H7+H = CH3+C2H5                     5.90E+23   -2.81    10009.   ! (52) 88TSA RRKM 0.1 atm
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iC3H7+O=CH3CHO+CH3                      9.60E+13    0.00        0.   ! (52) Tsang 88
iC3H7+O2=C3H6+HO2                       1.26E+11    0.00        0.   ! (52) Tsang 88
iC3H7+HO2=CH3CHO+OH+CH3                 2.41E+13    0.00        0.   ! (52) Tsang 88
iC3H7+OH=C3H6+H2O                       2.41E+13    0.00        0.   ! (52) Tsang 88
iC3H7+CH3=CH4+C3H6                      2.19E+14   -0.68        0.   ! (52) Tsang 88
iC3H7+C2H5=C3H6+C2H6                    2.30E+13   -0.35        0.   ! (52) Tsang 88
iC3H7+C2H5=C3H8+C2H4                    1.84E+13   -0.35        0.   ! (52) Tsang 88
iC3H7+C2H3=C2H4+C3H6                    1.52E+14   -0.70        0.   ! (52) Tsang 88
iC3H7+C2H3=C3H8+C2H2                    1.52E+14   -0.70        0.   ! (52) Tsang 88
iC3H7+C2H2=CH3+iiiC4H6                  2.77E+10    0.00     6504.   ! (52) Tsang 88
iC3H7+C2H=C3H6+C2H2                     3.60E+12    0.00        0.   ! (52) Tsang 88
iC3H7+iC3H7=C3H8+C3H6                   2.11E+14   -0.70        0.   ! (52) Tsang 88
iC3H7+HCO=CO+C3H8                       1.20E+14    0.00        0.   ! (52) Tsang 88
iC3H7+CH3O=C3H8+CH2O                    1.21E+13    0.00        0.   ! (52) Tsang 88
iC3H7+CH2SING=C3H6+CH3                  1.04E+13    0.00        0.   ! (52) Tsang 88
iC3H7+CH2=C3H6+CH3                      3.01E+13    0.00        0.   ! (52) Tsang 88
iC3H7+CH2OH=C3H6+CH3OH                  2.89E+12    0.00        0.   ! (52) Tsang 88
iC3H7+CH2OH=C3H8+CH2O                   2.35E+12    0.00        0.   ! (52) Tsang 88
!
!---------C3H6 chemistry------------
!
CH3+C2H3(+M)=C3H6(+M)                   2.50E+13    0.00        0.   ! (50) Qin/Wan 00
  LOW                                  /4.27E+58  -11.94     9770./
  TROE /0.175 1341 60000 10140/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H2/3.00/ AR/0.7/
C3H6+H=H2+AC3H5                         1.70E+05    2.50    2492.    ! (84) Tsang 91
C3H6+H=C2H4+CH3                         8.80E+16    -1.05   6461.    ! (84) Tsang 91 0.1 atm
C3H6+H=SC3H5+H2                         7.81E+05    2.50   12285.    ! (85) Tsang 92
C3H6+H(+M)=nC3H7(+M)                    1.33E+13    0.00    3260.7   ! (84) Tsang 91
  LOW                                  /6.26E+38   -6.66    7000./
  TROE /1.000 1000.  1310.  48097./
  H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/
 C3H6+H(+M)=iC3H7(+M)                   1.33E+13    0.00    1559.8   ! (84) Tsang 91
  LOW                                 /8.70E+42   -7.50    4721.8/
  TROE /1.000 1000.   645.4  6844.3 /
  H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/
C3H6+H=TC3H5+H2                         3.90E+05    2.50    5821.    ! (85) Tsang 92
C3H6=H2+AC3H4                           4.00E+13    0.00   80000.    ! (87) Hidaka 92
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C3H6=CH4+C2H2                          3.50E+12    0.00   70000.    ! (87) Hidaka 92
C3H6+O=C2H5+HCO                        3.50E+07    1.65    -972.    ! (84) Tsang 91
C3H6+O=AC3H5+OH                        1.75E+11    0.70    5884.    ! (84) Tsang 91
C3H6+O=SC3H5+OH                        1.21E+11    0.70    8960.    ! (84) Tsang 91
C3H6+O=TC3H5+OH                        6.03E+10    0.70    7633.    ! (84) Tsang 91
C3H6+O=CH3+H+CH2CO                     1.20E+08    1.65     327.    ! (84) Tsang 91
C3H6+OH=AC3H5+H2O                      3.12E+06    2.00    -298.    ! (84) Tsang 91
C3H6+OH=SC3H5+H2O                      2.14E+06    2.00    2778.    ! (84) Tsang 91
C3H6+OH=TC3H5+H2O                      1.11E+06    2.00    1451.    ! (84) Tsang 91
C3H6+HO2=AC3H5+H2O2                    9.63E+03    2.60   13910.    ! (84) Tsang 91
C3H6+O2=AC3H5+HO2                      6.03E+13    0.00   47590.    ! (84) Tsang 91
C3H6+CH3=AC3H5+CH4                     2.20E+00    3.50    5675.    ! (84) Tsang 91
C3H6+CH3=TC3H5+CH4                     8.40E-01    3.50   11660.    ! (84) Tsang 91
C3H6+C2H5=AC3H5+C2H6                   2.23E+00    3.50    6637.    ! (84) Tsang 91
C3H6+C2H2=AC3H5+C2H3                   4.04E+13    0.00   46818.    ! (84) Tsang 91
C3H6+C2H3=AC3H5+C2H4                   2.21E+00    3.50    4682.    ! (84) Tsang 91
C3H6+C2H3=SC3H5+C2H4                   1.35E+00    3.50   10842.    ! (84) Tsang 91
C3H6+C2H3=TC3H5+C2H4                   8.40E-01    3.50    9670.    ! (84) Tsang 91
C3H6+C2H3=iiiC4H6+CH3                  7.23E+11    0.00    5008.    ! (84) Tsang 91
C3H6+C2H4=AC3H5+C2H5                   5.78E+13    0.00   51584.    ! (84) Tsang 91
C3H6+C2H4=nC3H7+C2H3                   6.03E+13    0.00   75446.    ! (84) Tsang 91
C3H6+CH2OH=AC3H5+CH3OH                 6.03E+01    2.95   12000.    ! (84) Tsang 91
C3H6+nC3H7=AC3H5+C3H8                  2.23E+00    3.50    6637.    ! (84) Tsang 91
C3H6+nC3H7=IC4H8+C2H5                  2.23E+00    3.50   -2000.    ! (84) Tsang 91
C3H6+iC3H7=C3H8+AC3H5                  6.62E-02    4.00    8066.    ! (84) Tsang 91
C3H6+C3H6=AC3H5+nC3H7                  2.53E+14    0.00   55179.    ! (84) Tsang 91
C3H6+C3H6=AC3H5+iC3H7                  4.88E+13    0.00   52309.    ! (84) Tsang 91
!
!---------C3H5 chemistry------------
!
CH3+C2H3=AC3H5+H                       1.50E+24   -2.83   18618.    ! (88) Davis/Wang 99
CH3+C2H3=SC3H5+H                       3.20E+35   -7.76   13300.    ! (88) Davis/Wang 99
CH3+C2H3=TC3H5+H                       4.99E+22   -4.39   18850.    ! (88) Davis/Wang 99
AC3H5+H(+M)=C3H6(+M)                   2.00E14     0.00       0.    ! (84) Tsang 91
  LOW                                 /1.33E+60  -12.00    5967.8/
  TROE /0.02 1097 10967 6860/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
AC3H5+H=AC3H4+H2                       1.80E+13    0.00       0.    ! (84) Tsang 91
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TC3H5+H=AC3H4+H2                      3.30E+12    0.00       0.    ! (83) Dagaut 92
SC3H5+H=AC3H4+H2                      3.30E+12    0.00       0.    ! (83) Dagaut 92
AC3H5+O=C2H3CHO+H                     6.00E+13    0.00       0.    ! (84) Tsang 91
AC3H5+O=C2H3+CH2O                     1.80E+14    0.00       0.    ! (89) Westmoreland PC
SC3H5+O=CH2CO+CH3                     1.81E+14    0.00       0.    ! (83) Dagaut 92
TC3H5+O=H+HCCO+CH3                    1.81E+14    0.00       0.    ! (83) Dagaut 92
AC3H5+OH = C2H3CHO+H+H                5.30E+37   -6.71   29306.    ! (84) Tsang 91 RRKM 0.1atm
AC3H5+OH=AC3H4+H2O                    6.00E+12    0.00       0.    ! (84) Tsang 91
AC3H5+O2=AC3H4+HO2                    4.99E+15   -1.40   22428.    ! (90) Boz/Dean 93
AC3H5+O2=CH2O+CH3CO                   1.19E+15   -1.01   20128.    ! (90) Boz/Dean 93
AC3H5+O2=OH+C2H3CHO                   1.82E+13   -0.41   22859.    ! (90) Boz/Dean 93
SC3H5+O2=CH3CHO+HCO                   4.34E+12    0.00       0.    ! (83) Dagaut 92
TC3H5+O2=CH3CHO+HCO                   4.34E+12    0.00       0.    ! (83) Dagaut 92
AC3H5+HO2=C2H3+CH2O+OH                6.60E+12    0.00       0.    ! (10) Baulch 94
AC3H5+CH3=AC3H4+CH4                   3.00E+12   -0.32    -131.    ! (84) Tsang 91
AC3H5+CH3(+M)=IC4H8(+M)               1.00E+14   -0.32    -262.    ! (84) Tsang 91
  LOW                                /3.51E+60   -12.97   6000./
  TROE /0.896 60000 1606 6118/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
SC3H5+CH3=AC3H4+CH4                   1.00E+11    0.00       0.    ! (83) Dagaut 92
TC3H5+CH3=AC3H4+CH4                   1.00E+11    0.00       0.    ! (83) Dagaut 92
AC3H5+C2H3=AC3H4+C2H4                 1.00E+12    0.00       0.    ! (83) Dagaut 92
SC3H5+C2H3=AC3H4+C2H4                 1.00E+11    0.00       0.    ! (83) Dagaut 92
TC3H5+C2H3=AC3H4+C2H4                 1.00E+11    0.00       0.    ! (83) Dagaut 92
AC3H5+CH2O=C3H6+HCO                   1.26E+08    1.90   18191.    ! (83) Dagaut 92
AC3H5+HCO=C3H6+CO                     6.00E+13    0.00       0.    ! (84) Tsang 91
AC3H5+AC3H5=AC3H4+C3H6                8.43E+10    0.00    -262.    ! (84) Tsang 91
AC3H5+CH2=iiiC4H6+H                   3.00E+13    0.00       0.    ! (84) Tsang 91
AC3H5+nC3H7=AC3H4+C3H8                7.23E+11    0.00    -131.    ! (84) Tsang 91
AC3H5+iC3H7=AC3H4+C3H8                4.58E+12   -0.35    -131.    ! (84) Tsang 91
AC3H5=TC3H5                           3.90E+59   -15.42  75400.    ! (88) Davis/Wang 99
AC3H5=SC3H5                           1.30E+55   -14.53  73800.    ! (88) Davis/Wang 99
TC3H5=SC3H5                           1.60E+44   -12.16  52200.    ! (88) Davis/Wang 99
!
!---------C3H4 chemistry------------
!
AC3H4=PC3H4                          6.0256E+53 -12.18   84276.    ! (91) JAM/SJK 03
AC3H4+H=AC3H5                        1.241E52   -12.02   17839.    ! (92) JAM/JPS 08
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  DUPLICATE
AC3H4+H=AC3H5                    6.923E36    -8.19    7462.    ! (92) JAM/JPS 08
  DUPLICATE
AC3H4+H=TC3H5                    1.554E53   -13.10   14472.    ! (92) JAM/JPS 08
  DUPLICATE
AC3H4+H=TC3H5                    0.988E45   -11.21    8212.    ! (92) JAM/JPS 08
  DUPLICATE
PC3H4+H=TC3H5                    3.174E52   -12.69   14226.    ! (92) JAM/JPS 08
  DUPLICATE
PC3H4+H=TC3H5                    2.589E45   -11.23    8046.    ! (92) JAM/JPS 08
  DUPLICATE
PC3H4+H=AC3H5                    3.379E49   -12.75   14072.    ! (92) JAM/JPS 08
  DUPLICATE
PC3H4+H=AC3H5                    2.981E43   -11.43    8736.    ! (92) JAM/JPS 08
  DUPLICATE
AC3H4+H=PC3H4+H                  1.476E13    0.26     4103.    ! (92) JAM/JPS 08
AC3H4+H=CH3+C2H2                 2.722E9     1.20     6834.    ! (92) JAM/JPS 08
PC3H4+H=CH3+C2H2                 3.891E10    0.989    4114.    ! (92) JAM/JPS 08
C2H2+CH3=AC3H5                  -0.681E+49  -12.27  16642.    ! (92) JAM/JPS 08
  DUPLICATE
C2H2+CH3=AC3H5                   1.524E+44  -10.73  15256.    ! (92) JAM/JPS 08
  DUPLICATE
C2H2+CH3=TC3H5                   6.80E+20    -4.16   18000.    ! (88) Davis/Wang 99 0.1 atm
C2H2+CH3=SC3H5                   1.40E+32    -7.14   10000.    ! (88) Davis/Wang 99 0.1 atm
AC3H4+H=C3H3+H2                  6.604E+3     3.095   5522.    ! (92) JAM/JPS 08
PC3H4+H=C3H3+H2                  3.57E+4      2.825   4821.    ! (92) JAM/JPS 08
AC3H4+O=C2H4+CO                  2.00E+07     1.80    1000.    ! (93) Davis/Wang 99
AC3H4+OH=C3H3+H2O                1.00E+07     2.00    1000.    ! (46) Miller 92
AC3H4+C2H=C3H3+C2H2              1.00E+13     0.00       0.    ! (54) Wang 97
AC3H4+CH3=C3H3+CH4               1.30E+12     0.00    7700.    ! (88) Davis/Wang 99
PC3H4+O=HCCO+CH3                 7.30E+12     0.00    2250.    ! (94) Adusei 96
PC3H4+O=C2H4+CO                  1.00E+13     0.00    2250.    ! (94) Adusei 96
PC3H4+O=C3H3+OH                  3.44E+04     2.16    4830.    ! (94) Adusei 96
PC3H4+OH=C3H3+H2O                1.00E+07     2.00    1000.    ! (46) Miller 92
PC3H4+C2H=C3H3+C2H2              1.00E+13     0.00       0.    ! (54) Wang 97
PC3H4+CH3=C3H3+CH4               1.80E+12     0.00    7700.    ! (88) Davis/Wang 99
!
!---------C3H3 chemistry------------
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!
C3H3+H=PC3H4                          3.6308E+36  -7.36    6039.    ! (91) JAM/SJK 03
C3H3+H=AC3H4                          3.3884E+36  -7.41    6337.    ! (91) JAM/SJK 03
C3H3+CH3(+M)=iiC4H6(+M)               1.50E+12     0.00       0.    ! (54) Wang 97
  LOW                                /2.60E+57    -11.94   9770./
  TROE /0.175 1341 60000 9770/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
C2H3+C2H3=iiiC4H6                     7.00E+57    -13.82  17629.    ! (54) Wang 97 RRKM 20 Torr
C3H3+H=C3H2+H2                        5.00E+13     0.00    3000.    ! (46) Miller 92
C3H3+O=>C2H2+HCO                      1.385E+14    0.00       0.    ! (95) Slagle 90
C3H3+O=C2H3+CO                        4.615E+13    0.00       0.    ! (95) Slagle 90
C3H3+O=C2H+CH2O                       4.615E+13    0.00       0.    ! (95) Slagle 90
C3H3+O=>C2H2+CO+H                     4.615E+13    0.00       0.    ! (95) Slagle 90
C3H3+OH=C3H2+H2O                       2.00E+13    0.00       0.    ! (34) Miller 89
C3H3+HCO=AC3H4+CO                      2.50E+13    0.00       0.    ! (54) Wang 97
C3H3+HCO=PC3H4+CO                      2.50E+13    0.00       0.    ! (54) Wang 97
C3H3+CH=iC4H3+H                        5.00E+13    0.00       0.    ! (54) Wang 97
C3H3+CH2=C4H4+H                        5.00E+13    0.00       0.    ! (46) Miller 92
C3H3+O2=CH2CO+HCO                      3.00E+10    0.00    2868.    ! (99) Slagle 88
C3H3+HCCO=C4H4+CO                      2.50E+13    0.00       0.    ! (54) Wang 97
C3H3+HO2=OH+CO+C2H3                    8.00E+11    0.00       0.    ! (93) Davis/Wang 99
C3H3+HO2=AC3H4+O2                      3.00E+11    0.00       0.    ! (93) Davis/Wang 99
C3H3+HO2=PC3H4+O2                      2.50E+12    0.00       0.    ! (93) Davis/Wang 99
C3H2+O2=H+CO+HCCO                      2.00E+12    0.00    1000.    ! (61) Pauwels 95
C3H2+O=C2H2+CO                         6.80E+13    0.00       0.    !(100) Warnatz 83
C3H2+OH=C2H2+HCO                       6.80E+13    0.00       0.    !(100) Warnatz 83
C3H2+H=C3H3                             1.1E+40   -8.0    84700.    !(101) HAR/KLI 07,WestmQRRK
C3H2+CH=C4H2+H                         5.00E+13    0.00       0.    ! (54) Wang 97
C3H2+CH2=nC4H3+H                       5.00E+13    0.00       0.    ! (54) Wang 97
C3H2+CH3=C4H4+H                        5.00E+12    0.00       0.    ! (54) Wang 97
C3H2+HCCO=nC4H3+CO                     1.00E+13    0.00       0.    ! (54) Wang 97
!
!---------C3HxO chemistry------------
!
C2H3CO+M=>C2H3+CO+M                    8.51E+15  0.00     23000.    ! (76) Wilk 89
C2H3+CO+M=>C2H3CO+M                    1.58E+11  0.00      6000.    ! (76) Wilk 89
C2H3CHO+HO2=>C2H3CH2O+O2               1.29E+11  0.00     32000.    ! (76) Wilk 89
C2H3CH2O=>C2H3CHO+H                    1.00E+14  0.00     19000.    ! (76) Wilk 89
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C2H3CHO+H=>C2H3CH2O                    1.00E+08  0.00     10000.    ! (76) Wilk 89
C2H3CHO+OH=>C2H3CO+H2O                 1.00E+13  0.00         0.    ! (76) Wilk 89
C2H3CO+H2O=>C2H3CHO+OH                 1.91E+13  0.00     36620.    ! (76) Wilk 89
C2H3CHO+H=>C2H3CO+H2                   3.98E+13  0.00      4200.    ! (76) Wilk 89
C2H3CO+H2=>C2H3CHO+H                   1.78E+13  0.00     23670.    ! (76) Wilk 89
C2H3CHO+O=>C2H3CO+OH                   5.01E+12  0.00      1790.    ! (76) Wilk 89
C2H3CO+OH=>C2H3CHO+O                   1.00E+12  0.00     19160.    ! (76) Wilk 89
C2H3CHO+HO2=>C2H3CO+H2O2               1.70E+12  0.00     10700.    ! (76) Wilk 89
C2H3CO+H2O2=>C2H3CHO+HO2               1.00E+12  0.00     14100.    ! (76) Wilk 89
C2H3CHO+CH3=>C2H3CO+CH4                1.74E+12  0.00      8440.    ! (76) Wilk 89
C2H3CO+CH4=>C2H3CHO+CH3                1.51E+13  0.00     28000.    ! (76) Wilk 89
C2H3CH2O+O2=>C2H3CHO+HO2               1.74E+11  0.00      1750.    ! (76) Wilk 89
C2H3CH2O=>CH2O+C2H3                    1.00E+14  0.00     21600.    ! (76) Wilk 89
CH2O+C2H3=>C2H3CH2O                    1.00E+11  0.00         0.    ! (76) Wilk 89
!
!---------C4H2 chemistry------------
!
C4H2+OH=CO+C3H3                      1.69E+28  -4.59      20140.   !(103) JPS/SJK/JAM 07
C4H2+H=nC4H3                         1.4375E+63 -15.66    24018    !(102) SJK/JAM 05
  DUPLICATE
C4H2+H=nC4H3                         4.165E+32 -6.4928     9726.1  !(102) SJK/JAM 05
  DUPLICATE
C4H2+H(+M)=iC4H3(+M)                  4.31E10    1.158      1752.9  !(102) SJK/JAM 05
  LOW                                /2.30E45   -8.095      2506.6 /
  TROE /0.0748 1.0E-50 -4215.9 1.0E50/
  H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/
C4H2+O=C3H2+CO                        2.70E+13   0.00       1720.   !  (3) Warnatz 84
C4H2+C2H=C6H2+H                       9.60E+13   0.00          0.   ! (54) Wang 97
C4H2+C2H=C6H3                         1.10E+30  -6.30       2790.   ! (54) Wang 97 20 Torr
!
!---------C4H3 chemistry------------
!
nC4H3=iC4H3                           3.70E+61 -15.81      54890.   ! (54) Wang 97 20 Torr
nC4H3+H=iC4H3+H                       2.40E+11   0.79       2410.   ! (54) Wang 97 20 Torr
nC4H3+H=C2H2+H2CC                     1.60E+19  -1.60       2220.   ! (54) Wang 97 20 Torr
nC4H3+H=C4H4                          1.10E+42  -9.65       7000.   ! (54) Wang 97 20 Torr
nC4H3+H=C4H2+H2                       3.00E+13   0.00          0.   ! (54) Wang 97
nC4H3+OH=C4H2+H2O                     2.00E+12   0.00          0.   ! (54) Wang 97
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nC4H3+C2H2=l-C6H4+H                 3.70E+16  -1.21      11100.   ! (54) Wang 97 20 Torr
nC4H3+C2H2=A1                       2.30E+68 -17.65      24400.   ! (54) Wang 97 20 Torr
nC4H3+C2H2=c-C6H4+H                 1.90E+36  -7.21      17900.   ! (54) Wang 97 20 Torr
iC4H3+H=C2H2+H2CC                   2.40E+19  -1.60       2800.   ! (54) Wang 97 20 Torr
iC4H3+H=C4H4                        4.20E+44 -10.27       7890.   ! (54) Wang 97 20 Torr
iC4H3+H=C4H2+H2                     5.00E+13   0.00          0.   ! (46) Miller 92
iC4H3+OH=C4H2+H2O                   4.00E+12   0.00          0.   ! (54) Wang 97
iC4H3+O2=HCCO+CH2CO                 7.86E+16  -1.80          0.   ! (54) Wang 97
!
!---------C4H4 chemistry------------
!
C4H4+H=n-C4H5                       4.20E+50 -12.34      12500.   ! (54) Wang 97 20Torr
C4H4+H=i-C4H5                       9.60E+52 -12.85      14300.   ! (54) Wang 97 20Torr
C4H4+H=nC4H3+H2                     6.65E+05   2.53      12240.   ! (54) Wang 97
C4H4+H=iC4H3+H2                     3.33E+05   2.53       9240.   ! (54) Wang 97
C4H4+OH=nC4H3+H2O                   3.10E+07   2.00       3430.   ! (54) Wang 97
C4H4+OH=iC4H3+H2O                   1.55E+07   2.00        430.   ! (54) Wang 97
C4H4+O=C3H3+HCO                     6.00E+08   1.45       -860.   ! (54) Wang 97
C4H4+C2H=l-C6H4+H                   1.20E+13   0.00          0.   ! (54) Wang 97
!
!---------C4H5 chemistry------------
!
n-C4H5=i-C4H5                       1.30E+62 -16.38      49600.   ! (54) Wang 97 20Torr
n-C4H5+H=i-C4H5+H                   1.00E+36  -6.26      17486.   ! (54) Wang 97 20Torr
n-C4H5+H=C4H4+H2                    1.50E+13   0.00          0.   ! (54) Wang 97
n-C4H5+OH=C4H4+H2O                  2.00E+12   0.00          0.   ! (54) Wang 97
n-C4H5+HCO=iiiC4H6+CO               5.00E+12   0.00          0.   ! (54) Wang 97
n-C4H5+HO2=C2H3+CH2CO+OH            6.60E+12   0.00          0.   ! (54) Wang 97
n-C4H5+H2O2=iiiC4H6+HO2             1.21E+10   0.00       -596.   ! (54) Wang 97
n-C4H5+HO2=iiiC4H6+O2               6.00E+11   0.00          0.   ! (54) Wang 97
n-C4H5+O2=HCO+C2H3CHO               9.20E+16  -1.39       1010.   ! (54) Wang 97
i-C4H5+H=C4H4+H2                    3.00E+13   0.00          0.   ! (54) Wang 97
i-C4H5+H=C3H3+CH3                   1.0E+14    0.00          0.   ! (66) Hansen/Miller 08
i-C4H5+OH=C4H4+H2O                  4.00E+12   0.00          0.   ! (54) Wang 97
i-C4H5+HCO=iiiC4H6+CO               5.00E+12   0.00          0.   ! (54) Wang 97
i-C4H5+HO2=iiiC4H6+O2               6.00E+11   0.00          0.   ! (54) Wang 97
i-C4H5+HO2=C2H3+CH2CO+OH            6.60E+12   0.00          0.   ! (54) Wang 97
i-C4H5+H2O2=iiiC4H6+HO2             1.21E+10   0.00       -596.   ! (54) Wang 97
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i-C4H5+O2=CH2CO+CH2CHO                2.16E+10   0.00       2500.   ! (54) Wang 97
n-C4H5+C6H5OH=iiiC4H6+C6H5O           6.0E+12    0.00          0.   !(137) Klotz/Brez 98
i-C4H5+C6H5OH=iiiC4H6+C6H5O           6.0E+12    0.00          0.   !(137) Klotz/Brez 98
n-C4H5+C5H6=iiiC4H6+C5H5              6.0E+12    0.00          0.   !(137) Klotz/Brez 98
i-C4H5+C5H6=iiiC4H6+C5H5              6.0E+12    0.00          0.   !(137) Klotz/Brez 98
i-C4H5+C6H5CH3=iiiC4H6+C6H5CH2        6.0E+12    0.00          0.   !(137) Klotz/Brez 98
!
!---------C4H6 chemistry------------
!
iiiC4H6 = i-C4H5 + H                 8.20E+51  -10.92    118409.    ! (54) Wang 97 20Torr
iiiC4H6 = n-C4H5 + H                 3.50E+61  -13.87    129677.    ! (54) Wang 97 20Torr
iiiC4H6=C4H4+H2                      2.50E+15    0.00     94700.    !(106) Hidaka 96
iiiC4H6+H=n-C4H5+H2                  1.33E+06    2.5      12240.    ! (66) Hansen/Miller 08 JAM Est
iiiC4H6+H=i-C4H5+H2                  6.65E+05    2.5       9240.    ! (66) Hansen/Miller 08 JAM Est
C2H4 + C2H3 = iiiC4H6 + H            7.40E+14   -0.66      8420.    ! (54) Wang 97 20Torr
iiiC4H6+H=PC3H4+CH3                  2.00E+12    0.00      7000.    ! (86) Wang USC_II 07
iiiC4H6+H=AC3H4+CH3                  2.00E+12    0.00      7000.    ! (86) Wang USC_II 07
iiiC4H6+O=n-C4H5+OH                  7.50E+06    1.90      3740.    ! (86) Wang USC_II 07
iiiC4H6+O=i-C4H5+OH                  7.50E+06    1.90      3740.    ! (86) Wang USC_II 07
iiiC4H6+O=HCO+AC3H5                  6.02E+08    1.45      -858.    ! (66) Hansen/Miller 08
iiiC4H6+OH=CH3CHO+C2H3                 6.3E12    0.00      -874.    ! (66) Hansen/Miller 08 JAM Est
iiiC4H6+OH=AC3H5+CH2O                  6.3E12    0.00      -874.    ! (66) Hansen/Miller 08
iiiC4H6+OH=n-C4H5+H2O                6.20E+06    2.00      3430.    !(107) Liu 88
iiiC4H6+OH=i-C4H5+H2O                3.10E+06    2.00       430.    ! (86) Wang USC_II 07
iiiC4H6+CH3=n-C4H5+CH4               2.00E+14    0.00     22800.    !(106) Hidaka 96
iiiC4H6+CH3=i-C4H5+CH4               1.00E+14    0.00     19800.    !(106) Hidaka 96
iiiC4H6+C2H3=n-C4H5+C2H4             5.00E+13    0.00     22800.    !(106) Hidaka 96
iiiC4H6+C2H3=i-C4H5+C2H4             2.50E+13    0.00     19800.    !(106) Hidaka 96
iiiC4H6+C3H3=n-C4H5+AC3H4            1.00E+13    0.00     22500.    !(106) Hidaka 96
iiiC4H6+C3H3=i-C4H5+AC3H4            5.00E+12    0.00     19500.    !(106) Hidaka 96
iiiC4H6+AC3H5=n-C4H5+C3H6            1.00E+13    0.00     22500.    ! (86) Wang USC_II 07
iiiC4H6+AC3H5=i-C4H5+C3H6            5.00E+12    0.00     19500.    ! (86) Wang USC_II 07
iiiC4H6+C2H3=A+H2+H                  5.62E+11    0.00      3240.    !(108) Leung/Linstedt 95
iiC4H6=i-C4H5+H                      4.20E+15    0.00     92600.    !(108) Leung/Linstedt 95
iiC4H6+H=iiiC4H6+H                   2.00E+13    0.00      4000.    ! (86) Wang USC_II 07
iiC4H6+H=i-C4H5+H2                   1.70E+05    2.50      2490.    ! (86) Wang USC_II 07
iiC4H6+H=AC3H4+CH3                   2.00E+13    0.00      2000.    ! (86) Wang USC_II 07
iiC4H6+H=PC3H4+CH3                   2.00E+13    0.00      2000.    ! (86) Wang USC_II 07
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iiC4H6+CH3=i-C4H5+CH4                 7.00E+13    0.00     18500.    ! (86) Wang USC_II 07
iiC4H6+O=CH2CO+C2H4                   1.20E+08    1.65       327.    ! (86) Wang USC_II 07
iiC4H6+O=i-C4H5+OH                    1.80E+11    0.70      5880.    ! (86) Wang USC_II 07
iiC4H6+OH=i-C4H5+H2O                  3.10E+06    2.00      -298.    ! (86) Wang USC_II 07
iiC4H6=iiiC4H6                        3.00E+13    0.00     65000.    ! (86) Wang USC_II 07
!
!---------1-C4H8 1-butene chemistry------------
!
IC4H8+H=C2H4+C2H5                     1.60E+22   -2.39     11180.    ! (86) Wang USC_II 07
IC4H8+H=C3H6+CH3                      3.20E+22   -2.39     11180.    ! (86) Wang USC_II 07
IC4H8+H=C4H7+H2                       6.50E+05    2.54      6756.    ! (86) Wang USC_II 07
IC4H8+O=nC3H7+HCO                     3.30E+08    1.45      -402.    !(109) Ko/Adusei 91
IC4H8+O=C4H7+OH                       1.50E+13    0.00      5760.    !(109) Ko/Adusei 91
  DUPLICATE
IC4H8+O=C4H7+OH                       2.60E+13    0.00      4470.    !(109) Ko/Adusei 91
  DUPLICATE
IC4H8+OH=C4H7+H2O                     7.00E+02    2.66       527.    ! (86) Wang USC_II 07
IC4H8+O2=C4H7+HO2                     2.00E+13    0.00     50930.    ! (86) Wang USC_II 07
IC4H8+HO2=C4H7+H2O2                   1.00E+12    0.00     14340.    ! (86) Wang USC_II 07
IC4H8+CH3=C4H7+CH4                    4.50E-01    3.65      7153.    ! (86) Wang USC_II 07
C4H7=iiiC4H6+H                        2.48E+53  -12.3       52000.    ! (86) Wang USC_II 07
C4H7+H(+M)=IC4H8(+M)                  3.60E+13    0.00          0.    ! (86) Wang USC_II 07
  LOW                                /3.01E+48   -9.32      5833.6/
  TROE /0.498 1314 1314 50000/
  H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
C4H7+H=CH3+AC3H5                      2.00E+21   -2.00     11000.    ! (86) Wang USC_II 07
C4H7+H=iiiC4H6+H2                     1.80E+12    0.00          0.    ! (86) Wang USC_II 07
C4H7+O2=iiiC4H6+HO2                   1.00E+11    0.00          0.    ! (86) Wang USC_II 07
C4H7+HO2=CH2O+OH+AC3H5                2.40E+13    0.00          0.    ! (86) Wang USC_II 07
C4H7+HCO=IC4H8+CO                     6.00E+13    0.00          0.    ! (86) Wang USC_II 07
C4H7+CH3=iiiC4H6+CH4                  1.10E+13    0.00          0.    ! (86) Wang USC_II 07
C2H4+C2H3=C4H7                        1.23E+35   -7.76      9930.    ! (54) Wang 97 RRKM 0.1 atm
!
!---------1-butyl nC4H9 chemistry from USC_Mech_II:                   (86) Wang USC_II 07
! (86) 2007 Hai Wang USC_II
IC4H8+H(+M) = nC4H9(+M)               1.33E+13    0.00     3260.7    !=(C3H6+H) TS5 600 cm-1
  LOW                                /6.26E+38   -6.66     7000./
  TROE /1.000  1000.   1310.  48097.  /
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  H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/
C2H4+C2H5 = nC4H9                     1.50E+11    0.00     7300.     ! KP, P
nC4H9+H = IC4H8+H2                    1.80E+12    0.00        0.     ! =(nC3H7+H) TS4
nC4H9+O = nC3H7+CH2O                  9.60E+13    0.00        0.     ! =(nC3H7+O) TS3 ka+kb
nC4H9+OH = IC4H8+H2O                  2.40E+13    0.00        0.     ! =(nC3H7+OH) TS3
nC4H9+O2 = IC4H8+HO2                  2.70E+11    0.00        0.     ! BB75
nC4H9+HO2 = nC3H7+OH+CH2O             2.40E+13    0.00        0.     ! =(nC3H7+HO2) TS3 ?
!pC4H9+HCO = C4H10+CO                 9.00E+13    0.00        0.     ! =(nC3H7+HCO) TS3
nC4H9+CH3 = IC4H8+CH4                 1.10E+13    0.00        0.     ! =(nC3H7+CH3) TS3
!C4H10+H = pC4H9+H2                   9.20E+05    2.54     6756.     ! =(C3H8+H scaled to BBW at 753K)
!
!---------C5H5/C5H6, C5HxO chemistry------------
!
C5H5+H=C5H6                           2.71E+63  -14.79    21050.    !(111) Zhong/Bozzelli 97/8
C5H5=C3H3+C2H2                        2.79E+79  -18.30   130834.    !(113) Mos/Lin 00
C5H5+O=n-C4H5+CO                      7.27E+13   -0.28      470.    !(111) Zhong/Bozzelli 97/8
C5H5+O=C5H5O                          1.84E+03    1.03    -6960.    !(111) Zhong/Bozzelli 97/8
C5H5+O=C5H4O+H                        6.71E+13   -0.03       40.    !(111) Zhong/Bozzelli 97/8
C5H5+HO2=C5H5O+OH                     3.0E+13     0.00        0.    !(114) Emdee/Brezinsky 92
C5H5O=n-C4H5+CO                       2.51E+11    0.00    43900.    !(137) Klotz/Brez 98
C5H5O=C5H4O+H                         2.90E+32   -6.50    21220.    !(116) Alzueta 00
C5H5O=i-C4H5+CO                       1.10E+79  -19.62    66250.    !(116) Alzueta 00
C5H5+OH=iiiC4H6+CO                    1.2E14      0.00     4500.    !(143) Ristori 01 * 0.3
C5H5+OH=C5H4OH+H                      2.15E+30   -4.61    25050.    !(111) Zhong/Bozzelli 97/8
C5H4O+H=C5H4OH                        1.10E+69  -16.018   37130.    !(121) Richter2002 QRRK,20torr
C5H4OH+O2=C5H4O+HO2                   3.00E+13    0.00     5000.    !(116) Alzueta 00
C5H4O+H=n-C4H5+CO                     2.10E+61  -13.27    40810.    !(116) Alzueta 00
C5H4O+O=C4H4+CO2                      1.00E+13    0.00     2000.    !(116) Alzueta 00
C5H4O=2C2H2+CO                        1.10E+47   -9.63    99500.    !(117) Wang/Brezinsky98 0.1atm
C5H6+H=C5H5+H2                        2.80E+13    0.00     2259.    !(118) Roy 98
C5H6+H=AC3H5+C2H2                     6.60E+14    0.00    12345.    !(118) Roy 98
C5H6+OH=C5H5+H2O                      3.08E+06    2.          0.    !(111) Zhong/Bozzelli 97/8
C5H6+O=C5H5+OH                        4.77E+04    2.71     1106.    !(111) Zhong/Bozzelli 97/8
C5H6+O2=C5H5+HO2                      4.00E+13    0.00    37150.    !(111) Zhong/Bozzelli 97/8
C5H6+HO2=C5H5+H2O2                    1.10E+04    2.60    12900.    !(111) Zhong/Bozzelli 97/8
C5H6+CH3=C5H5+CH4                     1.80E-01    4.0         0.    !(111) Zhong/Bozzelli 97/8
C5H6+C2H3=C5H5+C2H4                   1.20E-01    4.0         0.    !(111) Zhong/Bozzelli 97/8
C5H6+A1=C5H5+A                        1.00E-01    4.0         0.    !(111) Zhong/Bozzelli 97/8
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!
!---------C6Hx chemistry------------
!
C6H2+H=C6H3                          4.30E+45  -10.15     13250.    ! (54) Wang 97
C6H3+H=C4H2+C2H2                     2.40E+19   -1.60      2800.    ! (54) Wang 97
C6H3+H=l-C6H4                        4.20E+44  -10.27      7890.    ! (54) Wang 97
C6H3+H=C6H2+H2                       3.00E+13    0.00         0.    ! (54) Wang 97
C6H3+OH=C6H2+H2O                     5.00E+12    0.00         0.    ! (54) Wang 97
C6H3+O2=>CO+C3H2+HCCO                5.00E+11    0.00         0.    ! (54) Wang 97
l-C6H4+H=n-C6H5                      3.30E+44  -10.04     18800.    ! (54) Wang 97
l-C6H4+H=A1                          3.60E+77  -20.09     28100.    ! (54) Wang 97
c-C6H4+H=A1                           3.0E17     0.00     36300.    ! (54) Wang 97
l-C6H4+H=C6H3+H2                     6.65E+06    2.53      9240.    ! (54) Wang 97
l-C6H4+OH=C6H3+H2O                   3.10E+06    2.00       430.    ! (54) Wang 97
n-C6H5=A1                            1.30E+62  -15.94     35800.    ! (54) Wang 97
n-C6H5=c-C6H4+H                      2.70E+65  -15.93     59700.    ! (54) Wang 97
n-C6H5+H=i-C6H5+H                    2.40E+11    0.79      2410.    ! (54) Wang 97
n-C6H5+H=l-C6H6                      1.10E+42   -9.65      7000.    ! (54) Wang 97
i-C6H5+H=l-C6H6                      4.20E+44  -10.27      7890.    ! (54) Wang 97
n-C6H5+H=l-C6H4+H2                   1.50E+13    0.00         0.    ! (54) Wang 97
i-C6H5+H=l-C6H4+H2                   3.00E+13    0.00         0.    ! (54) Wang 97
n-C6H5+OH=l-C6H4+H2O                 2.50E+12    0.00         0.    ! (54) Wang 97
i-C6H5+OH=l-C6H4+H2O                 5.00E+12    0.00         0.    ! (54) Wang 97
n-C6H5+O2=>C4H4+HCO+CO               4.16E+10    0.00      2500.    ! (54) Wang 97
i-C6H5+O2=>CH2CO+CH2CO+C2H           7.86E+16   -1.80         0.    ! (54) Wang 97
n-C6H5=nC4H3+C2H2                    4.00E+16    0.00     39100.    !(120) Lindstedt 94
l-C6H6+H+M=n-C6H7+M                  2.90E+17   -0.52      1000.    ! (54) Wang 97
  H2/2.0/ H2O/6.0/ CO/1.5/ CO2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/
l-C6H6+H+M=CYC6H7+M                  1.70E+28   -4.72      2800.    ! (54) Wang 97
  H2/2.0/ H2O/6.0/ CO/1.5/ CO2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/
l-C6H6+H=n-C6H5+H2                   6.65E+05    2.53     12240.    ! (54) Wang 97
l-C6H6+H=i-C6H5+H2                   3.33E+05    2.53      9240.    ! (54) Wang 97
l-C6H6+OH=n-C6H5+H2O                 6.20E+06    2.00      3430.    ! (54) Wang 97
l-C6H6+OH=i-C6H5+H2O                 3.10E+06    2.00       430.    ! (54) Wang 97
n-C6H7=CYC6H7                        4.10E+24   -7.11      3900.    ! (54) Wang 97
n-C6H7=A+H                           8.40E+21   -4.22     11300.    ! (54) Wang 97
n-C6H7+H=i-C6H7+H                    4.00E+41   -8.09     19200.    ! (54) Wang 97
i-C6H7+H=C6H8                        1.20E+60  -13.86     21000.    ! (54) Wang 97
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```
n-C6H7+H=C6H8                       8.70E+69  -17.01     24000.    ! (54) Wang 97
n-C6H7+H=l-C6H6+H2                  1.50E+13    0.00         0.    ! (54) Wang 97
i-C6H7+H=l-C6H6+H2                  3.00E+13    0.00         0.    ! (54) Wang 97
n-C6H7+OH=l-C6H6+H2O                2.50E+12    0.00         0.    ! (54) Wang 97
i-C6H7+OH=l-C6H6+H2O                5.00E+12    0.00         0.    ! (54) Wang 97
n-C6H7+O2=>iiiC4H6+CO+HCO           4.16E+10    0.00      2500.    ! (54) Wang 97
i-C6H7+O2=>CH2CO+CH2CO+C2H3         7.86E+16   -1.80         0.    ! (54) Wang 97
C6H8+H=n-C6H7+H2                    1.33E+06    2.53     12240.    ! (54) Wang 97
C6H8+H=i-C6H7+H2                    6.65E+05    2.53      9240.    ! (54) Wang 97
C6H8+OH=n-C6H7+H2O                  6.20E+06    2.00      3430.    ! (54) Wang 97
C6H8+OH=i-C6H7+H2O                  3.10E+06    2.00       430.    ! (54) Wang 97
!
!----------Phenyl Reactions----------
!
A1+O2=C6H5O+O                       2.39E21    -2.62      4400.    !(121) Richter 02
A1+HO2=C6H5O+OH                     5.00E13     0.0       1000.    !(108) Leung/Linstedt 95
A1+O=C5H5+CO                        9.00E13     0.0          0.    !(122) Frank 1994
CH2SING+A=A1+CH3                    1.7E14      0.0          0.    ! (77) Wagner 90
A1+OH=C6H5O+H                       5.00E+13    0.0          0.    ! (46) Miller 92
!
!----------C6H6 formation reactions----------
!
C3H3+C3H3=l-C6H6                    6.48E68   -16.686      2872.    ! Miller email???
  DUPLICATE
C3H3+C3H3=l-C6H6                    1.54E36    -7.797      5580.    ! Miller email???
  DUPLICATE
C3H3+C3H3=FC6H6                     7.25E65   -16.015     25035.    ! (98) Hansen/Miller 09 PCI
  DUPLICATE
C3H3+C3H3=FC6H6                     4.19E39    -8.958      6098.    ! (98) Hansen/Miller 09 PCI
  DUPLICATE
C3H3+C3H3=A                         1.64E66   -15.902     27529.    ! (98) Hansen/Miller 09 PCI
  DUPLICATE
C3H3+C3H3=A                         1.20E35    -7.435      5058.    ! (98) Hansen/Miller 09 PCI
  DUPLICATE
C3H3+C3H3=A1+H                      2.02E33    -6.05      15940.    ! (98) Hansen/Miller 09 PCI
C3H3+AC3H5=FC6H6+H+H                3.26E29    -5.397      3390.    !(125) YG/JAM/SJK 07
nC4H3+C2H3=A                        2.87E+14    0.00        817.    !(138) Lindstedt 96
n-C4H5+C2H2=A+H                     2.94E+16   -1.09       9257.    !(104) JPS/JAM 07 C4+C2
```

```
n-C4H5+C2H2=l-C6H6+H                1.14E+09    1.39     17338.    !(104) JPS/JAM 07 C4+C2
n-C4H5+C2H2=FC6H6+H                 1.52E+15   -0.76      8762.    !(104) JPS/JAM 07 C4+C2
i-C4H5+C2H2=A+H                     1.47E+23   -3.28     24907.    !(104) JPS/JAM 07 C4+C2
i-C4H5+C2H2=FC6H6+H                 1.01E+34   -5.94     28786.    !(104) JPS/JAM 07 C4+C2
n-C4H5+C2H3=A+H2                    1.84E-13    7.07     -3611.    !(105) Westm 89
FC6H6=A                             5.62E+81  -19.36   121500.    ! (91) JAM/SJK 03
FC6H6=A1+H                          2.57E+97  -23.16   153470.    ! (91) JAM/SJK 03
FC6H6+H=A+H                         3.00E+12     0.5      2000.    !(127) Marinov 98
CYC6H7=A+H                          3.16E+13     0.00    28500.    !(123) Dean 85
CY13C6H8=A+H2                       2.50E+13     0.0     59000.    !(131) Alfassi & Benson
!
!----------C6H6 consumption reactions----------
!
A=A1+H                              1.35E+108 -25.81   181750.0   ! (91) JAM/SJK 03
A+H=A1+H2                           2.50E+14     0.00    16000.0   ! (54) Wang 97
A+OH=A1+H2O                         1.63E+08     1.42     1450.0   ! (45) Baulch 92
A+O2=A1+HO2                         6.3E+13      0.00    60000.0   !(114) Emdee/Bre 92
A+O=A1+OH                           2.00E+13     0.00    14704.0   !(126) Leidreiter/Wagner 89
A+O=C6H5O+H                         3.560E+01    3.8       940.0   ! (10) Baulch 94
C6H5OH+H=A+OH                       5.36E6       2.0      5470.    !(128) Tok/Lin 02
!
!----------C6H5O phenoxy reactions------------
!
C6H5O+H=C6H5OH                      4.43E+60  -13.232   30010.    !(121) Richter 02
C6H5O=C5H5+CO                       2.51E+11     0.00    43900.    !(129) Lin/Lin 86
C6H5O+O=C5H5+CO2                    1.00E+13     0.00        0.    !(116) Alzueta 00
!
!----------C6H5OH (phenol) reactions----------
!
C6H5OH=C5H6+CO                      1.00E+12     0.00    60802.    !(130) Horn 1998
C6H5OH+H=C6H5O+H2                   1.15E+14     0.00    12400.    !(114) Emdee/Bre 92
C6H5OH+O=C6H5O+OH                   2.81E+13     0.00     7352.    !(114) Emdee/Bre 92
C6H5OH+HO2=C6H5O+H2O2               3.00E+13     0.00    15000.    !(132) Bittker 91
C6H5OH+C2H3=C2H4+C6H5O              6.00E+12     0.00        0.    !(114) Emdee/Bre 92
C6H5OH+A1=A+C6H5O                   4.91E+12     0.00     4400.    !(114) Emdee/Bre 92
C6H5O+C5H6=C5H5+C6H5OH              3.16E+11     0.00     8000.    !(114) Emdee/Bre 92
C6H5OH+OH=H2O+C6H5O                 1.39E+08     1.43     -962.    !(131) Shandross 96
!
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!
!
!-------------------------1-hexene sub mechanism reactions------------------------------
*******************************************************************************************
hex1yl=hexene1+H                    1.30E+13      0.0     39000.     !Westbrook87
hex2yl=hexane1+H                    2.00E+13      0.0     40400.     !Westbrook87
!--------------------1-Hexene sub-model from (136) Yahyaoui/Dagaut 06 Hexene model-------------------------
!M. Yahyaoui, N. Djebaili-Chaumeix, P. Dagaut, C. E. Paillard and S. Gail, Combust. Flame 147 (1-2) (2006)
67-78.
!-------------------------------------------------------------------------------------------------------
hex1yl=hex2yl                        2.00E+11      0.0     11100.     !(WB93 30/06/2000)
hex1yl=hex3yl                        2.00E+11      0.0     18100.     !(WB93 30/06/2000)
hex2yl+O2=>CH3CHO+IC4H8+OH          2.100E+11      0.0      6858.     !(=C2H5+O2)
hex2yl+HO2=>CH3CHO+nC4H9+OH         1.000E+13      0.0         0.     !(ESTIMEE)
hex2yl+OH=hexene1+H2O               3.645E+13      0.0         0.     !(=BC7H15+OH)
hex2yl+O=CH3CHO+nC4H9               1.610E+13      0.0         0.     !(=hex1yl+O)
hex3yl=IC4H8+C2H5                   6.000E+13      0.0     29700.     !(03/07/2000 NanCy)
hex2yl=C3H6+nC3H7                   5.000E+13      0.0     28700.     !(03/07/2000 NanCy*2.5)
hex1yl=C2H4+nC4H9                   1.000E+13      0.0     28700.     !(03/07/2000 NanCy/2)
hex1yl+H=hexene1+H2                 1.810E+12      0.0         0.     !(=NC3H7+H/88TSA)
hex2yl+O2=hexene1+HO2               3.000E+12      0.0      4500.     !(WESTB.87)
hex1yl+O2=hexene1+HO2               2.000E+12      0.0      2000.     !(WESTB.87)
hex1yl+OH=hexene1+H2O               2.430E+13      0.0         0.     !(=AC7H15+OH)
hex1yl+CH3=hexene1+CH4              1.000E+12      0.0         0.     !(ALLARA 80)
hex1yl+C2H5=hexene1+C2H6            1.000E+12      0.0         0.     !(ALLARA 80)
hex1yl+C2H3=hexene1+C2H4            1.000E+12      0.0         0.     !(ALLARA 80)
hex1yl+AC3H5=hexene1+C3H6           1.000E+12      0.0         0.     !(ALLARA 80)
hex2yl+CH3=hexene1+CH4              1.000E+12      0.0         0.     !(ALLARA 80)
hex2yl+C2H5=hexene1+C2H6            1.000E+12      0.0         0.     !(ALLARA 80)
hex2yl+C2H3=hexene1+C2H4            1.000E+12      0.0         0.     !(ALLARA 80)
hex2yl+AC3H5=hexene1+C3H6           1.000E+12      0.0         0.     !(ALLARA 80)
hexene1=AC3H5+nC3H7                  1.08E+80    -19.331    95177.     !Kiefer JPCA09 25 torr
hexene1=C6H6+C3H6                    4.00E+12      0.0     57430.     !Mohammed(TSANG)
C2H3+nC4H9=hexene1                  1.000E+13      0.0         0.     !(30/06/2000)
hexene1+O2=C6H11-13+HO2             4.000E+12      0.0     40000.     !Mohammed(EST/ C4H8+O2)
hexene1+O2=C6H11-15+HO2             2.800E+13      0.0     48300.     !Mohammed(EST/ C7H16)
hexene1+O2=C6H11-14+HO2             2.800E+13      0.0     48300.     !Mohammed(EST/ C7H16)
hexene1+O2=C6H11+HO2                2.100E+13      0.0     51300.     !Mohammed(EST/ C7H16)
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hexene1+HO2=C6H11-14+H2O2         6.800E+12      0.0     17000.     !Mohammed(EST/ C7H16)
hexene1+HO2=C6H11-15+H2O2         6.800E+12      0.0     17000.     !Mohammed(EST/ C7H16)
hexene1+HO2=C6H11+H2O2            5.600E+12      0.0     19400.     !Mohammed(EST/ C7H16)
hexene1+HO2=C6H11-13+H2O2         1.000E+11      0.0     17060.     !(EST/ C4H8+HO2)
hexene1+O=C6H11+OH                0.42E+03       3.47     3092.     !Mohammed(EST/ C7H16)
hexene1+O=C6H11-15+OH             2.25E+03       3.26     1653.     !Mohammed(EST/ C7H16)
hexene1+O=C6H11-14+OH             2.25E+03       3.26     1653.     !Mohammed(EST/ C7H16)
hexene1+O=C6H11-13+OH             4.00E+13       0.0      4000.     !(WESTB.87)
hexene1+H=C6H11+H2                2.80E+07       2.0      7700.     !Mohammed(EST/ C7H16)
hexene1+H=C6H11-15+H2             9.10E+06       0.0      5000.     !Mohammed(EST/ C7H16)
hexene1+H=C6H11-14+H2             9.10E+06       0.0      5000.     !Mohammed(EST/ C7H16)
hexene1+H=C6H11-13+H2             6.55E+12       0.0      4445.     !(= C4H8)
hexene1+OH=C6H11+H2O              2.85E+05       2.314     236.     !Mohammed(EST/ C7H16)
hexene1+OH=C6H11-15+H2O           6.35E+06       1.96     -500.     !Mohammed(EST/ C7H16)
hexene1+OH=C6H11-14+H2O           6.35E+06       1.96     -500.     !Mohammed(EST/ C7H16)
hexene1+OH=C6H11-13+H2O           6.00E+13       0.0      1230.     !Mohammed(2*Curran2002)
hexene1+CH3=C6H11+CH4             1.47E+12       0.0     11722.     !Mohammed(EST/ C7H16)
hexene1+CH3=C6H11-15+CH4          6.60E+11       0.0     10120.     !Mohammed(EST/ C7H16)
hexene1+CH3=C6H11-14+CH4          6.60E+11       0.0     10120.     !Mohammed(EST/ C7H16)
hexene1+CH3=C6H11-13+CH4          2.00E+11       0.0      6800.     !(WESTB.87)
hexene1+C2H3=C6H11-13+C2H4        2.00E+11       0.0      6800.     !(WESTB.87)
hexene1+C2H3=C6H11-14+C2H4        6.60E+12       0.0     10120.     !Mohammed(est C7H16)
hexene1+C2H3=C6H11-15+C2H4        6.60E+12       0.0     10120.     !Mohammed(est C7H16)
hexene1+C2H3=C6H11+C2H4           2.94E+12       0.0     11722.     !Mohammed(est C7H16)
C6H11-13+H=hexene1                1.00E+13       0.0         0.     !(RTI)
hexene1+nC3H7=C6H11-13+C3H8       1.00E+11       0.0      8300.     !(est C4H8+C2H5)
C6H11-13+HO2=>nC3H7+C2H3CHO+OH    1.00E+12       0.0      8000.     !(07/09/2000)
C6H11=C6H11-12                    1.00E+11       0.0     20320.     !Mohammed (Handford styring 95)
C6H11-12=C6H11-15                 2.00E+11       0.0     18100.     !(RTI)
C6H11-12=nC3H7+AC3H4              1.00E+12       0.0     33000.     !Mohammed(Yahyaoui et al. 05)
C6H11-14=C2H3+IC4H8               4.00E+13       0.0     35500.     !Mohammed(Yahyaoui et al. 05)
C6H11-15=AC3H5+C3H6               4.00E+13       0.0     35500.     !Mohammed(Yahyaoui et al. 05)
!-------------------------------------------------------------------------------------------------
!
C6H11=C6H11-13                    3.67E+12      -0.6     15300.     !(135) Silke et al. 07
iiiC4H6+C2H5=C6H11-13             1.32E+04       2.48     6130.     !(135) Silke et al. 07
C6H11=C4H7+C2H4                   2.00E+13       0.00    28700.     !(124) Dayma 03
!*************************************************************************************************
```

```
!
!!----------------------------------Cyclohexane subset below---------------------------------
!*****************************************************************************************
!
!  CYC6H12, Cyclohexane
!
CYC6H12=hexene1                  5.588E+37    -7.3256    73554.7    !(133) Kiefer 09 WLi Fit
CYC6H12+M=CYC6H11+H+M            3.00E+16      0.0       95000.     !(134) Voisin 98
CYC6H12+O2=CYC6H11+HO2           7.50E+13      0.0       49000.     !(134) Voisin 98
CYC6H12+HO2=CYC6H11+H2O2         1.20E+13      0.0       17057.     !(134) Voisin 98
CYC6H12+OH=CYC6H11+H2O           2.25E+07      2.0        -765.     !(134) Voisin 98
CYC6H12+O=CYC6H11+OH             2.60E+06      2.6        2563.     !(134) Voisin 98
CYC6H12+H=CYC6H11+H2             6.00E+14      0.0        8373.     !(134) Voisin 98
CYC6H12+CH3=CYC6H11+CH4          1.35E+12      0.0        9540.     !(134) Voisin 98
CYC6H12+C2H3=CYC6H11+C2H4        1.35E+12      0.0        9540.     !(134) Voisin 98
CYC6H12+C2H5=CYC6H11+C2H6        1.35E+12      0.0        9540.     !(134) Voisin 98
CYC6H12+AC3H5=CYC6H11+C3H6       1.35E+12      0.0        9540.     !(134) Voisin 98
CYC6H12+SC3H5=CYC6H11+C3H6       1.35E+12      0.0        9540.     !(134) Voisin 98
CYC6H12+TC3H5=CYC6H11+C3H6       1.35E+12      0.0        9540.     !(134) Voisin 98
CYC6H12+CH3O=CYC6H11+CH3OH       4.32E+11      0.0        4473.     !(134) Voisin 98
CYC6H12+HCO=CYC6H11+CH2O         1.35E+12      0.0        9540.     !(134) Voisin 98
!
!
!  CYC6H11
!
CYC6H11=C6H11                    4.00E+13      0.0       27700.     !(124) Dayma 03
CYC6H11=CYC6H10+H               2.52E+13       0.0       35613.     !(134) Voisin 98
CYC6H11+O2=CYC6H10+HO2           3.2E+12       0.0        5000.     !(124) Dayma 03
CYC6H11+HO2=CYC6H10+H2O2        2.00E+12       0.0        2000.     !(134) Voisin 98
CYC6H11+OH=CYC6H10+H2O          4.80E+13       0.0           0.     !(134) Voisin 98
CYC6H11+O=CYC6H10+OH            9.64E+13       0.0           0.     !(134) Voisin 98
CYC6H11+H=CYC6H10+H2            2.00E+11       0.0           0.     !(134) Voisin 98
CYC6H11+CH3=CYC6H10+CH4         4.00E+12       0.0           0.     !(134) Voisin 98
CYC6H11+HCO=CYC6H10+CH2O        4.00E+12       0.0           0.     !(134) Voisin 98
!
!  CYC6H10
!
CYC6H10=iiiC4H6+C2H4            1.50E+15       0.0       66900.     !(124) Dayma 03
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CYC6H10=CYC6H9+H                7.08E+65    -14.5      110278.     !WL/PRW QRRK, this Work
CYC6H10+O2=CYC6H9+HO2           7.20E+13      0.0       34800.     !(124) Dayma 03
CYC6H10+HO2=CYC6H9+H2O2         2.00E+11      0.0       17060.     !(134) Voisin 98
CYC6H10+OH=CYC6H9+H2O           6.00E+13      0.0         300.     !(134) Voisin 98
CYC6H10+O=CYC6H9+OH             6.20E+12      0.0        4445.     !(134) Voisin 98
CYC6H10+H=CYC6H9+H2             6.20E+12      0.0        4445.     !(134) Voisin 98
CYC6H10+CH3=CYC6H9+CH4          1.65E+11      0.0        4118.     !(134) Voisin 98
CYC6H10+HCO=CYC6H9+CH2O         1.65E+11      0.0        4118.     !(134) Voisin 98
!
!   CYC6H9
!
CYC6H9=CY13C6H8+H               1.20E+14      0.0       49300.     !(134) Voisin 98
CYC6H9=C6H9                     1.30E+13      0.0       35900.     !(124) Dayma 03
CYC6H9+O2=CY13C6H8+HO2          1.60E+12      0.0       15160.     !(124) Dayma 03
CYC6H9+HO2=CY13C6H8+H2O2        1.00E+12      0.0           0.     !(134) Voisin 98
CYC6H9+OH=CY13C6H8+H2O          6.02E+12      0.0           0.     !(134) Voisin 98
CYC6H9+O=CY13C6H8+OH            1.80E+13      0.0           0.     !(134) Voisin 98
CYC6H9+H=CY13C6H8+H2            3.16E+13      0.0           0.     !(134) Voisin 98
CYC6H9+CH3=CY13C6H8+CH4         8.00E+12      0.0           0.     !(134) Voisin 98
CYC6H9+HCO=CY13C6H8+CH2O        4.00E+12      0.0           0.     !(134) Voisin 98
!
!   CY13C6H8
!
CY13C6H8=CYC6H7+H               2.60E+14      0.0       77100.     !(124) Dayma 03
CY13C6H8+O2=CYC6H7+HO2          8.31E+11      0.0       24858.     !(134) Voisin 98
CY13C6H8+HO2=CYC6H7+H2O2        4.00E+12      0.0       17057.     !(134) Voisin 98
CY13C6H8+OH=CYC6H7+H2O          6.00E+06      2.0       -1520.     !(124) Dayma 03
CY13C6H8+O=CYC6H7+OH            1.40E+13      0.0        -795.     !(134) Voisin 98
CY13C6H8+H=CYC6H7+H2            1.10E+05      2.5       -1900.     !(124) Dayma 03
CY13C6H8+CH3=CYC6H7+CH4         1.23E+11      0.0        5201.     !(134) Voisin 98
CY13C6H8+C2H3=CYC6H7+C2H4       1.23E+11      0.0        5201.     !(134) Voisin 98
CY13C6H8+HCO=CYC6H7+CH2O        1.23E+11      0.0        5201.     !(134) Voisin 98
CY13C6H8+C2H2=A+C2H4            3.10E+10      0.0       27200.     !(134) Voisin 98
!
!   CYC6H7
!
C2H2+n-C4H5=CYC6H7              2.78E+11      0.0        3509.     !(134) Voisin 98
CYC6H7+O2=A+HO2                 1.00E+12      0.0           0.     !(134) Voisin 98
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CYC6H7+HO2=A+H2O2              1.00E+12       0.0           0.     !(134) Voisin 98
CYC6H7+HO2=C5H6+HCO+OH         4.50E+12       0.0           0.     !(134) Voisin 98
CYC6H7+OH=A+H2O                6.02E+12       0.0           0.     !(134) Voisin 98
CYC6H7+O=A+OH                  1.80E+13       0.0           0.     !(134) Voisin 98
CYC6H7+O=C5H6+HCO              8.26E+13       0.0           0.     !(134) Voisin 98
CYC6H7+H=A+H2                  3.16E+13       0.0           0.     !(134) Voisin 98
CYC6H7+CH3=A+CH4               8.00E+12       0.0           0.     !(134) Voisin 98
CYC6H7+HCO=A+CH2O              4.00E+12       0.0           0.     !(134) Voisin 98
!
!   C6H11
!
C6H11=C6H10+H                  3.20E+13       0.0       38000.     !(124) Dayma 03
C6H11+H=C6H10+H2               1.80E+12       0.0           0.     !Estimated (C4H7+H=iiiC4H6+H2)
C6H11+O2=C6H10+HO2             1.00E+11       0.0           0.     !Estimated (C4H7+O2=iiiC4H6+HO2)
C6H11+CH3=C6H10+CH4            1.10E+13       0.0           0.     !Estimated (C4H7+CH3=iiiC4H6+CH4)
C6H11+O=C6H10+OH               4.82E+13       0.0           0.     !Estimated 2*(C6H11+OH=C6H10+H2O)
C6H11+OH=C6H10+H2O             2.41E+13       0.0           0.     !Estimated (nC3H7+OH=C3H6+H2O)
!
!   C6H10
!
C6H10+H=C6H9+H2                1.33E+06       2.53      12240.     !Estimated (iiiC4H6+H=n-C4H5+H2)
C6H10+H=C4H7+C2H4              1.46E+30      -4.34      21647.     !Estimated (iiiC4H6+H=C2H4+C2H3)
C6H10+O=C6H9+OH                7.50E+06       1.90       3740.     !Estimated (iiiC4H6+O=n-C4H5+OH)
C6H10+O=CH2CO+C4H7+H           1.20E+08       1.65        327.     !Estimated (C3H6+O=CH3+H+CH2CO)
C6H10+OH=C6H9+H2O              6.20E+06       2.00       3430.     !Est (iiiC4H6+OH==n-C4H5+H2O)
!
!   C6H9
!
C6H9=n-C4H5+C2H4               2.00E+13       0.0       35500.     !(124) Dayma 03
C6H9=C6H8+H                    3.20E+13       0.0       34800.     !(124) Dayma 03
C6H9+O2=C6H8+HO2               1.60E+12       0.0        5000.     !(124) Dayma 03
C6H9+H=C6H10                   1.00E+14       0.0           0.     !(124) Dayma 03
C6H9+H=C6H8+H2                 1.80E+12       0.0           0.     !Estimated (C4H7+H=iiiC4H6+H2)
C6H9+CH3=C6H8+CH4              1.10E+13       0.0           0.     !Estimated (C4H7+CH3=iiiC4H6+CH4)
C6H9+O=C6H8+OH                 4.82E+13       0.0           0.     !Estimated 2*(C6H9+OH=C6H8+H2O)
C6H9+OH=C6H8+H2O               2.41E+13       0.0           0.     !Estimated (nC3H7+OH=C3H6+H2O)
!
!   C6H8
```

```
!
C6H8+O=CH2CO+n-C4H5+H           1.20E+08       1.65        327.0    !Estimated (C3H6+O=CH3+H+CH2CO)
!
!
!**********************************Toluene sub-model reactions*****************************************
!
! Most of these reactions are from (138) Lindstedt 96 toluene model
!
! C6H5CH3
!
C6H5CH3=C6H5CH2+H               3.00E+15       0.00      88194.     !(115) Dagaut 02
C6H5CH3=A1+CH3                  8.91E+12       0.00      72565.     !1987PAM/KER from Lindstedt 96
C6H5CH3+O2=C6H5CH2+HO2           3.0E+14       0.00      41400.     !(114) Emdee/Bre 92
C6H5CH3+OH=C6H5CH2+H2O          5.19E+09       1.00        874.3    !Baulch 92 from Lindstedt 96
C6H5CH3+OH=C6H5CH2O+H2          2.29E+12       0.00       -358.3    !Baulch 92 from Lindstedt 96
C6H5CH3+OH=C6H5CH2OH+H          6.60E+12       0.00      10588.     !Adj,Baulch 92 from Lindstedt 96
C6H5CH3+H=C6H5CH2+H2            3.97E+02       3.44       3120.     !BAU/COB 92 from Lindstedt 96
C6H5CH3+H=A+CH3                 1.20E+13       0.00       5148.     !(114) Emdee/Bre92
C6H5CH3+O=OC6H4CH3+H            3.10E+13       0.00       3973.     !Hoff 90 from Lindstedt 96
C6H5CH3+O=C6H5CH2O+H            1.55E+13       0.00       3973.     !Hoff 90 from Lindstedt 96
C6H5CH3+O=C6H5CH2+OH            6.30E+11       0.00          0.     !Hoff 90 from Lindstedt 96
C6H5CH3+O=C6H5OCH3              6.30E+11       0.00          0.     !Hoff 90 from Lindstedt 96
C6H5CH3+CH3=C6H5CH2+CH4         3.16E+12       0.00      11094.     !adj&colket&seer94 Lindstedt 96
C6H5CH3+AC3H5=C6H5CH2+C3H6      5.00E+12       0.00      14000.     !(144) Colket 94
C6H5CH3+C2H3=C6H5CH2+C2H4       3.98E+12       0.00       8000.     !(144) Colket 94
C6H5CH3+HO2=C6H5CH2+H2O2       3.975E+11       0.00      14061.     !Baulch 94 from Lindstedt 96
C6H5CH3+OH=C6H4CH3+H2O           1.6E08        1.42       1450.     !(140) Bounaceur/Battin 05
C6H4CH3+H=C6H5CH3                1.0E14        0.0           0.     !(140) Bounaceur/Battin 05
C6H5CH3+HO2=C6H4CH3+H2O2        5.48E+12       0.00      28798.     !Baulch 94 from Lindstedt 96
C6H5CH3+A1=C6H5CH2+A            2.10E+12       0.00       4400.     !(114) Emdee/Bre 92
n-C4H5+AC3H4=C6H5CH3+H          2.00E+11       0.00       3698.     !Kern 88 from Lindstedt 96
n-C4H5+PC3H4=C6H5CH3+H          3.16E+11       0.00       3698.     !Cole 88 from Lindstedt 96
A+CH2SING=C6H5CH3               1.20E+14       0.00          0.     !Bohland 89 from Lindstedt 96
A+CH2=C6H5CH3                   5.00E+10       0.00       8958.     !Bohland 89 from Lindstedt 96
!
! C6H5OCH3
!
C6H5OCH3=C6H5O+CH3              2.00E+15       0.00      63566.7    !Arends 93 from Lindstedt 96
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C6H5OCH3+H=C6H5OH+CH3           7.08E+12       0.00       5387.     !Arends 93 from Lindstedt 96
C6H5OCH3+O=C6H5OCH2+OH          1.67E+13       0.00       2938.4    !Koch 92 from Lindstedt 96
C6H5OCH3+OH=C6H5OCH2+H2O        1.20E+12       0.00       -501.7    !Perry 77 from Lindstedt 96
C6H5OCH3+CH3=C6H5OCH2+CH4       5.01E+11       0.00      10492.     !Mulcahy 67 from Lindstedt 96
C6H5OCH2=C6H5CHO+H              3.16E+12       0.00      20989.     !Mulcahy 67 from Lindstedt 96
C6H5OH+C6H5CH2=C6H5CH3+C6H5O    1.05E+11       0.00       9500.     !(114) Emdee/Bre 92
HOC6H4CH3+C6H5CH2=OC6H4CH3+C6H5CH3 1.05E+11    0.00       9500.     !(114) Emdee/Bre 92
!
! C6H5CH2
!
C6H5CH2=C4H4+C3H3               2.00E+14       0.00      83600.     !(144) Colket 94
C6H5CH2=C5H5+C2H2               6.03E+13       0.00      70000.     !(144) Colket 94
C6H5CH2+O=C6H5CHO+H             3.50E+13       0.00          0.     ! Lindstedt 96
C6H5CH2+O=A1+CH2O               8.00E+13       0.00          0.     !(114) Emdee/Bre 92
C6H5CH2+O=A+HCO                 3.50E+13       0.00          0.     ! Lindstedt 96
C6H5CH2+HO2=C6H5CHO+H+OH        5.00E+14       0.00          0.     !(137) Klotz/Brez 98
C6H5CH2+HO2=A+HCO+OH            3.50E+13       0.00          0.     !Adj,Hipple91 in Lindstedt 96
C6H5CH2+HO2=A1+CH2O+OH          8.00E+13       0.00          0.     !(114) Emdee/Bre 92
C6H5CH2+OH=C6H5CH2OH            6.00E+13       0.00          0.     !(114) Emdee/Bre 92
C6H5CH2+O2=C6H5CH2O+O           6.31E+12       0.00      42979.     !Brezinsky84 from Lindstedt 96
C6H5CH2+O2=C6H5CH2OO            4.58E+11       0.00       -377.4    !Brezinsky84 from Lindstedt 96
!
 C6H5CH2OO

C6H5CH2OO=C6H5CHO+OH            1.00E+10       0.00      28906.     !Adj, Clothier95 from Lindstedt 96
!
!------------Methyl phenyl from Bounaceur/Battin 2005 Toluene model----------------------------------------
C6H4CH3+O2=OC6H4CH3+O            2.6E13        0.0        6100.     !(140) Bounaceur/Battin 05
C6H4CH3+O2=C6H4O2+CH3            3.0E13        0.0        9000.     !(140) Bounaceur/Battin 05
C6H4CH3+O=OC6H4CH3               1.0E14        0.0         0.0      !(140) Bounaceur/Battin 05
C6H4CH3+OH=HOC6H4CH3             1.0E13        0.0         0.0      !(140) Bounaceur/Battin 05
C6H4CH3+H=C6H5CH2+H              1.0E13        0.0         0.0      ! (46) Miller 92
!-------------------------------------------------------------------------------------------------------
!
! C6H5CH2O
!
C6H5CH2O+M=C6H5CHO+H+M          2.50E+11       0.00          0.     !Hoffman 90 from Lindstedt 96
C6H5CH2O+H=C6H5CHO+H2           3.00E+13       0.00          0.     ! Lindstedt 96
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C6H5CH2O+O=C6H5CHO+OH           4.20E+13       0.00          0.     ! Lindstedt 96
C6H5CH2O+OH=C6H5CHO+H2O         2.40E+13       0.00          0.     ! Lindstedt 96
C6H5CH2O+O2=C6H5CHO+HO2         1.00E+13       0.00       5016.7    ! Lindstedt 96
C6H5CH2O+H=C6H5CH2OH            2.50E+13       0.00       5016.7    ! Lindstedt 96
!
! C6H5CH2OH
!
C6H5CH2OH+O2=C6H5CHO+HO2+H      2.00E+14       0.00      41400.     !(114) Emdee/Bre 92
C6H5CH2OH+OH=C6H5CHO+H2O+H      8.43E+12       0.00       2583.     !(114) Emdee/Bre 92
C6H5CH2OH+OH=C6H5CH2O+H2O       5.00E+12       0.00          0.     !Hippler 91 from Lindstedt 96
C6H5CH2OH+H=C6H5CHO+H2+H        8.00E+13       0.00       8235.     !(114) Emdee/Bre 92
C6H5CH2OH+H=C6H5CH2O+H2         8.00E+13       0.00       8234.6    ! Lindstedt 96
C6H5CH2OH+H=A+CH2OH             1.20E+13       0.00       5148.     !(114) Emdee/Bre 92
C6H5CH2OH+C6H5CH2=C6H5CHO+C6H5CH3+H 2.11E+11   0.00       9500.     !(114) Emdee/Bre 92
C6H5CH2OH+A1=C6H5CHO+A+H        1.40E+12       0.00       4400.     !(114) Emdee/Bre 92
!
! C6H5CHO
!
C6H5CHO=C6H5CO+H                3.98E+15       0.00      83660.     !Grela and Colussi 1986
C6H5CHO+O2=C6H5CO+HO2           1.02E+13       0.00      38950.     !(114) Emdee/Bre 92
C6H5CHO+OH=C6H5CO+H2O           1.71E+09       1.18       -447.     !(114) Emdee/Bre 92
C6H5CHO+H=C6H5CO+H2             5.00E+13       0.00       4928.     !(114) Emdee/Bre 92
C6H5CHO+H=A+HCO                 1.20E+13       0.00       5148.     !(114) Emdee/Bre 92
C6H5CHO+O=C6H5CO+OH             9.04E+12       0.00       3080.     !(114) Emdee/Bre 92
C6H5CHO+HO2=C6H5CO+H2O2         2.00E+12       0.0       11660.3    ! Lindstedt 96
C6H5CHO+C6H5CH2=C6H5CO+C6H5CH3  2.77E+03       2.81       5773.     !(114) Emdee/Bre 92
C6H5CHO+CH3=C6H5CO+CH4          2.77E+03       2.81       5773.     !(114) Emdee/Bre 92
C6H5CHO+A1=C6H5CO+A             7.01E+11       0.00       4400.     !(114) Emdee/Bre 92
C6H5CO=A1+CO                    3.98E+14       0.00      29400.     !(114) Emdee/Bre 92
C6H5CO+H=A+CO                   3.00E+13       0.00          0.     !Buth 92 from Lindstedt 96
!
! HOC6H4CH3
!
C6H5CH3+OH=HOC6H4CH3+H          2.29E+12       0.00       -358.3    !Adj,Baulch 92 in Lindstedt 96
OC6H4CH3+H=HOC6H4CH3            2.50E+14       0.00          0.     !(114) Emdee/Bre 92
OC6H4CH3=A+H+CO                 2.51E+11       0.00      43900.     !(114) Emdee/Bre 92
OC6H4CH3+H2O=HOC6H4CH3+OH       6.88E+12       0.36      32541.2    !(114) Emdee/Bre 92
HOC6H4CH3+H=OC6H4CH3+H2         1.15E+14       0.00      12400.     !(114) Emdee/Bre 92
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```
HOC6H4CH3+H=C6H5OH+CH3          1.20E+13       0.00       5148.     !(114) Emdee/Bre 92


!
! C6H5CH2CH3
!
C6H5CH2+CH3=C6H5CH2CH3          1.00E+13       0.00          0.     !Adj&Colket 94 fm Lindstedt 96
C6H5CH2CH3+OH=C6H5CHCH2+H2O+H   8.43E+12       0.00       2583.     !(114) Emdee/Bre 92
C6H5CH2CH3+H=C6H5CHCH2+H2+H     8.00E+13       0.00       8235.     !(114) Emdee/Bre 92
C6H5CH2CH3+O2=C6H5CHCH2+HO2+H   2.00E+14       0.00      41400.     !(114) Emdee/Bre 92
C6H4CCH+H=C6H5CCH               7.83E+13       0.00          0.     ! Lindstedt 96 Toluene
C6H5CCH+H=A1+C2H2               2.00E+14       0.00       9698.     !HER/FRA 92 from Lindstedt 96
C6H5CCH+H=C6H4CCH+H2            2.70E+13       0.00       9698.     !HER/FRA 92 from Lindstedt 96
C6H5CCH+O=C6H4CCH+OH            1.00E+13       0.00       8122.3    ! Lindstedt 96 Toluene
C6H5CCH+OH=C6H4CCH+H2O          2.10E+13       0.00       4562.8    !Frenklach94 from Lindstedt 96
A1+C2H2=C6H5CHCH                3.60E+12       0.00       8065.     ! Lindstedt 96
C6H5CHCH+H=C6H5CHCH2            5.40E+12       0.00       2410.4    ! Lindstedt 96
C6H5CHCH+H=C6H5CCH+H2           1.00E+13       0.00          0.     ! Lindstedt 96
C6H5CHCH+O=C6H5CCH+OH           1.00E+13       0.00          0.     ! Lindstedt 96
C6H5CHCH+OH=C6H5CCH+H2O         1.00E+13       0.00          0.     ! Lindstedt 96
A1+C2H3=C6H5CHCH2               5.00E+12       0.00          0.     ! Lindstedt 96
A+C2H3=C6H5CHCH2+H              7.94E+11       0.00       6395.1    !Fahr&Stein 89 in Lindstedt 96
A1+C2H4=C6H5CHCH2+H             2.51E+12       0.00       6196.8    !Fahr&Stein89 from Lindstedt 96
i-C4H5+C4H4=C6H5CHCH2+H         3.61E+11       0.00        599.6    !Cole 84 from Lindstedt 96
C6H5CH2CH2=C6H5CHCH2+H          3.16E+13       0.00      50645.     !Muller&Troe88 in Lindstedt 96
C6H5CH2CH3=C6H5CH2CH2+H         2.51E+15       0.00      81223.     !Muller&Troe88 in Lindstedt 96
C6H5CH2CH3+H=C6H5CH2CH2+H2      0.126E+3       3.44       3117.5    ! Lindstedt 96
C6H5CH2CH3+O=C6H5CH2CH2+OH      2.20E+12       0.00       3798.4    !Adj&Frerichs91 in Lindstedt 96
C6H5CH2CH3+OH=C6H5CH2CH2+H2O    5.00E+11       0.00          0.     ! Lindstedt 96
C6H5CH2CH3+HO2=C6H5CH2CH2+H2O2  2.65E+11       0.00      11280.5    !Baulch94 in Lindstedt 96
C6H5CH2CH3+A1=C6H5CH2CH2+A      5.00E+11       0.00          0.     !Adj,Muller&Troe88in Lindstedt 96
C6H5CH2+CH2SING=C6H5CHCH2+H     2.40E+14       0.00          0.     !Adj,Bohland89 in Lindstedt 96
C6H5CH2+CH2=C6H5CHCH2+H         7.00E+13       0.00       8958.4    !Adj,Bohland89 in Lindstedt 96
!
! Other oxidation and growth
!
C6H5O+O=C6H4O2+H                8.50E+13       0.00          0.     !(139) Sivaramakrishnan 04
A1+O2=C6H4O2+H                  3.00E+13       0.00       8982.     !(139) Sivaramakrishnan 04
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```
C6H4O2=C5H4O+CO                 7.40E+11       0.00      59020.     !(139) Sivaramakrishnan 04
A1+A1=C6H5C6H5                  5.70E+12       0.00          0.     !HEC/HIP 96 from Lindstedt 96
A+A1=C6H5C6H5+H                 2.00E+12       0.00       3996.7    !FAH/STE 89 from Lindstedt 96
C6H5CH2+C6H5CH2=BiBenzyl        2.51E+11       0.40          0.     !(114) Emdee/Bre92
BiBenzyl+H=C6H5CHCH2+A1+H2      5.01E+13       0.00      13000.     !(144) Colket 94
!
!
!
END
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Thermodynamic properties used for flame simulation

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! Thermochemistry in Chemkin format for
! portion of C/H/O reaction set used for cyclohexane model (Nov 1, 2010).
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!
THERMO
   300.000  1000.000  5000.000
H                 L 7/88H   1               G   200.000  3500.000  1000.000    1
 2.50000001E+00-2.30842973E-11 1.61561948E-14-4.73515235E-18 4.98197357E-22    2
 2.54736599E+04-4.46682914E-01 2.50000000E+00 7.05332819E-13-1.99591964E-15    3
 2.30081632E-18-9.27732332E-22 2.54736599E+04-4.46682853E-01                   4
H2                TPIS78H   2               G   200.000  3500.000  1000.000    1
 3.33727920E+00-4.94024731E-05 4.99456778E-07-1.79566394E-10 2.00255376E-14    2
-9.50158922E+02-3.20502331E+00 2.34433112E+00 7.98052075E-03-1.94781510E-05    3
 2.01572094E-08-7.37611761E-12-9.17935173E+02 6.83010238E-01                   4
CH                JUN03 C   1H   1          G   200.000  6000.000  1000.000    1
 0.25209369E+01 0.17653639E-02-0.46147660E-06 0.59289675E-10-0.33474501E-14    2
 0.70946769E+05 0.74051829E+01 0.34897583E+01 0.32432160E-03-0.16899751E-05    3
 0.31628420E-08-0.14061803E-11 0.70612646E+05 0.20842841E+01 0.71658188E+05    4
CH2               JUN03 C   1H   2          G   200.000  6000.000  1000.000    1
 0.31463189E+01 0.30367126E-02-0.99647444E-06 0.15048358E-09-0.85733552E-14    2
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 0.46041260E+05 0.47234171E+01 0.37175785E+01 0.12739126E-02 0.21734725E-05    3
-0.34885850E-08 0.16520887E-11 0.45872387E+05 0.17529794E+01 0.47050492E+05    4
CH2SING           JUN03 C   1H   2          G   200.000  6000.000  1000.000    1
 0.31350169E+01 0.28959393E-02-0.81666809E-06 0.11357270E-09-0.63626284E-14    2
 0.50504050E+05 0.40603062E+01 0.41933133E+01-0.23310518E-02 0.81567645E-05    3
-0.66298598E-08 0.19323320E-11 0.50366225E+05-0.74673431E+00 0.51572728E+05    4
CH3               JUN03 C   1H   3          G   200.000  6000.000  1000.000    1
 0.29781206E+01 0.57978520E-02-0.19755800E-05 0.30729790E-09-0.17917416E-13    2
 0.16509513E+05 0.47224799E+01 0.36571797E+01 0.21265979E-02 0.54583883E-05    3
-0.66181003E-08 0.24657074E-11 0.16422716E+05 0.16735354E+01 0.17643935E+05    4
O                 L 1/90O   1              G   200.000  3500.000  1000.000    1
 2.56942078E+00-8.59741137E-05 4.19484589E-08-1.00177799E-11 1.22833691E-15    2
 2.92175791E+04 4.78433864E+00 3.16826710E+00-3.27931884E-03 6.64306396E-06    3
-6.12806624E-09 2.11265971E-12 2.91222592E+04 2.05193346E+00                   4
CH4               L 8/88C   1H   4          G   200.000  3500.000  1000.000    1
 7.48514950E-02 1.33909467E-02-5.73285809E-06 1.22292535E-09-1.01815230E-13    2
-9.46834459E+03 1.84373180E+01 5.14987613E+00-1.36709788E-02 4.91800599E-05    3
-4.84743026E-08 1.66693956E-11-1.02466476E+04-4.64130376E+00                   4
OH                JUN03 O   1H   1          G   200.000  6000.000  1000.000    1
 0.28385303E+01 0.11074129E-02-0.29400021E-06 0.42069873E-10-0.24228989E-14    2
 0.36978081E+04 0.58449465E+01 0.39919842E+01-0.24010666E-02 0.46166403E-05    3
-0.38791631E-08 0.13631950E-11 0.33688984E+04-0.10399848E+00 0.44861538E+04    4
H2O               L 8/89H   2O   1          G   200.000  3500.000  1000.000    1
 3.03399249E+00 2.17691804E-03-1.64072518E-07-9.70419870E-11 1.68200992E-14    2
-3.00042971E+04 4.96677010E+00 4.19864056E+00-2.03643410E-03 6.52040211E-06    3
-5.48797062E-09 1.77197817E-12-3.02937267E+04-8.49032208E-01                   4
C2H               L 1/91C   2H   1          G   200.000  3500.000  1000.000    1
 3.16780652E+00 4.75221902E-03-1.83787077E-06 3.04190252E-10-1.77232770E-14    2
 6.71210650E+04 6.63589475E+00 2.88965733E+00 1.34099611E-02-2.84769501E-05    3
 2.94791045E-08-1.09331511E-11 6.68393932E+04 6.22296438E+00                   4
C2H2              L 1/91C   2H   2          G   200.000  3500.000  1000.000    1
 4.14756964E+00 5.96166664E-03-2.37294852E-06 4.67412171E-10-3.61235213E-14    2
 2.59359992E+04-1.23028121E+00 8.08681094E-01 2.33615629E-02-3.55171815E-05    3
 2.80152437E-08-8.50072974E-12 2.64289807E+04 1.39397051E+01                   4
H2CC              L12/89H   2C   2    0    0G   200.000  6000.000  1000.000    1
 0.42780340E+01 0.47562804E-02-0.16301009E-05 0.25462806E-09-0.14886379E-13    2
 0.48316688E+05 0.64023701E+00 0.32815483E+01 0.69764791E-02-0.23855244E-05    3
-0.12104432E-08 0.98189545E-12 0.48621794E+05 0.59203910E+01 0.49887266E+05    4
```

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C2H3               L 2/92C   2H   3          G   200.000  3500.000  1000.000    1
 3.01672400E+00 1.03302292E-02-4.68082349E-06 1.01763288E-09-8.62607041E-14    2
 3.46128739E+04 7.78732378E+00 3.21246645E+00 1.51479162E-03 2.59209412E-05    3
-3.57657847E-08 1.47150873E-11 3.48598468E+04 8.51054025E+00                   4
CO                 TPIS79C   1O   1          G   200.000  3500.000  1000.000    1
 2.71518561E+00 2.06252743E-03-9.98825771E-07 2.30053008E-10-2.03647716E-14    2
-1.41518724E+04 7.81868772E+00 3.57953347E+00-6.10353680E-04 1.01681433E-06    3
 9.07005884E-10-9.04424499E-13-1.43440860E+04 3.50840928E+00                   4
C2H4               L 1/91C   2H   4          G   200.000  3500.000  1000.000    1
 2.03611116E+00 1.46454151E-02-6.71077915E-06 1.47222923E-09-1.25706061E-13    2
 4.93988614E+03 1.03053693E+01 3.95920148E+00-7.57052247E-03 5.70990292E-05    3
-6.91588753E-08 2.69884373E-11 5.08977593E+03 4.09733096E+00                   4
HCO                L12/89H   1C   1O   1     G   200.000  3500.000  1000.000    1
 2.77217438E+00 4.95695526E-03-2.48445613E-06 5.89161778E-10-5.33508711E-14    2
 4.01191815E+03 9.79834492E+00 4.22118584E+00-3.24392532E-03 1.37799446E-05    3
-1.33144093E-08 4.33768865E-12 3.83956496E+03 3.39437243E+00                   4
C2H5               L12/92C   2H   5          G   200.000  3500.000  1000.000    1
 1.95465642E+00 1.73972722E-02-7.98206668E-06 1.75217689E-09-1.49641576E-13    2
 1.28575200E+04 1.34624343E+01 4.30646568E+00-4.18658892E-03 4.97142807E-05    3
-5.99126606E-08 2.30509004E-11 1.28416265E+04 4.70720924E+00                   4
CH2O               L 8/88H   2C   1O   1     G   200.000  3500.000  1000.000    1
 1.76069008E+00 9.20000082E-03-4.42258813E-06 1.00641212E-09-8.83855640E-14    2
-1.39958323E+04 1.36563230E+01 4.79372315E+00-9.90833369E-03 3.73220008E-05    3
-3.79285261E-08 1.31772652E-11-1.43089567E+04 6.02812900E-01                   4
C2H6               L 8/88C   2H   6          G   200.000  3500.000  1000.000    1
 1.07188150E+00 2.16852677E-02-1.00256067E-05 2.21412001E-09-1.90002890E-13    2
-1.14263932E+04 1.51156107E+01 4.29142492E+00-5.50154270E-03 5.99438288E-05    3
-7.08466285E-08 2.68685771E-11-1.15222055E+04 2.66682316E+00                   4
CH2OH              JUN03 C   1H   3O   1     G   200.000  6000.000  1000.000    1
 0.50931437E+01 0.59476126E-02-0.20649746E-05 0.32300817E-09-0.18812590E-13    2
-0.40340964E+04-0.18469149E+01 0.44783436E+01-0.13507031E-02 0.27848498E-04    3
-0.36486906E-07 0.14790745E-10-0.35007289E+04 0.33091350E+01-0.20446277E+04    4
CH3O               JUN03 C   1H   3O   1     G   200.000  6000.000  1000.000    1
 0.47577924E+01 0.74414247E-02-0.26970518E-05 0.43809050E-09-0.26353710E-13    2
 0.37811194E+03-0.19668003E+01 0.37118050E+01-0.28046331E-02 0.37655097E-04    3
-0.47307209E-07 0.18658842E-10 0.12956976E+04 0.65724086E+01 0.25257166E+04    4
CH3OH              L 8/88C   1H   4O   1     G   200.000  3500.000  1000.000    1
 1.78970791E+00 1.40938292E-02-6.36500835E-06 1.38171085E-09-1.17060220E-13    2
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-2.53748747E+04 1.45023623E+01 5.71539582E+00-1.52309129E-02 6.52441155E-05    3
-7.10806889E-08 2.61352698E-11-2.56427656E+04-1.50409823E+00                   4
O2                TPIS89O   2               G   200.000  3500.000  1000.000    1
 3.28253784E+00 1.48308754E-03-7.57966669E-07 2.09470555E-10-2.16717794E-14    2
-1.08845772E+03 5.45323129E+00 3.78245636E+00-2.99673416E-03 9.84730201E-06    3
-9.68129509E-09 3.24372837E-12-1.06394356E+03 3.65767573E+00                   4
HO2               L 5/89H   1O   2          G   200.000  3500.000  1000.000    1
 4.01721090E+00 2.23982013E-03-6.33658150E-07 1.14246370E-10-1.07908535E-14    2
 1.11856713E+02 3.78510215E+00 4.30179801E+00-4.74912051E-03 2.11582891E-05    3
-2.42763894E-08 9.29225124E-12 2.94808040E+02 3.71666245E+00                   4
H2O2              L 7/88H   2O   2          G   200.000  3500.000  1000.000    1
 4.16500285E+00 4.90831694E-03-1.90139225E-06 3.71185986E-10-2.87908305E-14    2
-1.78617877E+04 2.91615662E+00 4.27611269E+00-5.42822417E-04 1.67335701E-05    3
-2.15770813E-08 8.62454363E-12-1.77025821E+04 3.43505074E+00                   4
C3H2              121686C   3H   2          G  0300.00   5000.00  1000.00     1
 0.06530853E+02 0.05870316E-01-0.01720777E-04 0.02127498E-08-0.08291910E-13    2
 0.05115214E+06-0.01122728E+03 0.02691077E+02 0.01480366E+00-0.03250551E-04    3
-0.08644363E-07 0.05284878E-10 0.05219072E+06 0.08757391E+02                   4
C3H3              T 5/99C   3H   3    0    0G   200.000  6000.000              1
 7.14221880E+00 7.61902005E-03-2.67459950E-06 4.24914801E-10-2.51475415E-14    2
 3.89087427E+04-1.25848436E+01 1.35110927E+00 3.27411223E-02-4.73827135E-05    3
 3.76309808E-08-1.18540923E-11 4.01057783E+04 1.52058924E+01 4.16139977E+04    4
AR                120186AR  1               G   300.000  5000.000  1000.000    1
 0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-0.07453750E+04 0.04366000E+02 0.02500000E+02 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-0.07453750E+04 0.04366000E+02                   4
AC3H4             L 8/89C   3H   4    0    0G   200.000  6000.000              1
 0.63168722E+01 0.11133728E-01-0.39629378E-05 0.63564238E-09-0.37875540E-13    2
 0.20117495E+05-0.10995766E+02 0.26130445E+01 0.12122575E-01 0.18539880E-04    3
-0.34525149E-07 0.15335079E-10 0.21541567E+05 0.10226139E+02 0.22962267E+05    4
PC3H4             T 2/90H   4C   3    0    0G   200.000  6000.000              1
 0.60252400E+01 0.11336542E-01-0.40223391E-05 0.64376063E-09-0.38299635E-13    2
 0.19620942E+05-0.86043785E+01 0.26803869E+01 0.15799651E-01 0.25070596E-05    3
-0.13657623E-07 0.66154285E-11 0.20802374E+05 0.98769351E+01 0.22302059E+05    4
HCCO              SRIC91H   1C   2O   1     G   300.00   4000.00   1000.000    1
 0.56282058E+01 0.40853401E-02-0.15934547E-05 0.28626052E-09-0.19407832E-13    2
 0.19327215E+05-0.39302595E+01 0.22517214E+01 0.17655021E-01-0.23729101E-04    3
 0.17275759E-07-0.50664811E-11 0.20059449E+05 0.12490417E+02                   4
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AC3H5             PD5/98C   3H   5    0    0G   300.000  3000.000             1
 0.65007877E+01 0.14324731E-01-0.56781632E-05 0.11080801E-08-0.90363887E-13    2
 0.17482449E+05-0.11243050E+02 0.13631835E+01 0.19813821E-01 0.12497060E-04    3
-0.33355555E-07 0.15846571E-10 0.19245629E+05 0.17173214E+02                   4
TC3H5             PD5/98C   3H   5    0    0G   300.000  3000.000             1
 0.54255528E+01 0.15511072E-01-0.56678350E-05 0.79224388E-09-0.16878034E-13    2
 0.27843027E+05-0.33527184E+01 0.17329209E+01 0.22394620E-01-0.51490611E-05    3
-0.67596466E-08 0.38253211E-11 0.29040498E+05 0.16568878E+02                   4
SC3H5             PD5/98C   3H   5    0    0G   300.000  3000.000             1
 0.53725281E+01 0.15780509E-01-0.59922850E-05 0.93089664E-09-0.36550966E-13    2
 0.29614760E+05-0.34186478E+01 0.91372931E+00 0.26432343E-01-0.11758950E-04    3
-0.23035678E-08 0.27715488E-11 0.30916867E+05 0.19989269E+02                   4
CH2CO             L 5/90C   2H   2O   1     G   200.000  3500.000  1000.000    1
 4.51129732E+00 9.00359745E-03-4.16939635E-06 9.23345882E-10-7.94838201E-14    2
-7.55105311E+03 6.32247205E-01 2.13583630E+00 1.81188721E-02-1.73947474E-05    3
 9.34397568E-09-2.01457615E-12-7.04291804E+03 1.22156480E+01                   4
C3H6              120186C   3H   6          G  0300.00   5000.00  1000.00     1
 0.06732257E+02 0.01490834E+00-0.04949899E-04 0.07212022E-08-0.03766204E-12    2
-0.09235703E+04-0.01331335E+03 0.01493307E+02 0.02092518E+00 0.04486794E-04    3
-0.01668912E-06 0.07158146E-10 0.01074826E+05 0.01614534E+03                   4
CH3CO             JUN03 C   2H   3O   1    0G   200.000  6000.000  1000.0     1
 0.53137165E+01 0.91737793E-02-0.33220386E-05 0.53947456E-09-0.32452368E-13    2
-0.36450414E+04-0.16757558E+01 0.40358705E+01 0.87729487E-03 0.30710010E-04    3
-0.39247565E-07 0.15296869E-10-0.26820738E+04 0.78617682E+01-0.12388039E+04    4
CH2CHO            SAND86O   1H   3C   2     G   300.000  5000.000  1000.000    1
 0.05975670E+02 0.08130591E-01-0.02743624E-04 0.04070304E-08-0.02176017E-12    2
 0.04903218E+04-0.05045251E+02 0.03409062E+02 0.10738574E-01 0.01891492E-04    3
-0.07158583E-07 0.02867385E-10 0.15214766E+04 0.09558290E+02                   4
nC3H7             P11/94C   3H   7    0    0G   300.000  3000.000             1
 0.77097479E+01 0.16031485E-01-0.52720238E-05 0.75888352E-09-0.38862719E-13    2
 0.79762236E+04-0.15515297E+02 0.10491173E+01 0.26008973E-01 0.23542516E-05    3
-0.19595132E-07 0.93720207E-11 0.10312346E+05 0.21136034E+02                   4
iC3H7             P11/94C   3H   7    0    0G   300.000  3000.000             1
 0.65192741E+01 0.17220104E-01-0.57364217E-05 0.84130732E-09-0.44565913E-13    2
 0.73227193E+04-0.90830215E+01 0.14449199E+01 0.20999112E-01 0.77036222E-05    3
-0.18476253E-07 0.71282962E-11 0.94223724E+04 0.20116317E+02                   4
C2H4O             J 9/65C   2H   4O   1    0G   300.000  5000.000             1
 0.59249249E 01 0.11120714E-01-0.37434083E-05 0.55413918E-09-0.29549886E-13    2
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-0.93028008E 04-0.93792849E 01-0.24173594E 00 0.20761095E-01 0.21481201E-05    3
-0.16948157E-07 0.81075771E-11-0.71720117E 04 0.24432190E 02                   4
CH3CHO            L 8/88C   2H   4O   1     G   200.000  6000.000  1000.000    1
 0.54041108E+01 0.11723059E-01-0.42263137E-05 0.68372451E-09-0.40984863E-13    2
-0.22593122E+05-0.34807917E+01 0.47294595E+01-0.31932858E-02 0.47534921E-04    3
-0.57458611E-07 0.21931112E-10-0.21572878E+05 0.41030159E+01                   4
C3H8              P11/94C   3H   8    0    0G   300.000  3000.000              1
 0.75244152E+01 0.18898282E-01-0.62921041E-05 0.92161457E-09-0.48684478E-13    2
-0.16564394E+05-0.17838375E+02 0.92851093E+00 0.26460566E-01 0.60332446E-05    3
-0.21914953E-07 0.94961544E-11-0.14057907E+05 0.19225538E+02                   4
CO2               L 7/88C   1O   2          G   200.000  3500.000  1000.000    1
 3.85746029E+00 4.41437026E-03-2.21481404E-06 5.23490188E-10-4.72084164E-14    2
-4.87591660E+04 2.27163806E+00 2.35677352E+00 8.98459677E-03-7.12356269E-06    3
 2.45919022E-09-1.43699548E-13-4.83719697E+04 9.90105222E+00                   4
C2H5O            JUN03  C   2O   1H   5     G   200.000  6000.000 1000.00     1
 0.66889982E+01 0.13125676E-01-0.47038840E-05 0.75858552E-09-0.45413306E-13    2
-0.47457832E+04-0.96983755E+01 0.43074268E+01 0.64147205E-02 0.31139714E-04    3
-0.43314083E-07 0.17276184E-10-0.34027524E+04 0.59025837E+01-0.16357022E+04    4
C4H2              P 1/93C   4H   2    0    0G   300.000  3000.000              1
 0.86637708E+01 0.67247189E-02-0.23593397E-05 0.37506380E-09-0.22230940E-13    2
 0.53252275E+05-0.21093503E+02-0.39201030E+00 0.51937565E-01-0.91737340E-04    3
 0.80471986E-07-0.26898218E-10 0.54845266E+05 0.20957794E+02                   4
nC4H3              82489C   4H   3          G  0300.00   4000.00  1000.00     1
 0.10752738E+02 0.05381153E-01-0.05549637E-05-0.03052266E-08 0.05761740E-12    2
 0.61979123E+05-0.02973025E+03 0.04153881E+02 0.01726287E+00-0.02389374E-05    3
-0.10187000E-07 0.04340504E-10 0.64145633E+05 0.06036506E+02                   4
iC4H3                  0C   4H   3    0    0G   200.000  5000.000 1200.00    0 1
 0.87092233E+01 0.88631021E-02-0.31303011E-05 0.50137975E-09-0.29878650E-13    2
 0.57500575E+05-0.18391950E+02 0.37694948E+01 0.23256639E-01-0.18531943E-04    3
 0.76188028E-08-0.12128742E-11 0.58835310E+05 0.69616708E+01                   4
C4H4              H6W/94C   4H   4    0    0G   300.000  3000.000              1
 0.66507092E+01 0.16129434E-01-0.71938875E-05 0.14981787E-08-0.11864110E-12    2
 0.31195992E+05-0.97952118E+01-0.19152479E+01 0.52750878E-01-0.71655944E-04    3
 0.55072423E-07-0.17286228E-10 0.32978504E+05 0.31419983E+02                   4
n-C4H5             82489C   4H   5          G  0300.00   4000.00  1000.00     1
 0.12865971E+02 0.07943369E-01-0.08626466E-05-0.04655635E-08 0.08951131E-12    2
 0.38695564E+05-0.04182502E+03 0.02995240E+02 0.02288456E+00 0.01975471E-04    3
-0.11482454E-07 0.03197823E-10 0.42282224E+05 0.12894539E+02                   4
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i-C4H5              82489C   4H   5          G  0300.00   4000.00  1000.00      1
 0.11997762E+02 0.07990580E-01-0.08098172E-05-0.04568733E-08 0.08636911E-12    2
 0.33423896E+05-0.03528494E+03 0.03879443E+02 0.01997663E+00 0.01872777E-04    3
-0.09306953E-07 0.02386116E-10 0.36407556E+05 0.09842152E+02                   4
iiC4H6              A 8/83C   4H   6    0    0G   300.     3000.     1000.0     1
  0.1781557E 02 -0.4257502E-02  0.1051185E-04 -0.4473844E-08  0.5848138E-12    2
  0.1267342E 05 -0.6982662E 02  0.1023467E 01  0.3495919E-01 -0.2200905E-04    3
  0.6942272E-08 -0.7879187E-12  0.1811799E 05  0.1975066E 02  0.1950807E+05    4
iiiC4H6             H6W/94C   4H   6    0    0G   300.000  3000.000            1
 0.88673134E+01 0.14918670E-01-0.31548716E-05-0.41841330E-09 0.15761258E-12    2
 0.91338516E+04-0.23328171E+02 0.11284465E+00 0.34369022E-01-0.11107392E-04    3
-0.92106660E-08 0.62065179E-11 0.11802270E+05 0.23089996E+02                   4
C2H3CO C3H3O        T05/99C   3H   3O   1    0G   200.000  6000.000            1
 6.95842227E+00 1.07193211E-02-3.85218494E-06 6.22009064E-10-3.72401640E-14    2
 5.64826498E+03-1.14745786E+01 3.21169467E+00 1.18422105E-02 1.67462582E-05    3
-3.06947176E-08 1.33048816E-11 7.12815750E+03 1.00881663E+01 8.70564832E+03    4
C4H7                AM1/94C   4H   7    0    0G   300.000  3000.000  1000.000    1
 0.11963392E+02 0.11425305E-01 0.78948909E-06-0.19858872E-08 0.36873645E-12    2
 0.16962977E+05-0.37542908E+02 0.28698254E+00 0.36964495E-01-0.86277441E-05    3
-0.15051821E-07 0.89891263E-11 0.20551301E+05 0.24484467E+02                   4
C2H3CHO             T 6/92C   3H   4O   1    0G   298.150  3000.0    1000.0     1
 0.48353180E+01 0.19772601E-01-0.10426628E-04 0.26525803E-08-0.26278207E-12    2
-0.11557837E+05 0.18853144E+01 0.11529584E+01 0.28040214E-01-0.15072153E-04    3
 0.15905842E-08 0.84930371E-12-0.10417694E+05 0.21453279E+02-0.89572567E+04    4
IC4H8               T 6/83C   4H   8    0    0G   300.000  5000.000            1
 0.20535841E+01 0.34350507E-01-0.15883197E-04 0.33089662E-08-0.25361045E-12    2
-0.21397231E+04 0.15543201E+02 0.11811380E+01 0.30853380E-01 0.50865247E-05    3
-0.24654888E-07 0.11110193E-10-0.17904004E+04 0.21062469E+02                   4
C2H3CH2O            96PRW1C   3H   5O   1    0G   300.00   3000.00  1000.00     1
+2.75835879D+00+2.71781452D-02-1.44239030D-05+3.66635155D-09-3.64832209D-13    2
+1.09685129D+04+1.15870981D+01+4.48935705D-01+3.24335892D-02-1.58843257D-05    3
+4.03948822D-10+1.43106465D-12+1.15934429D+04+2.36532883D+01                   4
nC4H9      BURCAT T 6/93C   4H   9    0     G   200.000  6000.000 1000.        1
 8.97401527E+00 2.39704154E-02-8.48703645E-06 1.35644127E-09-8.06234913E-14    2
 5.19161526E+03-2.31075609E+01 4.73737837E+00 9.69051565E-03 6.63846383E-05    3
-9.24799302E-08 3.74006099E-11 7.57382332E+03 4.91063455E+00 9.83838903E+03    4
C2H3OO              PRW84 C   2O   2H   3     G  0300.00   5000.00  1000.00     1
+1.07095497D+00+2.93293018D-02-2.26481331D-05+8.68753392D-09-1.30462650D-12    2
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+1.27909845D+04+2.07891307D+01+3.93381061D+00+1.98311250D-02-1.14186387D-05    3
+3.09270357D-09-3.22330856D-13+1.21364287D+04+6.51468027D+00                   4
C2H5OO            PW3/94C   2O   2H   5     G  0300.00   5000.00  1000.00     1
+2.10630563D+00+2.77943799D-02-1.44630852D-05+3.25545688D-09-2.46592854D-13    2
-2.64777663D+03+1.80691037D+01+2.10630563D+00+2.77943799D-02-1.44630852D-05    3
+3.25545688D-09-2.46592854D-13-2.64767408D+03+1.80671959D+01                   4
C5H5       HR 6/01BLYP00C   5H   5    0     G   300.000  5000.000 1403.000    1
 1.26805871E+01 1.27575785E-02-4.34788920E-06 6.73442111E-10-3.90092992E-14    2
 2.55507801E+04-4.67103980E+01-3.35979212E+00 5.80041481E-02-5.41839461E-05    3
 2.56964859E-08-4.80036435E-12 3.03384665E+04 3.66689604E+01                   4
C5H6       HR11/99BLYP00C   5H   6    0     G   300.000  5000.000 1402.000    1
 1.26575005E+01 1.53301203E-02-5.23821364E-06 8.12867095E-10-4.71504821E-14    2
 1.03083446E+04-4.75386061E+01-4.78259036E+00 6.09873033E-02-5.17363931E-05    3
 2.25173536E-08-3.92621113E-12 1.58382836E+04 4.43226201E+01                   4
C6H2              P 1/93C   6H   2    0    0G   300.000  3000.000             1
 0.13226281E+02 0.73904302E-02-0.22715381E-05 0.25875217E-09-0.55356741E-14    2
 0.80565258E+05-0.41201176E+02-0.15932624E+01 0.80530145E-01-0.14800649E-03    3
 0.13300031E-06-0.45332313E-10 0.83273227E+05 0.27980873E+02                   4
C6H3              H6W/94C   6H   3    0    0G   300.000  3000.000             1
 0.58188343E+01 0.27933408E-01-0.17825427E-04 0.53702536E-08-0.61707627E-12    2
 0.85188250E+05-0.92147827E+00 0.11790619E+01 0.55547360E-01-0.73076168E-04    3
 0.52076736E-07-0.15046964E-10 0.85647312E+05 0.19179199E+02                   4
l-C6H4            H6W/94C   6H   4    0    0G   300.000  3000.000             1
 0.12715182E+02 0.13839662E-01-0.43765440E-05 0.31541636E-09 0.46619026E-13    2
 0.57031148E+05-0.39464600E+02 0.29590225E+00 0.58053318E-01-0.67766756E-04    3
 0.43376762E-07-0.11418864E-10 0.60001371E+05 0.22318970E+02                   4
c-C6H4            H6W/94C   6H   4    0    0G   300.000  3000.000             1
 0.13849209E+02 0.78807920E-02 0.18243836E-05-0.21169166E-08 0.37459977E-12    2
 0.47446340E+05-0.50404953E+02-0.30991268E+01 0.54030564E-01-0.40839004E-04    3
 0.10738837E-07 0.98078490E-12 0.52205711E+05 0.37415207E+02                   4
n-C6H5            H6W/94C   6H   5    0    0G   300.000  3000.000             1
 0.16070068E+02 0.81899539E-02 0.17325165E-05-0.20624185E-08 0.36292345E-12    2
 0.64616867E+05-0.56163742E+02-0.61135769E+00 0.65082610E-01-0.78262397E-04    3
 0.53030828E-07-0.14946683E-10 0.68805375E+05 0.27635468E+02                   4
i-C6H5            H6W/94C   6H   5    0    0G   300.000  3000.000             1
 0.22501663E+02-0.81009977E-02 0.15955695E-04-0.72310371E-08 0.10310424E-11    2
 0.58473410E+05-0.91224777E+02-0.78585434E+00 0.60221825E-01-0.62890264E-04    3
 0.36310730E-07-0.87000259E-11 0.64942270E+05 0.28658905E+02                   4
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A1                H6W/94C   6H   5    0    0G   300.000  3000.000              1
 0.14493439E+02 0.75712688E-02 0.37894542E-05-0.30769500E-08 0.51347820E-12    2
 0.33189977E+05-0.54288940E+02-0.49076147E+01 0.59790771E-01-0.45639827E-04    3
 0.14964993E-07-0.91767826E-12 0.38733410E+05 0.46567780E+02                   4
A                 H6W/94C   6H   6    0    0G   300.000  3000.000              1
 0.17246994E+02 0.38420164E-02 0.82776232E-05-0.48961120E-08 0.76064545E-12    2
 0.26646055E+04-0.71945175E+02-0.48998680E+01 0.59806932E-01-0.36710087E-04    3
 0.32740399E-08 0.37600886E-11 0.91824570E+04 0.44095642E+02                   4
FC6H6             T03/97C   6H   6    0     G   200.000  6000.000  1000.0     1
 1.19233607E+01 1.98993861E-02-7.21223888E-06 1.17141499E-09-7.04278845E-14    2
 2.27199368E+04-4.13488172E+01 1.25853571E-01 3.04056534E-02 4.01806332E-05    3
-8.27651456E-08 3.77645005E-11 2.68838408E+04 2.44628931E+01 2.84820633E+04    4
l-C6H6            H6W/94C   6H   6    0    0G   300.000  3000.000              1
 0.17584442E+02 0.64486600E-02 0.48933980E-05-0.34696221E-08 0.56150749E-12    2
 0.34111988E+05-0.66017838E+02-0.10170622E+01 0.61794821E-01-0.59461061E-04    3
 0.31873491E-07-0.71717693E-11 0.39202707E+05 0.29460373E+02                   4
C4H5C2H                0C   6H   6    0    0G   200.000  5000.000 1100.00    0 1
 0.13903605E+02 0.17453182E-01-0.63026581E-05 0.10316520E-08-0.63440931E-13    2
 0.35975470E+05-0.47671401E+02-0.23220260E+00 0.54092928E-01-0.36134322E-04    3
 0.69104632E-08 0.13734168E-11 0.39978520E+05 0.25932864E+02                   4
CYC6H7     BURCAT T 6/93C   6H   7    0     G   200.000  6000.000 1000.        1
 0.12801758E+02 0.21924749E-01-0.79713001E-05 0.12972935E-08-0.78100416E-13    2
 0.17889539E+05-0.45804341E+02-0.10303140E+00 0.34393354E-01 0.39788466E-04    3
-0.85116612E-07 0.39012224E-10 0.22425515E+05 0.26022350E+02 0.24125213E+05    4
n-C6H7            H6W/94C   6H   7    0    0G   300.000  3000.000              1
 0.22577469E+02-0.30737517E-02 0.14225234E-04-0.69880848E-08 0.10232874E-11    2
 0.41228980E+05-0.91568619E+02 0.13248032E+00 0.57103366E-01-0.43712644E-04    3
 0.15538603E-07-0.12976356E-11 0.47730512E+05 0.25339081E+02                   4
i-C6H7            H6W/94C   6H   7    0    0G   300.000  3000.000              1
 0.20481506E+02 0.79439697E-03 0.11450761E-04-0.60991177E-08 0.91756724E-12    2
 0.37728426E+05-0.81812073E+02-0.17099094E+01 0.62486034E-01-0.54290707E-04    3
 0.26959682E-07-0.58999090E-11 0.44086621E+05 0.33344772E+02                   4
C5H4O     10/00BURCBLYP C   5H   4O   1     G   300.000  5000.000 1402.000     1
 1.37907739E+01 1.19738147E-02-4.11436106E-06 6.40954643E-10-3.72821366E-14    2
 2.74553951E+02-5.06296371E+01-3.01174376E+00 5.82012965E-02-5.36527132E-05    3
 2.48757306E-08-4.54630764E-12 5.38127213E+03 3.70844611E+01                   4
CY13C6H8   BURCAT T 2/90C   6H   8    0     G   200.000  6000.000 1000.        1
 0.11779870E+02 0.25519980E-01-0.92666947E-05 0.15068122E-08-0.90658701E-13    2
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 0.65486686E+04-0.41618805E+02 0.17265319E+01 0.14887612E-01 0.94809230E-04    3
-0.14083394E-06 0.58859873E-10 0.11021297E+05 0.19130886E+02 0.12784878E+05    4
C6H8              H6W/94C   6H   8    0    0G   300.000  3000.000              1
 0.28481979E+02-0.15702948E-01 0.26771697E-04-0.11780109E-07 0.16573427E-11    2
 0.93346445E+04-0.12500226E+03 0.15850439E+01 0.40215142E-01 0.78439543E-05    3
-0.38761325E-07 0.18545207E-10 0.17949613E+05 0.19112625E+02                   4
C5H5O     ZHONG/BOZ1998 C   5H   5O   1     G   300.000  5000.000 1395.000   1
 1.49072105E+01 1.36369619E-02-4.70762207E-06 7.36028654E-10-4.29314124E-14    2
 1.43724130E+04-5.69296345E+01-4.14628450E+00 6.23584874E-02-5.28374678E-05    3
 2.24628793E-08-3.80136191E-12 2.04992627E+04 4.37921058E+01                   4
C6H9       BURCAT T 2/92C   6H   9    0     G   298.150  3000.000 1000.       1
 0.21786938E+02 0.11894129E-01-0.21209124E-05 0.00000000E+00 0.00000000E+00    2
 0.20013752E+05-0.89218982E+02 0.20594889E+01 0.46753513E-01-0.18644505E-04    3
 0.00000000E+00 0.00000000E+00 0.27665639E+05 0.20293525E+02 0.30193000E+05    4
CYC6H9     BURCAT T 2/92C   6H   9    0     G   298.150  3000.000 1000.       1
 0.26295828E+02 0.86828857E-02-0.15770376E-05 0.00000000E+00 0.00000000E+00    2
 0.20863563E+04-0.12573825E+03-0.35714300E+01 0.61696043E-01-0.26928803E-04    3
 0.00000000E+00 0.00000000E+00 0.13657039E+05 0.39986250E+02 0.15096500E+05    4
C5H4OH    ALZUETA 2000  C   5H   5O   1     G   300.000  5000.000 1417.000   1
 1.54616992E+01 1.21543874E-02-3.97713729E-06 5.99530783E-10-3.40841280E-14    2
 1.18008962E+03-5.80092304E+01-3.36507049E+00 6.65211552E-02-6.40907012E-05    3
 3.04663074E-08-5.61147666E-12 6.55733089E+03 3.92124189E+01                   4
CYC6H10    BURCAT T 2/90C   6H  10    0     G   200.000  6000.000 1000.       1
 0.11773904E+02 0.30947360E-01-0.11234330E-04 0.18262494E-08-0.10985119E-12    2
-0.72028376E+04-0.42658688E+02 0.23662378E+01 0.10681712E-01 0.11822112E-03    3
-0.16567854E-06 0.67612802E-10-0.24824973E+04 0.16769357E+02-0.55324968E+03    4
C6H10      BURCAT T 2/92C   6H  10    0     G   298.150  3000.000 1000.       1
 0.23903966E+02 0.12046216E-01-0.19588306E-05 0.00000000E+00 0.00000000E+00    2
-0.43733937E+04-0.10376594E+03-0.96299362E+00 0.60880377E-01-0.28062414E-04    3
 0.00000000E+00 0.00000000E+00 0.45722054E+04 0.32010145E+02 0.67431033E+04    4
CYC6H11    BURCAT 12/98 C   6H  11    0     G   298.150  5000.000 1000.       1
 1.28647309E+01 3.52600147E-02-1.39450525E-05 2.51808759E-09-1.70899213E-13    2
 6.15531214E+02-4.88786148E+01-3.76580647E+00 5.88838077E-02 1.22955158E-07    3
-3.30729397E-08 1.42142299E-11 6.76556720E+03 4.36106643E+01 8.20243165E+03    4
C6H11-12                  C   6H  110   00   0G   300.00   5000.00  1000.00     1
 0.15903220E+02 0.23659610E-01-0.67095560E-05 0.94231160E-09-0.53289920E-13    2
 0.15837710E+05-0.54096690E+02 0.14245270E+00 0.61529150E-01-0.39403020E-04    3
 0.13625820E-07-0.21393720E-11 0.20807860E+05 0.29545670E+02                   4
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C6H11-13                C   6H  110   00   0G   300.00   5000.00  1000.00      1
 0.15939530E+02 0.24454600E-01-0.71328250E-05 0.10237720E-08-0.58843450E-13    2
 0.27317560E+04-0.56236800E+02-0.18343630E+00 0.62924820E-01-0.39494870E-04    3
 0.12901540E-07-0.19206490E-11 0.78098810E+04 0.29353710E+02                   4
C6H11-14                C   6H  11O   00   0G   300.00   5000.00  1000.00      1
 1.32786E+01    2.79515E-02   -8.47472E-06    1.23752E-09   -7.12640E-14       2
 1.22232E+04   -3.88114E+01   -1.06617E+00    7.16134E-02   -5.85771E-05       3
 2.71262E-08   -5.15786E-12    1.59829E+04    3.43102E+01                      4
C6H11-15                C   6H  110   00   0G   300.00   5000.00  1000.00      1
 0.16511810E+02 0.23103710E-01-0.65196350E-05 0.91279680E-09-0.51533620E-13    2
 0.11020680E+05-0.57226020E+02-0.65185990E+00 0.69069390E-01-0.55091450E-04    3
 0.26728390E-07-0.60813550E-11 0.16144180E+05 0.32558910E+02                   4
C6H11      BURCAT  2/92 C   6H  11    0     G   298.150  3000.000 1000.       1
 0.24938654E+02 0.13258801E-01-0.23302223E-05 0.00000000E+00 0.00000000E+00    2
 0.51145941E+04-0.10690338E+03 0.63802451E+00 0.56209452E-01-0.23047424E-04    3
 0.00000000E+00 0.00000000E+00 0.14624427E+05 0.28133981E+02 0.17109367E+05    4
CYC6H12    BURCAT 2/90  C   6H  12    0     G   200.000  5000.000 1000.       1
 0.10209166E+02 0.41894173E-01-0.17234045E-04 0.32239024E-08-0.22540929E-12    2
-0.21742125E+05-0.38990666E+02 0.40402264E+01-0.61827997E-02 0.17662080E-03    3
-0.22300383E-06 0.86393385E-10-0.16919808E+05 0.85269500E+01-0.14829497E+05    4
hexene1    BURCAT T 6/93C   6H  12    0     G   200.000  6000.000 1000.       1
 1.60616093E+01 2.75650562E-02-9.32973368E-06 1.49349013E-09-8.98810268E-14    2
-1.28042951E+04-5.69925586E+01 7.31509054E+00 3.71150329E-03 1.27250318E-04    3
-1.71556964E-07 6.89805935E-11-8.20916507E+03-5.94354365E-01-5.04539654E+03    4
hex1yl     BURCAT T 6/93C   6H  13    0     G   200.000  6000.000 1000.       1
 1.39163141E+01 3.48510892E-02-1.26898935E-05 2.07144196E-09-1.24756674E-13    2
-4.01785625E+03-4.33071846E+01 8.76348959E+00 2.16244832E-03 1.31674686E-04    3
-1.73828247E-07 6.92518175E-11-5.42630596E+02-5.91729689E+00 3.01881891E+03    4
hex2yl     BURCAT T 6/93C   6H  13    0     G   200.000  6000.000 1000.       1
 1.41986473E+01 3.46787125E-02-1.25515738E-05 2.02767674E-09-1.21224274E-13    2
-3.68102477E+03-4.23012097E+01 7.58145549E+00 1.89615514E-02 8.16571755E-05    3
-1.18091545E-07 4.81236008E-11-2.27328454E+02 5.28216352E-05 3.38664816E+03    4
hex3yl                  C   6H  130   00   0G   300.00   5000.00  1000.00      1
 0.18621920E+02 0.24911520E-01-0.68681720E-05 0.94495470E-09-0.52683770E-13    2
-0.51170230E+04-0.69174640E+02-0.17466440E+01 0.81867340E-01-0.74301960E-04    3
 0.43594630E-07-0.11843740E-10 0.94735310E+03 0.37018690E+02                   4
C6H4CH3           P 1/93C   7H   7    0    0G   300.000  2500.000             1
 0.11615498E+02 0.27431838E-01-0.10899345E-04 0.18641830E-08-0.10191607E-12    2
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 0.31209334E+05-0.38994637E+02-0.31415942E+01 0.56723077E-01-0.86885111E-05    3
-0.34249616E-07 0.19266902E-10 0.35738547E+05 0.39742840E+02                   4
C6H5CH2    5/11/93 thermC   7H   7    0    0g   300.000  5000.000 1380.000    1
 1.74066429e+01 1.94934914e-02-6.89552346e-06 1.09498206e-09-6.45370306e-14    2
 1.52488939e+04-7.16678643e+01-3.13104309e+00 6.45512922e-02-4.39082794e-05    3
 1.46756825e-08-1.95214937e-12 2.26869723e+04 3.96945254e+01                   4
C6H5CH3    5/19/93 thermC   7H   8    0    0g   300.000  5000.000 1389.000    1
 1.63091542e+01 2.25331612e-02-7.84281827e-06 1.23200630e-09-7.20675043e-14    2
-2.75804095e+03-6.66759774e+01-4.08982289e+00 6.86477374e-02-4.74716566e-05    3
 1.67001205e-08-2.39578007e-12 4.49937542e+03 4.34582591e+01                   4
C6H5O      HR 6/99 BLYP C   6H   5O   1     G   300.000  5000.000 1402.000    1
 1.63197375E+01 1.49421635E-02-5.14462138E-06 8.02578740E-10-4.67303957E-14    2
-1.19712631E+03-6.52157169E+01-4.17772040E+00 6.95185958E-02-6.15479047E-05    3
 2.74342242E-08-4.84615473E-12 5.19007431E+03 4.23910339E+01                   4
C6H5OH     HR 6/99 BLYP C   6H   6O   1     G   300.000  5000.000 1391.000    1
 1.68693795E+01 1.70838426E-02-5.98946836E-06 9.45398420E-10-5.54859198E-14    2
-1.97294434E+04-6.87883562E+01-4.92900267E+00 7.76036830E-02-7.29208148E-05    3
 3.51831137E-08-6.74079973E-12-1.29920911E+04 4.50935388E+01                   4
C6H4CCH           HW /94C   8H   5    0    0G   300.000  3000.000             1
 0.28686157E+02-0.13869863E-01 0.22721186E-04-0.99882271E-08 0.14085851E-11    2
 0.56047309E+05-0.12750334E+03-0.29324217E+01 0.66043675E-01-0.39500475E-04    3
-0.31830381E-08 0.85300387E-11 0.65324043E+05 0.38058685E+02                   4
C6H5CCH           H6W/94C   8H   6    0    0G   300.000  3000.000             1
 0.24090759E+02 0.78232400E-03 0.11453964E-04-0.61620504E-08 0.93346685E-12    2
 0.27429445E+05-0.10499631E+03-0.52645016E+01 0.84511042E-01-0.76597848E-04    3
 0.33216978E-07-0.47673063E-11 0.35566242E+05 0.46378815E+02                   4
C6H5CHCH          HW /94C   8H   7    0    0G   300.000  3000.000             1
 0.30433151E+02-0.13965182E-01 0.25416972E-04-0.11354174E-07 0.16092050E-11    2
 0.35738719E+05-0.13416492E+03-0.44899931E+01 0.78750789E-01-0.62376959E-04    3
 0.21952140E-07-0.16960955E-11 0.45902949E+05 0.47980759E+02                   4
C6H5CHCH2         T12/94C   8H   8    0    0G   298.150  5000.000             1
 0.16139277E+02 0.24210847E-01-0.72678359E-05 0.11392276E-08-0.72984881E-13    2
 0.10249251E+05-0.61169437E+02-0.10717708E+02 0.12666725E+00-0.17762493E-03    3
 0.14344049E-06-0.47616577E-10 0.16597133E+05 0.71526331E+02 0.17723291E+05    4
C6H5CO     2/25/94 thermC   7H   5O   1    0g   300.000  5000.000 1382.000    1
 1.77196103e+01 1.59990428e-02-5.54532150e-06 8.69582681e-10-5.08335220e-14    2
 4.57408086e+03-6.82553109e+01-1.93001550e+00 6.18799970e-02-4.60916515e-05    3
 1.70133701e-08-2.49869948e-12 1.13352170e+04 3.71779131e+01                   4
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C6H5CH2CH2        A11/04C   8H   9    0    0G   200.000  6000.000             1
 1.61326962E+01 2.82904273E-02-1.01801876E-05 1.64176637E-09-9.81375329E-14    2
 2.08791061E+04-6.00115413E+01 7.33299107E-01 4.59053158E-02 3.78257231E-05    3
-9.12367411E-08 4.25589678E-11 2.61572945E+04 2.50411074E+01 2.85902549E+04    4
C6H5CHO    2/25/94 thermC   7H   6O   1    0g   300.000  5000.000 1382.000    1
 1.75038056e+01 1.87911370e-02-6.51897523e-06 1.02244104e-09-5.97629759e-14    2
-1.31835944e+04-6.88975598e+01-2.70517666e+00 6.46821582e-02-4.57286415e-05    3
 1.60322213e-08-2.23734122e-12-6.07344750e+03 4.00414090e+01                   4
C6H5CH2CH3        A 6/83C   8H  10    0    0G   300.     3000.    1000.00     1
  0.3878978E 01  0.5810059E-01 -0.3196380E-04  0.8448993E-08 -0.8694825E-12    2
 -0.5024922E 03  0.3837099E 01 -0.7266845E 01  0.1003089E 00 -0.9651715E-04    3
  0.5565908E-07 -0.1453370E-10  0.1987290E 04  0.5857746E 02  0.3529492E+04    4
OC6H4CH3  EST/BUR P 1/93C   7H   7O   1    0G   300.000  2500.000             1
 0.22609371E+02 0.75646150E-02 0.65960894E-05-0.47150865E-08 0.80409063E-12    2
-0.82025244E+04-0.97292511E+02-0.28855777E+00 0.48003536E-01 0.18032993E-04    3
-0.61741488E-07 0.28852587E-10-0.68945581E+03 0.26720068E+02                   4
C6H5CH2O   4/14/94 thermC   7H   7O   1    0g   300.000  5000.000 1392.000    1
 1.78843033e+01 2.09011735e-02-7.21832713e-06 1.12839851e-09-6.57955260e-14    2
 4.93182818e+03-7.01304667e+01-4.77736690e+00 7.51049308e-02-5.68532831e-05    3
 2.18290029e-08-3.38134298e-12 1.26234438e+04 5.10429366e+01                   4
C6H5OCH2  1/ 1/80 therm C   7H   7O   1    0g   300.000  5000.000 1402.000    1
 2.21257590e+01 1.63629505e-02-5.55282773e-06 8.58992521e-10-4.97570425e-14    2
 2.27948250e+03-9.52304329e+01-5.69072376e+00 9.13768507e-02-8.35104568e-05    3
 3.76414300e-08-6.64543995e-12 1.07829618e+04 5.03483382e+01                   4
C6H4O2  O=C6H4=O  T10/97C   6H   4O   200  0G   200.000  6000.000 1000.       1
 1.43886174E+01 1.81624210E-02-6.69934678E-06 1.10097880E-09-6.67372266E-14    2
-2.12444054E+04-5.02572901E+01 3.79867882E+00 2.51676569E-02 3.79846917E-05    3
-7.06777516E-08 3.06126573E-11-1.72429606E+04 9.80455363E+00-1.478138819-04    4
C6H5OCH3   1/ 1/80 thermC   7H   8O   1    0g   300.000  5000.000 1393.000    1
 2.07553992e+01 2.02558450e-02-6.93113185e-06 1.07748801e-09-6.26048146e-14    2
-1.87342907e+04-8.82873516e+01-5.18552392e+00 8.57486409e-02-7.07576026e-05    3
 2.95162383e-08-4.92530544e-12-1.03019987e+04 4.91527969e+01                   4
HOC6H4CH3 AVG CRESOL6/87C   7H   8O   1    0G   200.000  6000.000 1000.00     1
 0.15932987E+02 0.27011160E-01-0.99448722E-05 0.16296689E-08-0.98513298E-13    2
-0.23592065E+05-0.59732841E+02 0.42258267E+00 0.45551636E-01 0.32012513E-04    3
-0.81121959E-07 0.37665658E-10-0.18202621E+05 0.26032903E+02-0.15911701E+05    4
C6H5CH2OH  4/14/94 thermC   7H   8O   1    0g   300.000  5000.000 1393.000    1
 1.83336336e+01 2.24113846e-02-7.68817710e-06 1.19642445e-09-6.95416019e-14    2
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-2.13970553e+04-7.22444987e+01-4.04500885e+00 7.57965615e-02-5.64777639e-05    3
 2.15225418e-08-3.32436586e-12-1.37783634e+04 4.74803479e+01                   4
C6H5CH2OO  3/ 4/94 thermC   7H   7O   2    0g   300.000  5000.000 1389.000     1
 2.18946260e+01 2.02701494e-02-7.14525361e-06 1.13208570e-09-6.66220534e-14    2
 3.93272947e+03-8.95685129e+01-3.77863659e+00 8.29484718e-02-6.64288143e-05    3
 2.69504875e-08-4.41844689e-12 1.25603231e+04 4.73269747e+01                   4
C6H5C6H5          L12/84C  12H  10    0    0G   300.000  5000.000              1
 0.24289017E 02 0.34006648E-01-0.11722408E-04 0.17729298E-08-0.96812532E-13    2
 0.10287000E 05-0.10802374E 03-0.40739527E 01 0.86973310E-01-0.42353613E-05    3
-0.64564460E-07 0.34150169E-10 0.19405965E 05 0.44741348E 02 0.21905340E 05    4
BiBenzyl          A 6/83C  14H  14    0    0G   300.     3000.    1000.00      1
  0.7292035E 01  0.9250200E-01 -0.5168641E-04  0.1362709E-07 -0.1381148E-11    2
  0.1031673E 05 -0.1132738E 02 -0.1388958E 02  0.1720984E 00 -0.1700660E-03    3
  0.9601888E-07 -0.2373253E-10  0.1503234E 05  0.9270736E 02  0.1721641E+05    4
```

Sources

[1] R. J. Kee, F. M. Rupley, and J. A. Miller, The CHEMKIN Thermodynamic Data Base. SAND87-8215, Sandia National Laboratories, Livermore, California (1987).

[2] G. P. Smith, D. M. Golden, M. Frenklach, N. W. Moriarty, B., M. Eiteneer, Goldenberg, C. T.,Bowman, R. K. Hanson, S. Song, W. C. Gardiner Jr., V. V. Lissianski, and Z. Qin, GRI-Mech 3.0, http://www.me.berkeley.edu/gri_mech/ (1999).

[3] H. Wang and M. Frenklach, Combust. Flame 110 (1997) 173.

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[5] S. W. Benson, Thermochemical Kinetics. John Wiley and Sons: New York (1976).

[6] T. Carrière, Combustion Modeling of Ethylene/Oxygen and Allene/Oxygen Mixtures: Chemical Oxidation Mechanisms and Numerical Solution of the Non-Adiabatic Flame Equations. Ph.D. Dissertation, University of Massachusetts Amherst (2005).

[7] M. E. Law, Molecular-Beam Mass Spectrometry of Ethylene and Cyclohexane Flames. Ph.D. Dissertation, University of Massachusetts Amherst (2005).

[8] N. Hansen, J. A. Miller, T. Kasper, K. Kohse-Höinghaus, P. R. Westmoreland, J. Wang, T. A. Cool, Proc. Combust. Inst. 32(1) (2009) 623-630.

Transport properties used for flame simulation

```
! Transport parameters in Chemkin TRANFIT format for
! portion of C/H/O reaction set used for cyclohexane model (Nov 1, 2010).
! Contributors:
!    Thierry Carriere, University of Massachusetts Amherst (UMass2002.mech)
!    Matthew E. Law (PhD, 2005).
!    Wenjun Li (PhD in preparation)
!    Phillip R. Westmoreland
!------------------------------Transport data----------------------------------
H                 0   145.000     2.050     0.000     0.000     0.000 !
H2                1    38.000     2.920     0.000     0.790   280.000 !
CH                1    80.000     2.750     0.000     0.000     0.000 !
CH2               1   144.000     3.800     0.000     0.000     0.000 !
CH2SING           1   144.000     3.800     0.000     0.000     0.000 !
CH3               1   144.000     3.800     0.000     0.000     0.000 !
O                 0    80.000     2.750     0.000     0.000     0.000 !
CH4               2   141.400     3.746     0.000     2.600    13.000 !
OH                1    80.000     2.750     0.000     0.000     0.000 !
H2O               2   572.400     2.605     1.844     0.000     4.000 !
C2H               1   209.000     4.100     0.000     0.000     2.500 !
C2H2              1   209.000     4.100     0.000     0.000     2.500 !
H2CC              2   238.000     4.07      0.0       0.0       2.5   !JAM(1/02)
C2H3              2   209.000     4.100     0.000     0.000     1.000 !
CO                1    98.100     3.650     0.000     1.950     1.800 !
C2H4              2   280.800     3.971     0.000     0.000     1.500 !
HCO               2   498.000     3.590     0.000     0.000     0.000 !
C2H5              2   252.300     4.302     0.000     0.000     1.500 !
```

```
CH2O              2   498.000     3.590     0.000     0.000     2.000 !
C2H6              2   252.300     4.302     0.000     0.000     1.500 !
CH3O              2   417.000     3.690     1.700     0.000     2.000 !
CH2OH             2   417.000     3.690     1.700     0.000     2.000 !
CH3OH             2   481.800     3.626     0.000     0.000     1.000 !
O2                1   107.400     3.458     0.000     1.600     3.800 !

HO2               2   107.400     3.458     0.000     0.000     1.000 !
H2O2              2   107.400     3.458     0.000     0.000     3.800 !
C3H2              2   209.000     4.100     0.000     0.000     1.000 !
C3H3              2   252.000     4.760     0.000     0.000     1.000 !(JAM)
AR                0   136.500     3.330     0.000     0.000     0.000 !
AC3H4             2   252.000     4.760     0.000     0.000     1.000 !
PC3H4             2   252.000     4.760     0.000     0.000     1.000 !
HCCO              2   150.000     2.500     0.000     0.000     1.000 !
AC3H5             2   260.000     4.850     0.000     0.000     1.000 !(JAM)
TC3H5             2   260.000     4.850     0.000     0.000     1.000 !(JAM)
SC3H5             2   260.000     4.850     0.000     0.000     1.000 !(JAM)
CH2CO             2   436.000     3.970     0.000     0.000     2.000 !
C3H6              2   266.800     4.982     0.000     0.000     1.000 !
CH3CO             2   436.000     3.970     0.000     0.000     2.000 !
CH2CHO            2   436.000     3.970     0.000     0.000     2.000 !estimated
nC3H7             2   266.800     4.982     0.000     0.000     1.000 !
iC3H7             2   266.800     4.982     0.000     0.000     1.000 !
C2H4O             2   436.000     3.970     0.000     0.000     2.000 !estimated
CH3CHO            2   436.000     3.970     0.000     0.000     2.000 !
C3H8              2   266.800     4.982     0.000     0.000     1.000 !
CO2               1   244.000     3.763     0.000     2.650     2.100 !
C2H5O             2   436.000     3.970     0.000     0.000     2.000 !estimated
C4H2              1   357.000     5.180     0.000     0.000     1.000 !
nC4H3             2   357.000     5.180     0.000     0.000     1.000 !est
iC4H3             2   357.000     5.180     0.000     0.000     1.000 !Wang
C4H4              2   357.000     5.180     0.000     0.000     1.000 !(JAM)
n-C4H5            2   357.000     5.180     0.000     0.000     1.000 !AB/97

i-C4H5            2   357.000     5.180     0.000     0.000     1.000 !AB/97
iiC4H6            2   357.000     5.176     0.000     0.000     1.000
iiiC4H6           2   357.000     5.176     0.000     0.000     1.000
```

```
C2H3CO          2   429.000     4.999     2.9       0.        1.    !est
C4H7            2   357.000     5.176     0.000     0.000     1.000
C2H3CHO         2   429.000     4.999     2.9       0.        1.    !PRW2/93
IC4H8           2   357.000     5.176     0.000     0.000     1.000
C2H3CH2O        2   429.000     4.999     2.9       0.        1.    !PRW5/93
nC4H9           2   357.000     5.176     0.000     0.000     1.000 !
C2H3OO          2   556.000     4.610     0.000     0.000     0.000 !est.
C2H5OO          2   576.7       4.549     0.000     0.000     1.000 !est.
C5H5            1   357.000     5.180     0.000     0.000     1.000 !same as C5H3
C5H6            2   354.700     5.13      0.000     0.000     1.000 !ab
C6H2            1   357.000     5.180     0.000     0.000     1.000 !
C6H3            2   412.300     5.349     0.000     0.000     1.000 !ab/97
l-C6H4          2   367.700     5.36      0.000     0.000     1.000 !ab/97
c-C6H4          2   367.700     5.36      0.000     0.000     1.000 !ab/97
n-C6H5          2   412.300     5.349     0.000     0.000     1.000 !ab/97
i-C6H5          2   412.300     5.349     0.000     0.000     1.000 !ab/97
A1              2   412.300     5.349     0.000     0.000     1.000 !ab/97
A               2   412.300     5.349     0.000     0.000     1.000 !ab/97
FC6H6           2   412.300     5.349     0.000     0.000     1.000 !ab/97
l-C6H6          2   412.300     5.349     0.000     0.000     1.000 !ab/97
C4H5C2H         2   412.3       5.349     0.00      0.00      1.00  !JAM(12/02)
CYC6H7          2   412.300     5.349     0.000     0.000     1.000 !est fm benzene
n-C6H7          2   412.300     5.349     0.000     0.000     1.000 !ab/97
i-C6H7          2   412.300     5.349     0.000     0.000     1.000 !ab/97
C5H4O           2   450.000     5.500     0.000     0.000     1.000 !    !
CY13C6H8        2   412.300     5.349     0.000     0.000     1.000 !est fm benzene
C6H8            2   412.300     5.349     0.000     0.000     1.000 !ab/97
C5H5O           2   450.000     5.500     0.000     0.000     1.000 !
C6H9            2   324.        6.093     0.000     0.000     1.000 !ab/97
CYC6H9          2   324.        6.093     0.000     0.000     1.000 !BSL60
C5H4OH          2   450.000     5.500     0.000     0.000     1.000 !
CYC6H10         2   324.        6.093     0.000     0.000     1.000 !BSL60
C6H10           2   399.3       5.949     0.000     0.000     1.000 !est
CYC6H11         2   324.        6.093     0.000     0.000     1.000 !BSL60
C6H11-12        2   399.3       5.949     0.000     0.000     1.000 !est fm C6H10
C6H11-13        2   399.3       5.949     0.000     0.000     1.000 !est fm C6H10
C6H11-14        2   399.3       5.949     0.000     0.000     1.000 !est fm C6H10
C6H11-15        2   399.3       5.949     0.000     0.000     1.000 !est fm C6H10
```

```
C6H11            2   399.3       5.949     0.000     0.000     1.000 !est fm C6H10
CYC6H12          2   324.        6.093     0.000     0.000     1.000 !BSL60
hexene1          2   413.        5.909     0.000     0.000     1.000 !BSL60 nC6H14
hex1yl           2   413.        5.909     0.000     0.000     1.000 !BSL60 nC6H14
hex2yl           2   413.        5.909     0.000     0.000     1.000 !BSL60 nC6H14
hex3yl           2   413.        5.909     0.000     0.000     1.000 !BSL60 nC6H14
C6H4CH3          2   495.300     5.680     0.000     0.000     1.000 !NMM
C6H5CH2          2   495.300     5.680     0.000     0.000     1.000 !NMM
C6H5CH3          2   495.300     5.680     0.430     12.30     1.000 !NMM
C6H5O            2   450.000     5.500     0.000     0.000     1.000 !(JAM)
C6H5OH           2   450.000     5.500     0.000     0.000     1.000 !
C6H4CCH          2   534.300     5.710     0.000     0.000     1.000 !NMM
C6H5CCH          2   534.300     5.710     0.770     0.000     1.000 !NMM
C6H5CHCH         2   546.200     6.000     0.000     0.000     1.000 !NMM
C6H5CHCH2        2   546.200     6.000     0.130     15.00     1.000 !NMM
C6H5CO           2   622.400     5.530     0.000     0.000     1.000 !NMM
C6H5CH2CH2       2   523.600     5.960     0.000     0.000     1.000 !Est by W Li
C6H5CHO          2   622.400     5.530     0.000     0.000     1.000 !NMM
C6H5CH2CH3       2   523.600     5.960     0.000     0.000     1.000 !NMM
OC6H4CH3         2   621.100     5.640     0.000     0.000     1.000 !NMM
C6H5CH2O         2   622.400     5.530     0.000     0.000     1.000 !NMM
C6H5OCH2         2   495.300     5.680     0.430     12.30     1.000 !Est
C6H4O2           2   621.100     5.640     0.000     0.000     1.000 !Est by W Li
C6H5OCH3         2   495.300     5.680     0.430     12.30     1.000 !Est
HOC6H4CH3        2   621.100     5.640     0.000     0.000     1.000 !NMM
C6H5CH2OH        2   622.400     5.530     0.000     0.000     1.000 !Est
C6H5CH2OO        2   622.400     5.530     0.000     0.000     1.000 !Est
C6H5C6H5         2   676.5       6.31      0.00     20.00      1.000 !
BiBenzyl         2   783.800     6.640     0.000     0.000     1.000 !NMM
```


General references for these transport data

[1] R. J. Kee, G. Dixon-Lewis, J. Warnatz,, M. E. Coltrin, J. A. Miller. The Chemkin-II Transport Database. Sandia Report #SAND 86-8246 (1986).

[2] G. P. Smith, D. M. Golden, M. Frenklach, N. W. Moriarty, B. Eiteneer, M. Goldenberg, C. T. Bowman, R. K. Hanson, S. Song, W. C. Gardiner Jr., V. V. Lissianski, Z. Qin, GRI-Mech 3.0, http://www.me.berkeley.edu/gri_mech/ (1999).

[3] H. Wang, M. Frenklach, Combust. Flame 110 (1997) 173.

[4] H. Wang, X.You, A. V. Joshi, S. G. Davis, A. Laskin, F. Egolfopoulos, C. K. Law, USC Mech Version II. High-Temperature Combustion Reaction Model of H2/CO/C1-C4 Compounds. http://ignis.usc.edu/USC_Mech_II.htm, May (2007).

[5] Properties for many species without transport data available were estimated by analogy with similar molecules.

CHEMKIN PREMIX INPUT FILE

```
/   BURNER STABILIZED, TEMP SPECIFIED
/  THIS KEYWORD FILE IS TO MODEL THE STOICHIOMETRIC ACETYLENE FLAME, T down by 100K
BURN
/WDIF
TGIV
/ENRG
/ASEN
RSTR
TDIF
MULT
CURV 0.50
GRAD 0.20
CDIF
MOLE
/   initial flowrate
FLRT   0.00191   (g/cm**2-s)
/  14 TORR
PRES  0.01842  (ATMOSPHERE)
/   initial grid and profile specification
NPTS      19
GRID  0.0
GRID  0.1
```

```
GRID  0.2
GRID  0.3
GRID  0.4
GRID  0.5
GRID  0.6
GRID  0.7
GRID  0.8
GRID  0.9
GRID  1.0
GRID  1.25
GRID  1.5
GRID  1.75
GRID  2.0
GRID  2.5
GRID  3.0
GRID  5.0
GRID  8.0
XEND    8.0 (cm)
XCEN    0.7 (cm)
WMIX      1  (cm)
/   unreacted fuel-oxidizer makeup (phi=2.0)
MOLE
REAC   C2H2    0.1120
REAC   O2      0.2924
REAC   AR      0.5956
/   estimated products mole fraction
PROD   H2O   0.18
PROD   CO2   0.033
PROD   CO    0.42
PROD   AR    0.23
PROD   H2    0.14
/   estimated intermediate mole fractions
INTM   H   0.002
INTM   CH3   0.001
INTM   CH4   0.0015
INTM   OH    0.001
INTM   C2H4  0.006
INTM   CH2O  0.01
```

```
INTM   C3H3     0.002
INTM   AC3H4     0.0003
INTM   PC3H4     0.0005
INTM   C3H6   0.0008
INTM   CH2CO   0.0008
INTM   C4H2   0.005
INTM   C4H4   0.0003
INTM   C6H2   0.0025
INTM   A   0.0001
/   tolerances for the Newton iteration
ATOL  1.0E-9
RTOL  1.0E-6
/   tolerances for the time step Newton iteration
ATIM  1.0E-9
RTIM  1.0E-6
/   print control print 1 is short, print 2 is long
PRNT 2
/   time step control
TIME  100  1.E-6   (s)
/      given temperature profile
TEMP    0       414
TEMP    0.025   506.368
TEMP    0.05    581.716
TEMP    0.075   646.3
TEMP    0.1     705.824
TEMP    0.125   766.452
TEMP    0.15    833.52
TEMP    0.175   907.488
TEMP    0.2     984.124
TEMP    0.225   1060.852
TEMP    0.25    1136.016
TEMP    0.275   1210.536
TEMP    0.3     1272.084
TEMP    0.325   1323.788
TEMP    0.35    1365.832
TEMP    0.375   1404.196
TEMP    0.4     1445.412
TEMP    0.425   1483.224
```

TEMP	0.45	1523.152
TEMP	0.475	1561.976
TEMP	0.5	1596.568
TEMP	0.525	1623.984
TEMP	0.55	1649.836
TEMP	0.575	1673.296
TEMP	0.6	1695.744
TEMP	0.625	1719.02
TEMP	0.65	1740.64
TEMP	0.675	1762.26
TEMP	0.7	1784.432
TEMP	0.725	1806.236
TEMP	0.75	1827.396
TEMP	0.775	1848.004
TEMP	0.8	1867.692
TEMP	0.825	1886.184
TEMP	0.85	1903.756
TEMP	0.875	1920.868
TEMP	0.9	1937.428
TEMP	0.925	1953.068
TEMP	0.95	1967.604
TEMP	0.975	1981.312
TEMP	1	1994.284
TEMP	1.025	2006.244
TEMP	1.05	2017.284
TEMP	1.075	2027.128
TEMP	1.1	2035.868
TEMP	1.125	2043.596
TEMP	1.15	2050.312
TEMP	1.175	2056.2
TEMP	1.2	2061.26
TEMP	1.225	2065.584
TEMP	1.25	2069.172
TEMP	1.275	2072.116
TEMP	1.3	2074.6
TEMP	1.325	2076.532
TEMP	1.35	2078.096
TEMP	1.375	2079.384

TEMP	1.4	2080.396
TEMP	1.425	2081.132
TEMP	1.45	2081.684
TEMP	1.475	2082.052
TEMP	1.5	2082.144
TEMP	1.525	2082.052
TEMP	1.55	2081.776
TEMP	1.575	2081.316
TEMP	1.6	2080.672
TEMP	1.625	2079.936
TEMP	1.65	2079.108
TEMP	1.675	2078.188
TEMP	1.7	2077.176
TEMP	1.725	2076.164
TEMP	1.75	2075.06
TEMP	1.775	2073.772
TEMP	1.8	2072.484
TEMP	1.825	2071.012
TEMP	1.85	2069.54
TEMP	1.875	2067.884
TEMP	1.9	2066.228
TEMP	1.925	2064.572
TEMP	1.95	2062.732
TEMP	1.975	2060.8
TEMP	2	2058.776
TEMP	2.025	2056.66
TEMP	2.05	2054.544
TEMP	2.075	2052.428
TEMP	2.1	2050.312
TEMP	2.125	2048.196
TEMP	2.15	2045.988
TEMP	2.175	2043.78
TEMP	2.2	2041.572
TEMP	2.225	2039.18
TEMP	2.25	2036.788
TEMP	2.275	2034.212
TEMP	2.3	2031.544
TEMP	2.325	2028.692

TEMP	2.35	2025.748
TEMP	2.375	2022.804
TEMP	2.4	2019.676
TEMP	2.425	2016.548
TEMP	2.45	2013.42
TEMP	2.475	2010.292
TEMP	2.5	2007.164
TEMP	2.525	2004.128
TEMP	2.55	2001
TEMP	2.575	1997.964
TEMP	2.6	1994.836
TEMP	2.625	1991.708
TEMP	2.65	1988.58
TEMP	2.675	1985.452
TEMP	2.7	1982.324
TEMP	2.725	1979.104
TEMP	2.75	1975.976
TEMP	2.775	1972.756
TEMP	2.8	1969.628
TEMP	2.825	1966.408
TEMP	2.85	1963.096
TEMP	2.875	1959.692
TEMP	2.9	1956.288
TEMP	2.925	1952.7
TEMP	2.95	1949.02
TEMP	2.975	1945.34
TEMP	3	1941.66
TEMP	3.025	1937.888
TEMP	3.05	1934.208
TEMP	3.075	1930.528
TEMP	3.1	1926.848
TEMP	3.125	1923.26
TEMP	3.15	1919.764
TEMP	3.175	1916.176
TEMP	3.2	1912.588
TEMP	3.225	1909.092
TEMP	3.25	1905.596
TEMP	3.275	1902.008

```
TEMP    3.3     1898.512
TEMP    3.325   1894.924
TEMP    3.35    1891.428
TEMP    3.375   1887.84
TEMP    3.4     1884.344
TEMP    3.425   1880.756
TEMP    3.45    1877.26
TEMP    3.475   1873.672
TEMP    3.5     1870.176
TEMP    3.525   1866.588
TEMP    3.55    1863.092
TEMP    3.575   1859.504
TEMP    3.6     1855.916
TEMP    3.625   1852.42
TEMP    3.65    1848.832
TEMP    3.675   1845.336
TEMP    3.7     1841.84
TEMP    3.725   1838.436
TEMP    3.75    1835.032
TEMP    3.775   1831.628
TEMP    3.8     1828.224
TEMP    3.825   1824.912
TEMP    3.85    1821.6
TEMP    3.875   1818.288
TEMP    3.9     1814.884
TEMP    3.925   1811.572
TEMP    3.95    1808.26
TEMP    3.975   1804.856
TEMP    4       1801.544
TEMP    8       1800.00
END
```

Appendix J.

MATLAB Code of Active Subspace Discovery

```
function Qfulldim = calculate_SM_ASD(response, gradient, designFullDim,
dim_AS)
%CALCULATE_SM_ASD calculates the surrogate model by Active Subspace
%Discovery.
%INPUT:
%response      - a struct of the responses from the flame simulations
%gradient      - a n_target dimensional cell array of gradient matrices %
for the candidate active parameters.
%designFullDim - the design matrix of active parameter candidate space.
%dim_AS        - the specified dimension of the active subspace.
%
%Written by:  Devin Yeates, UC Berkeley, 29 June 2010

n_targets = length(response(1).feature);
n_runs = length(response);

for ii = 1:n_targets
    %  Calculate the active subspace for for each feature
    [~,s,v] = svd(gradient{ii});

    S{ii} = v(:,1:dim_AS);  %linear transformation of active parameters to
active subspace dimension

    %Calculate the log10 transformation of the responses
    for jj = 1:n_runs
        y(jj) = log10(response(jj).feature(ii).value);
    end

    %make surrogate model fit in low-dim
    Qlowdim = qfit(designFullDim*S{ii},y');  %quadratic fitting function,
just does least squares

    %convert to full dim
    %y_fit = [1 z'*S]*Qlowdim*[1;S'z], so...
    Qfulldim{ii} = blkdiag(1,S{ii})*Qlowdim*blkdiag(1,S{ii}');
end

function Q = qfit(x,y)
%Q = qfit(x,y)
%  x is m-by-n
%  y is m-by-1
%  Q is n+1-by-n+1

if ~isvector(y)
    error('y should be a vector')
end
m = length(y);
```

```
if size(x,1)==m
    n = size(x,2);
elseif size(x,2)==m
    n=size(x,1);
    x=x';
else
    error('Input dimension mismatch')
end

A = zeros(m,(n+1)*(n+2)/2);
for i=1:m
    tmp = x(i,:)'*x(i,:);
    A(i,1:n+1) = [1 x(i,:)];
    idx = n+2;
    for j=1:n
        A(i,idx:idx+n-j) = tmp(j,j:n);
        idx = idx+n-j+1;
    end
end
q = A\y;

Q = zeros(n+1);
Q(:,1) = q(1:n+1,1);
idx = n+2;
for i=1:n
    Q(i+1:n+1,i+1) = q(idx:idx+n-i,1);
    idx = idx+n-i+1;
end
Q = 0.5*(Q+Q');
```

Appendix K.

Singular Value Plots and Fitting Errors for Surrogate Models of Targets and Prediction Features.

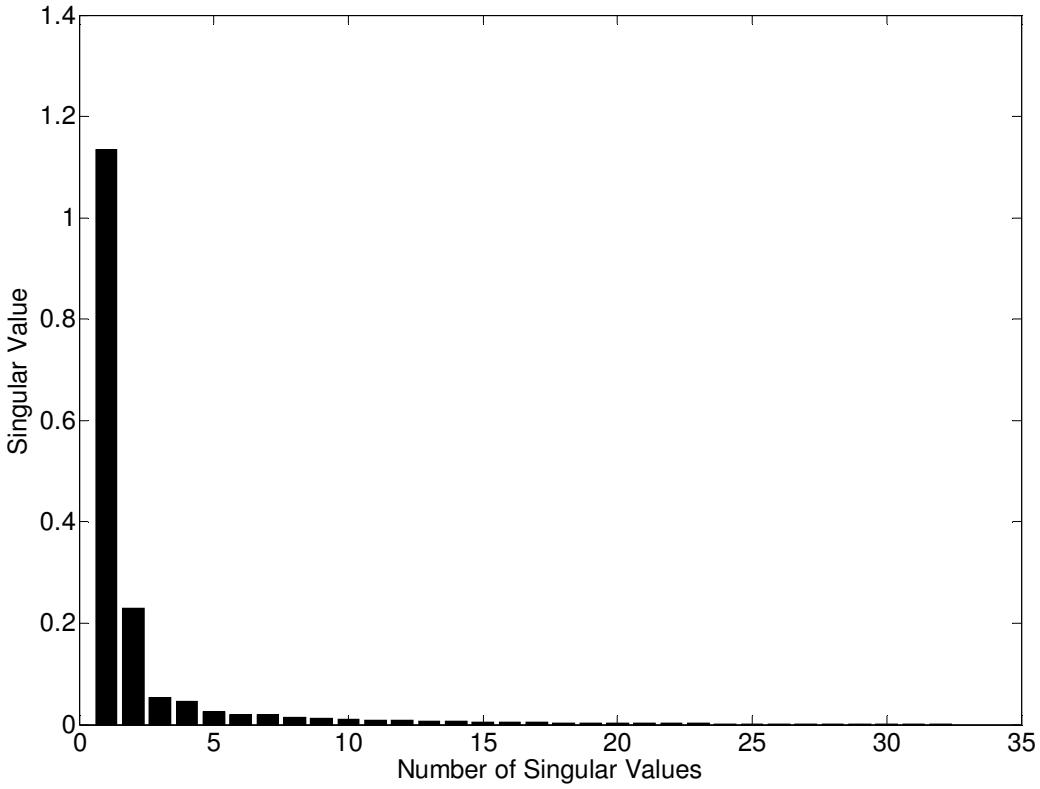

Figure K.10. Singular value plot of H2.PL target.

Table K.1. The relative average and maximum fitting errors in percentage of the surrogate model for H2.PL with increasing active subspace dimension.

Subspace Dimension	In-sample errors (%)		Out-of-sample errors (%)	
	Average	Maximum	Average	Maximum
1	4.42	17.37	3.66	11.87
2	1.69	4.96	1.85	7.01
3	1.43	3.45	1.55	9.23
4	0.92	2.29	1.23	3.87
5	0.64	1.66	1.99	7.10
6	0.17	0.66	4.71	17.78

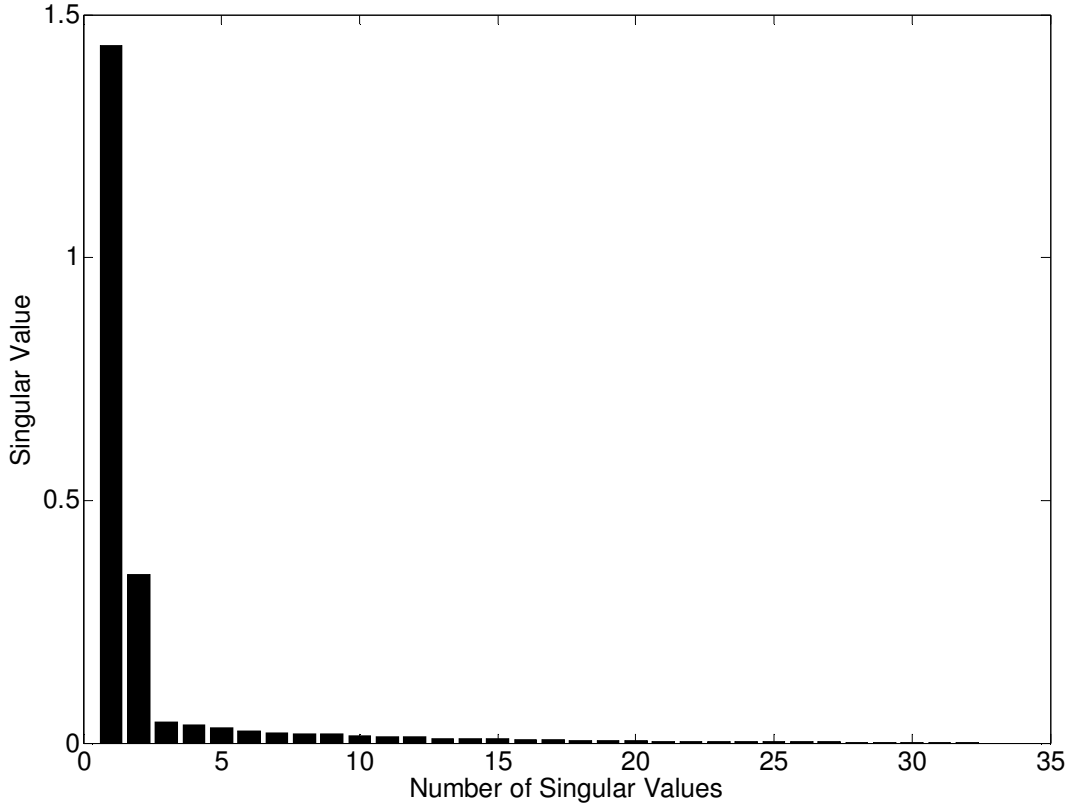

Figure K.11. Singular value plot of H2.PV target.

Table K.2. The relative average and maximum fitting errors in percentage of the surrogate model for H2.PV with increasing active subspace dimension.

Subspace Dimension	In-sample errors (%)		Out-of-sample errors (%)	
	Average	Maximum	Average	Maximum
1	6.03	20.89	5.78	18.31
2	1.24	4.25	1.46	4.57
3	0.98	2.73	1.08	3.88
4	0.60	2.02	0.99	3.39
5	0.44	1.47	1.13	3.75
6	0.10	0.42	1.40	4.92

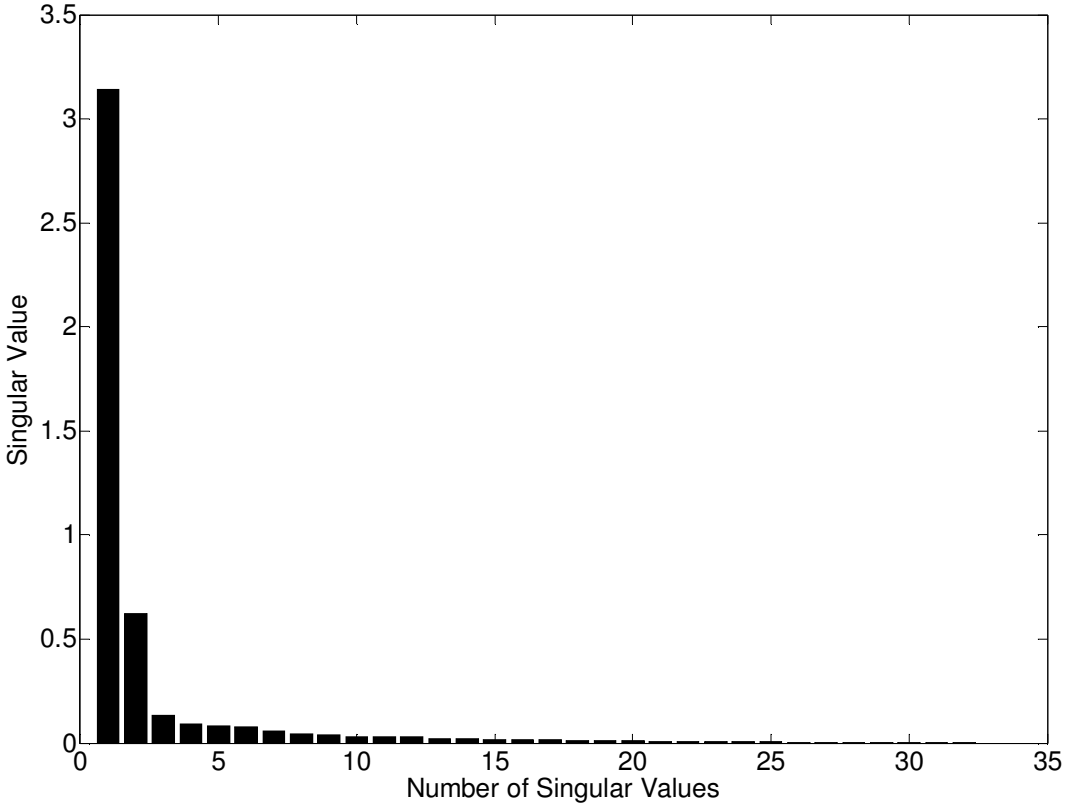

Figure K.12. Singular value plot of CH4.PL target.

Table K.3. The relative average and maximum fitting errors in percentage of the surrogate model for CH4.PL with increasing active subspace dimension.

Subspace Dimension	In-sample errors (%)		Out-of-sample errors (%)	
	Average	Maximum	Average	Maximum
1	11.90	43.04	14.81	191.21
2	4.47	16.20	4.14	39.40
3	3.10	7.14	4.25	26.01
4	2.73	6.40	4.59	15.17
5	1.63	4.82	7.88	16.22
6	1.14	5.37	7.05	54.56

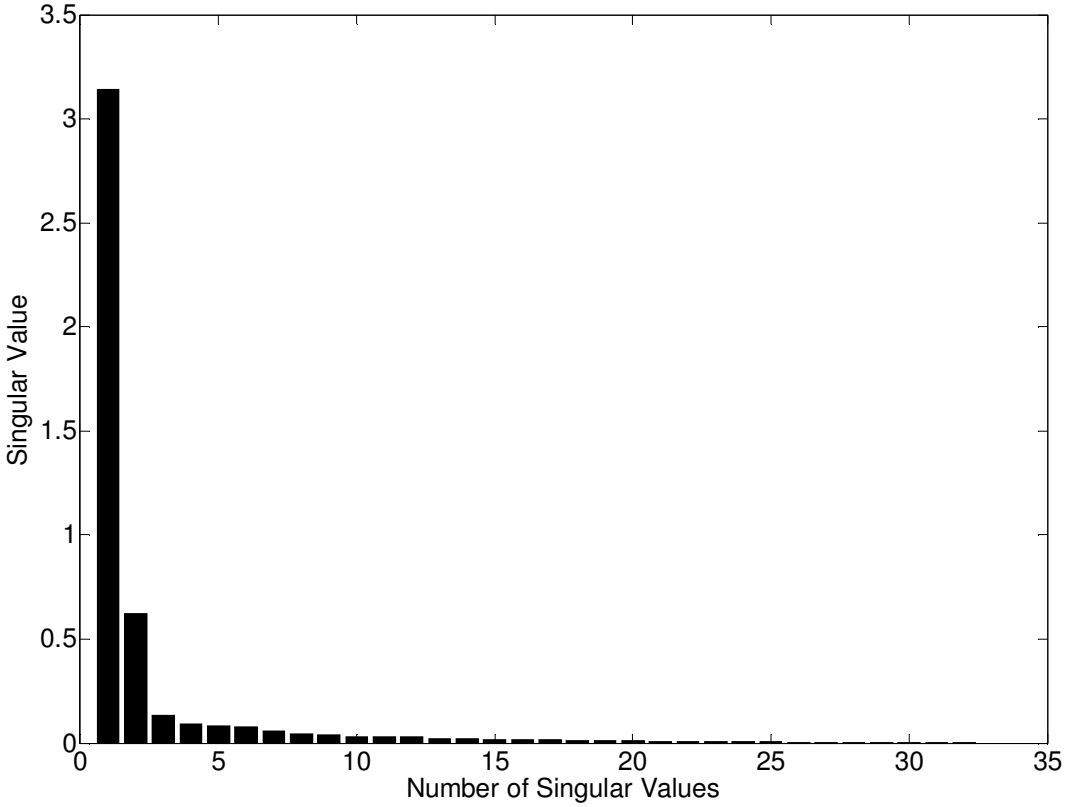

Figure K.13. Singular value plot of CH4.PV target.

Table K.4. The relative average and maximum fitting errors in percentage of the surrogate model for CH4.PV with increasing active subspace dimension.

Subspace Dimension	In-sample errors (%)		Out-of-sample errors (%)	
	Average	Maximum	Average	Maximum
1	28.44	83.51	33.90	191.21
2	4.38	14.18	10.40	39.40
3	3.01	11.99	7.10	26.01
4	2.50	12.79	5.32	15.17
5	1.86	10.93	6.02	16.22
6	1.54	8.70	11.56	54.56

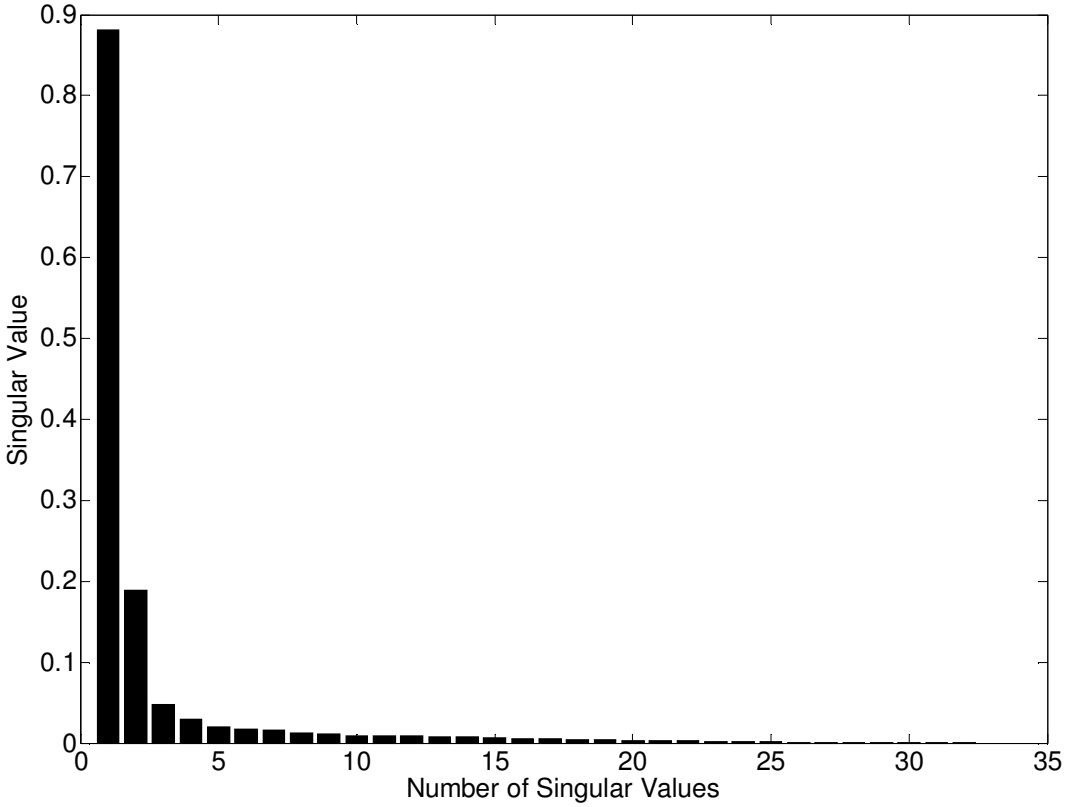

Figure K.14. Singular value plot of C2H2.HL target.

Table K.5. The relative average and maximum fitting errors in percentage of the surrogate model for C2H2.HL with increasing active subspace dimension.

Subspace Dimension	In-sample errors (%)		Out-of-sample errors (%)	
	Average	Maximum	Average	Maximum
1	3.67	11.77	3.70	12.03
2	0.70	2.40	1.00	3.37
3	0.54	2.05	0.81	2.50
4	0.44	1.68	0.68	2.30
5	0.22	0.86	0.88	2.19
6	0.13	0.46	0.99	2.19

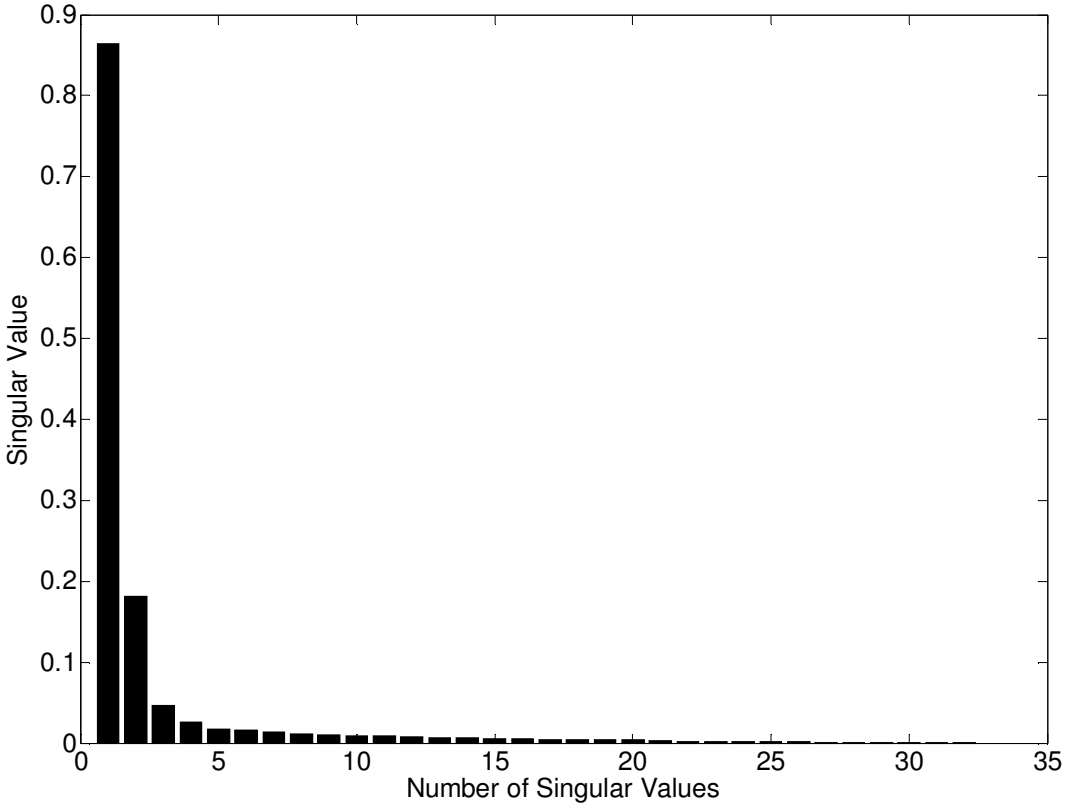

Figure K.15. Singular value plot of CO.PL target.

Table K.6. The relative average and maximum fitting errors in percentage of the surrogate model for CO.PL with increasing active subspace dimension.

Subspace Dimension	In-sample errors (%)		Out-of-sample errors (%)	
	Average	Maximum	Average	Maximum
1	3.62	10.36	3.46	12.21
2	0.69	1.82	0.87	3.40
3	0.44	1.40	0.62	2.08
4	0.40	1.26	0.60	2.29
5	0.26	1.16	0.88	3.36
6	0.13	0.32	0.75	2.09

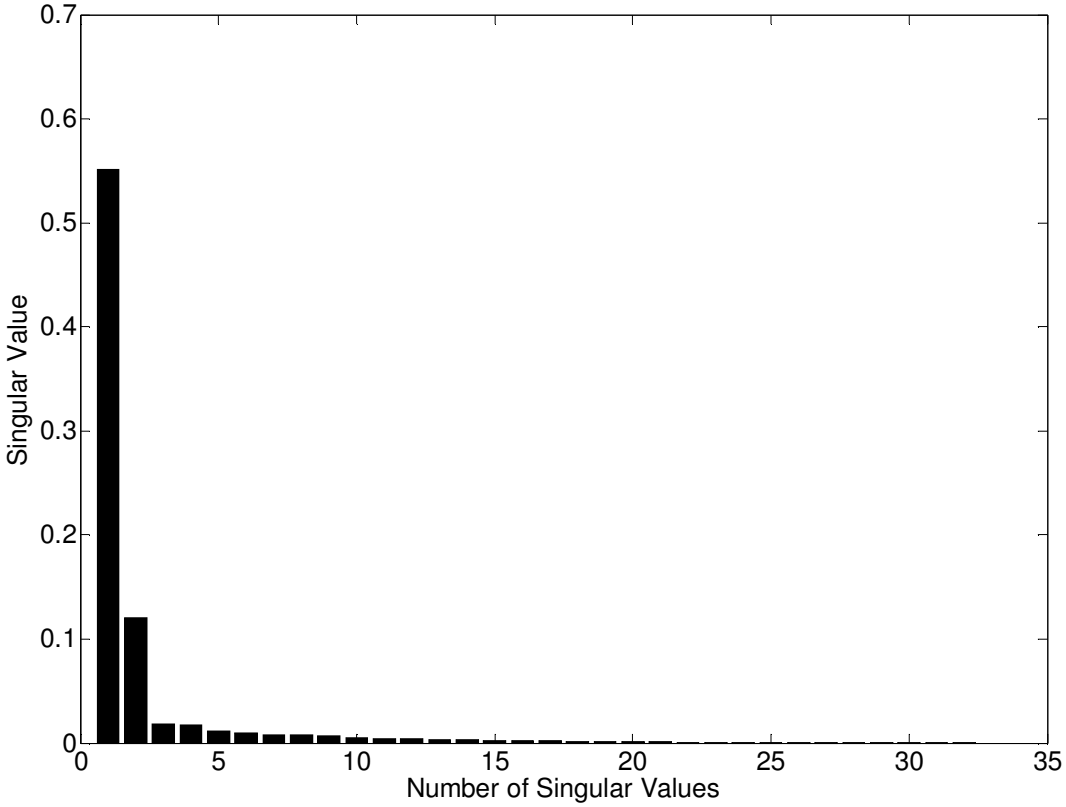

Figure K.16. Singular value plot of CO.PV target.

Table K.7. The relative average and maximum fitting errors in percentage of the surrogate model for CO.PV with increasing active subspace dimension.

Subspace Dimension	In-sample errors (%)		Out-of-sample errors (%)	
	Average	Maximum	Average	Maximum
1	2.32	4.97	1.96	5.30
2	0.36	1.17	0.41	1.38
3	0.29	0.74	0.48	1.28
4	0.18	0.46	0.42	1.11
5	0.14	0.47	0.58	1.61
6	0.07	0.26	0.60	2.57

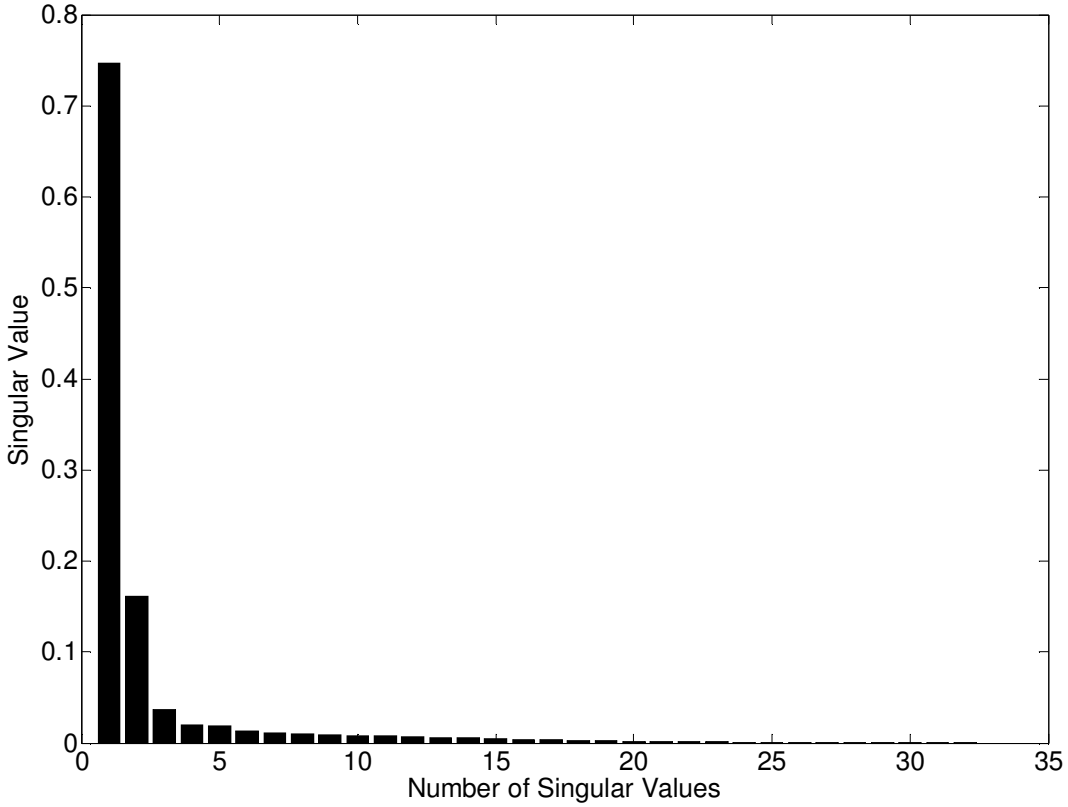

Figure K.17. Singular value plot of O2.HL target.

Table K.8. The relative average and maximum fitting errors in percentage of the surrogate model for O2.HL with increasing active subspace dimension.

Subspace Dimension	In-sample errors (%)		Out-of-sample errors (%)	
	Average	Maximum	Average	Maximum
1	2.96	11.28	2.63	7.04
2	0.52	1.77	0.74	2.23
3	0.48	1.40	0.69	2.68
4	0.39	1.26	0.79	2.20
5	0.17	0.58	0.57	1.45
6	0.04	0.16	0.93	2.43

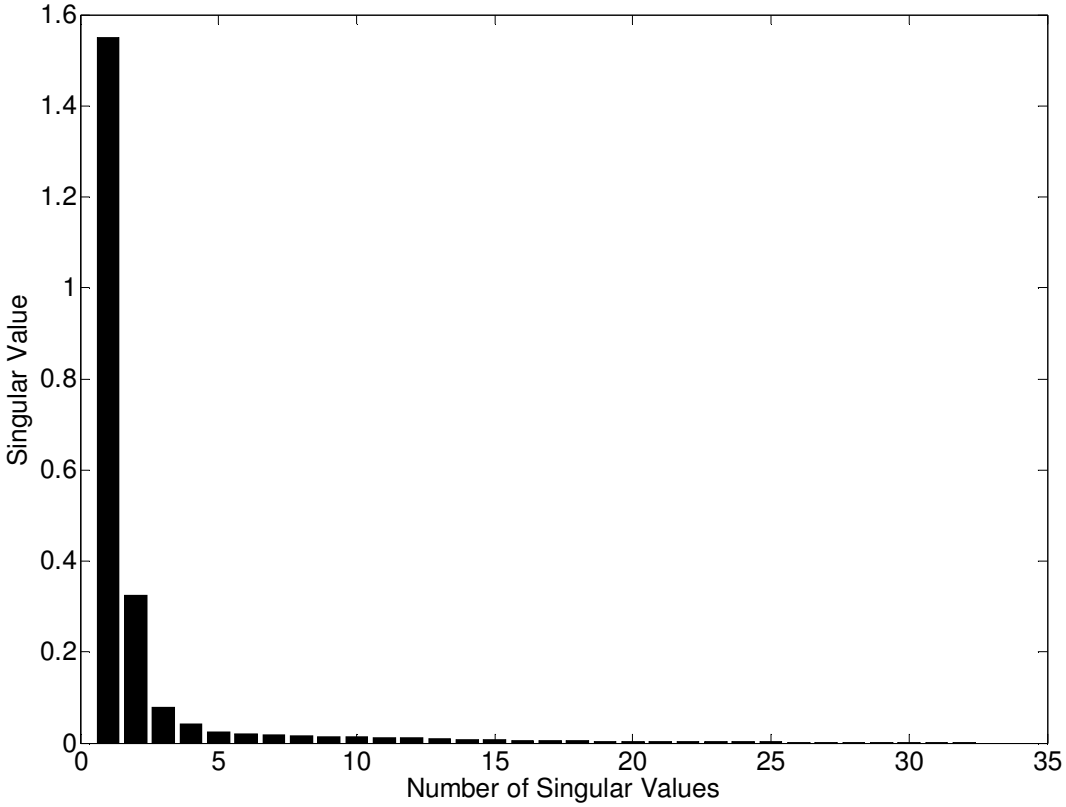

Figure K.18. Singular value plot of CO2.HL target.

Table K.9. The relative average and maximum fitting errors in percentage of the surrogate model for CO2.HL with increasing active subspace dimension.

Subspace Dimension	In-sample errors (%)		Out-of-sample errors (%)	
	Average	Maximum	Average	Maximum
1	5.72	20.01	7.03	22.44
2	1.03	2.34	1.09	2.93
3	0.72	2.09	1.00	4.09
4	0.46	1.07	1.02	3.84
5	0.37	1.16	1.68	6.33
6	0.10	0.33	2.13	12.53

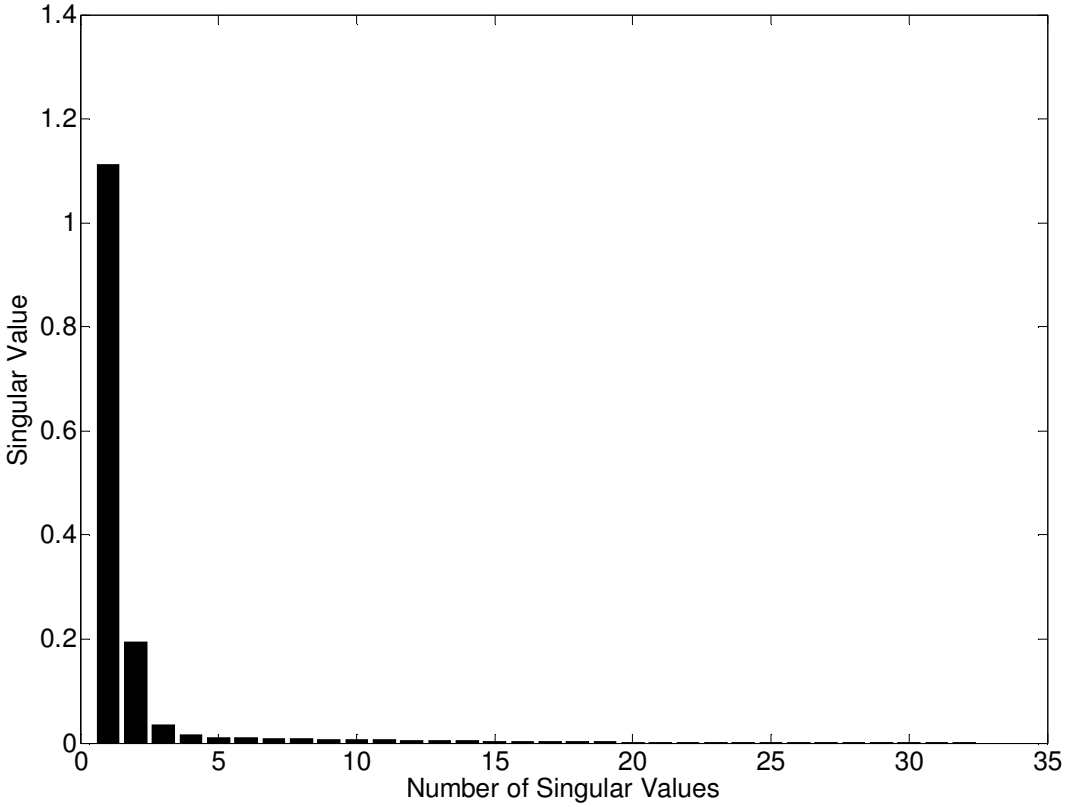

Figure K.19. Singular value plot of H2O.T1 target.

Table K.10. The relative average and maximum fitting errors in percentage of the surrogate model for H2O.T1 with increasing active subspace dimension.

Subspace Dimension	In-sample errors (%)		Out-of-sample errors (%)	
	Average	Maximum	Average	Maximum
1	3.21	11.67	2.59	8.36
2	0.67	1.82	0.50	1.09
3	0.39	1.38	0.40	1.18
4	0.23	0.71	0.52	1.67
5	0.17	0.50	0.77	2.28
6	0.10	0.28	0.71	2.20

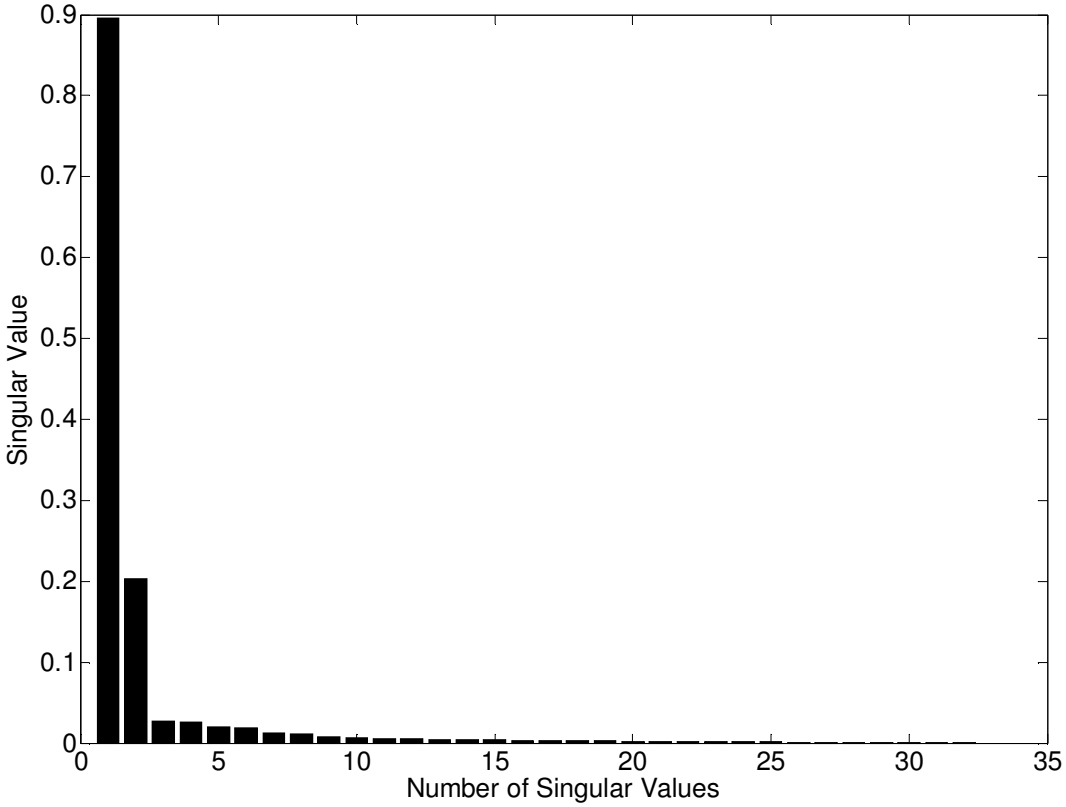

Figure K.20. Singular value plot of H2O.S0 target.

Table K.11. The relative average and maximum fitting errors in percentage of the surrogate model for H2O.S0 with increasing active subspace dimension.

Subspace Dimension	In-sample errors (%)		Out-of-sample errors (%)	
	Average	Maximum	Average	Maximum
1	3.87	11.00	3.11	8.56
2	0.88	2.05	1.19	3.40
3	0.73	1.88	1.37	3.74
4	0.44	1.46	0.92	2.77
5	0.24	0.63	1.03	3.44
6	0.13	0.31	0.92	2.65

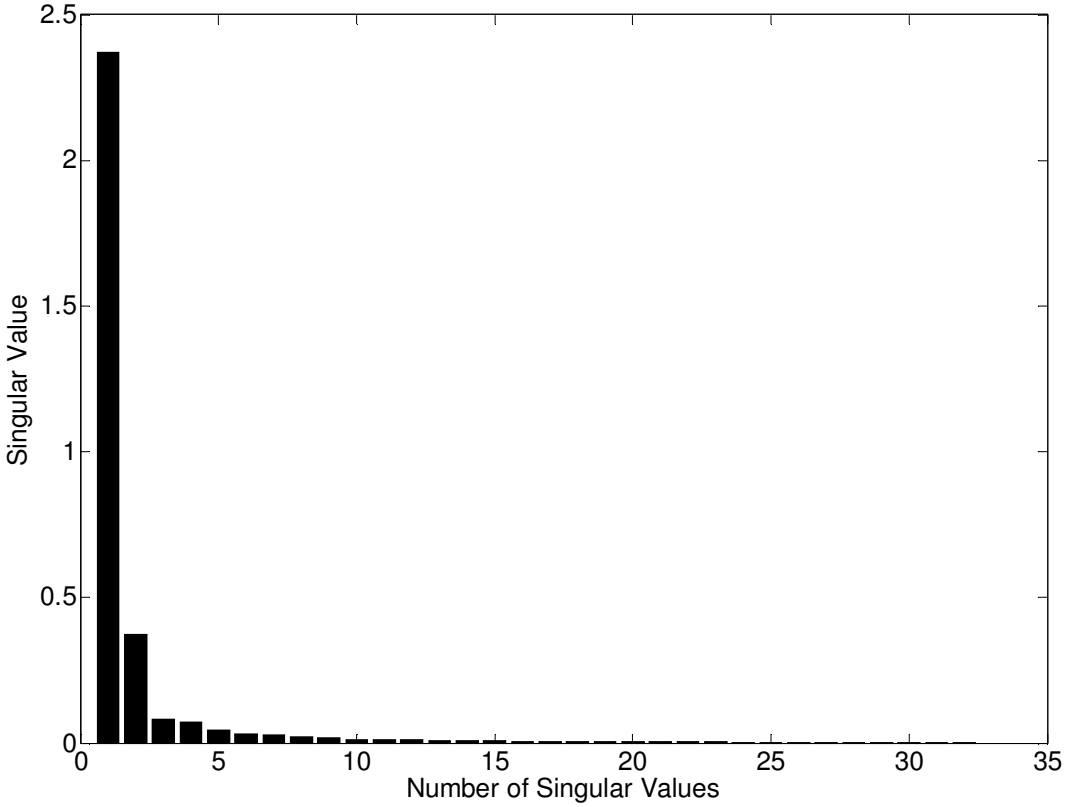

Figure K.21. Singular value plot of H.HL target.

Table K.12. The relative average and maximum fitting errors in percentage of the surrogate model for H.HL with increasing active subspace dimension.

Subspace Dimension	In-sample errors (%)		Out-of-sample errors (%)	
	Average	Maximum	Average	Maximum
1	9.18	28.35	10.67	29.70
2	1.73	4.71	2.32	5.92
3	1.39	3.61	1.91	6.99
4	0.96	2.73	1.63	5.10
5	0.70	1.90	1.71	4.76
6	0.36	1.02	3.71	8.10

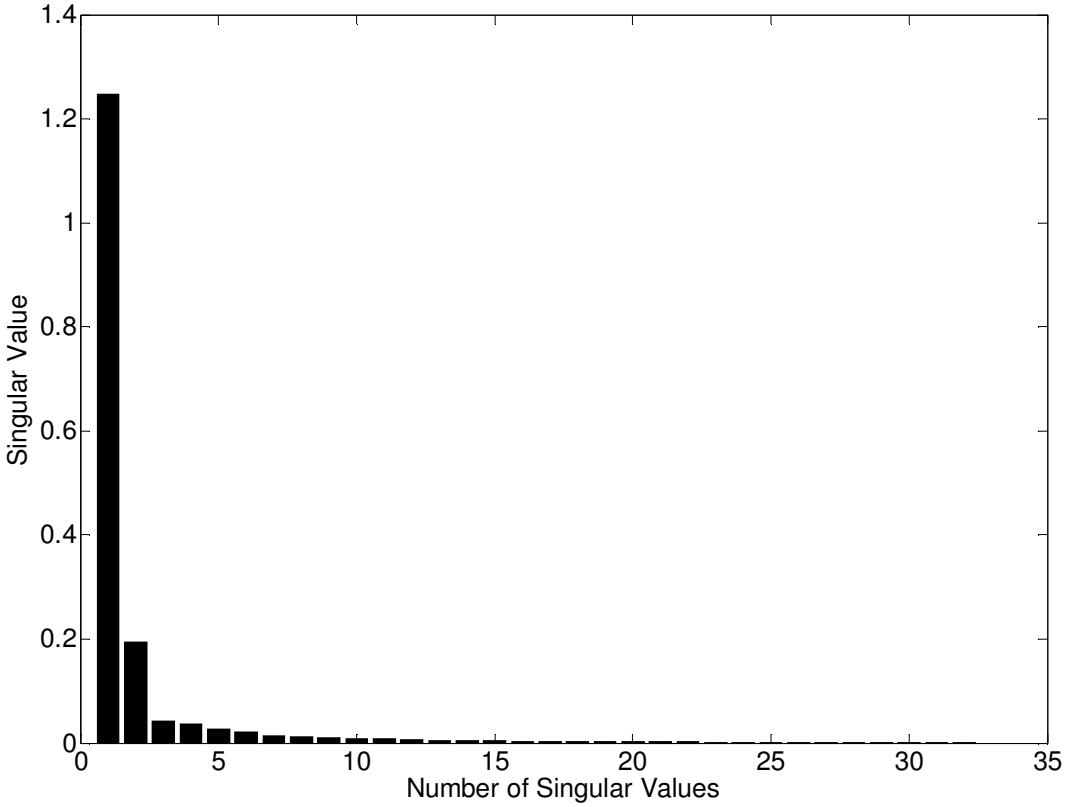

Figure K.22. Singular value plot for prediction of O.PV.

Table K.13. The relative average and maximum fitting errors in percentage of the surrogate model for O.PV with increasing active subspace dimension.

Subspace Dimension	In-sample errors (%)		Out-of-sample errors (%)	
	Average	Maximum	Average	Maximum
1	5.21	11.64	6.70	17.64
2	0.89	2.82	1.15	2.74
3	0.66	2.23	1.18	4.05
4	0.46	1.29	0.88	3.89
5	0.27	0.71	1.01	2.69
6	0.08	0.22	0.96	4.58

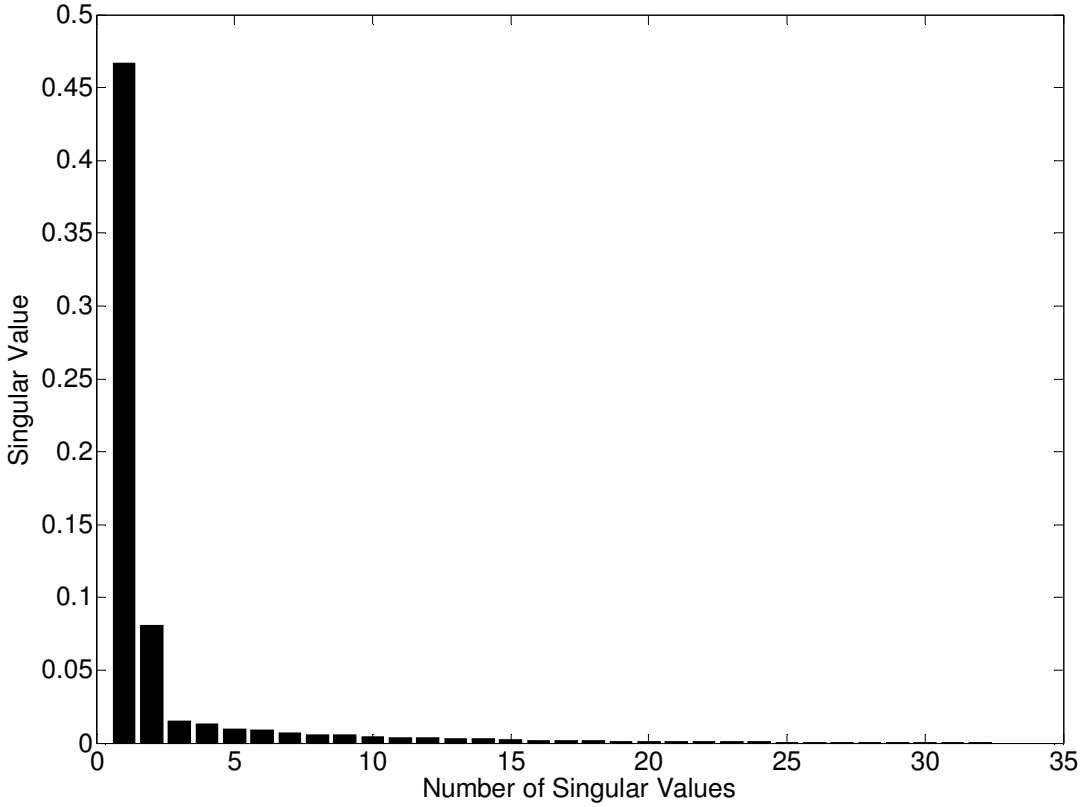

Figure K.23. Singular value plot for prediction of O.PL.

Table K.14. The relative average and maximum fitting errors in percentage of the surrogate model for O.PL with increasing active subspace dimension.

Subspace Dimension	In-sample errors (%)		Out-of-sample errors (%)	
	Average	Maximum	Average	Maximum
1	1.86	7.24	2.50	8.93
2	0.34	0.96	0.37	1.09
3	0.32	0.92	0.38	0.97
4	0.22	0.59	0.36	0.85
5	0.14	0.32	0.36	1.12
6	0.09	0.27	0.45	1.54

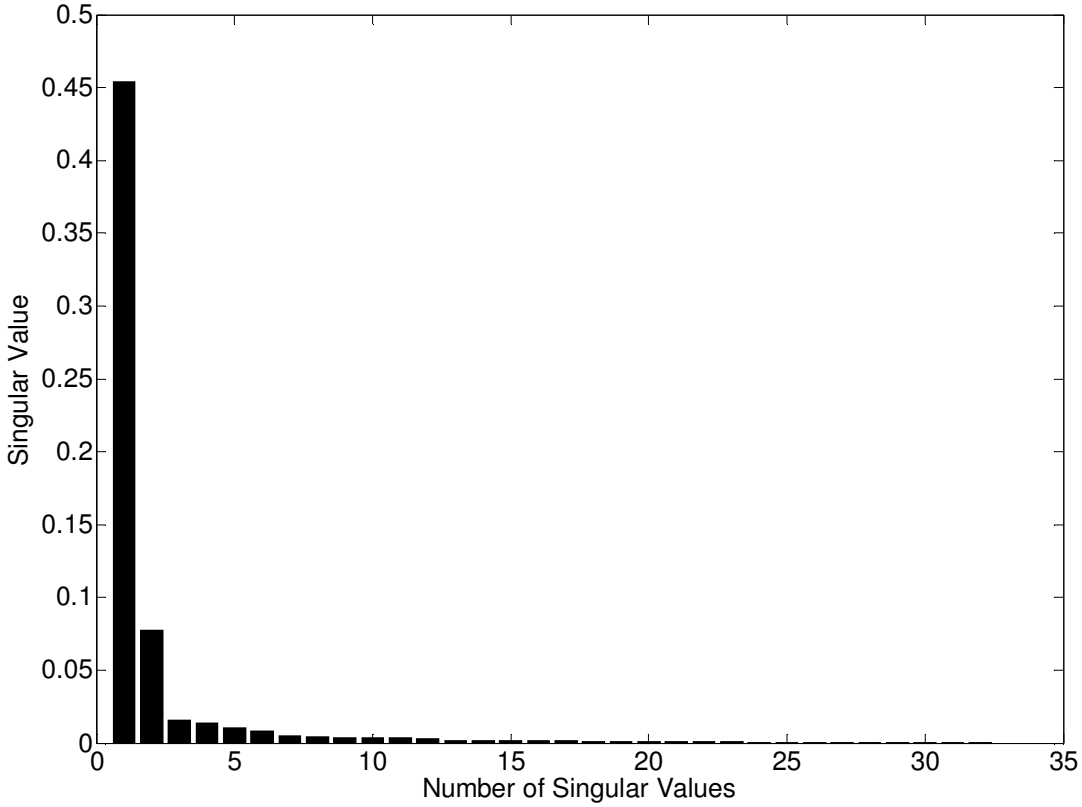

Figure K.24. Singular value plot for prediction of OH.PV.

Table K.15. The relative average and maximum fitting errors in percentage of the surrogate model for OH.PV with increasing active subspace dimension.

Subspace Dimension	In-sample errors (%)		Out-of-sample errors (%)	
	Average	Maximum	Average	Maximum
1	2.05	4.34	2.62	6.79
2	0.35	1.06	0.42	1.04
3	0.26	0.84	0.43	1.31
4	0.19	0.48	0.34	1.31
5	0.11	0.32	0.39	0.96
6	0.03	0.07	0.37	1.92

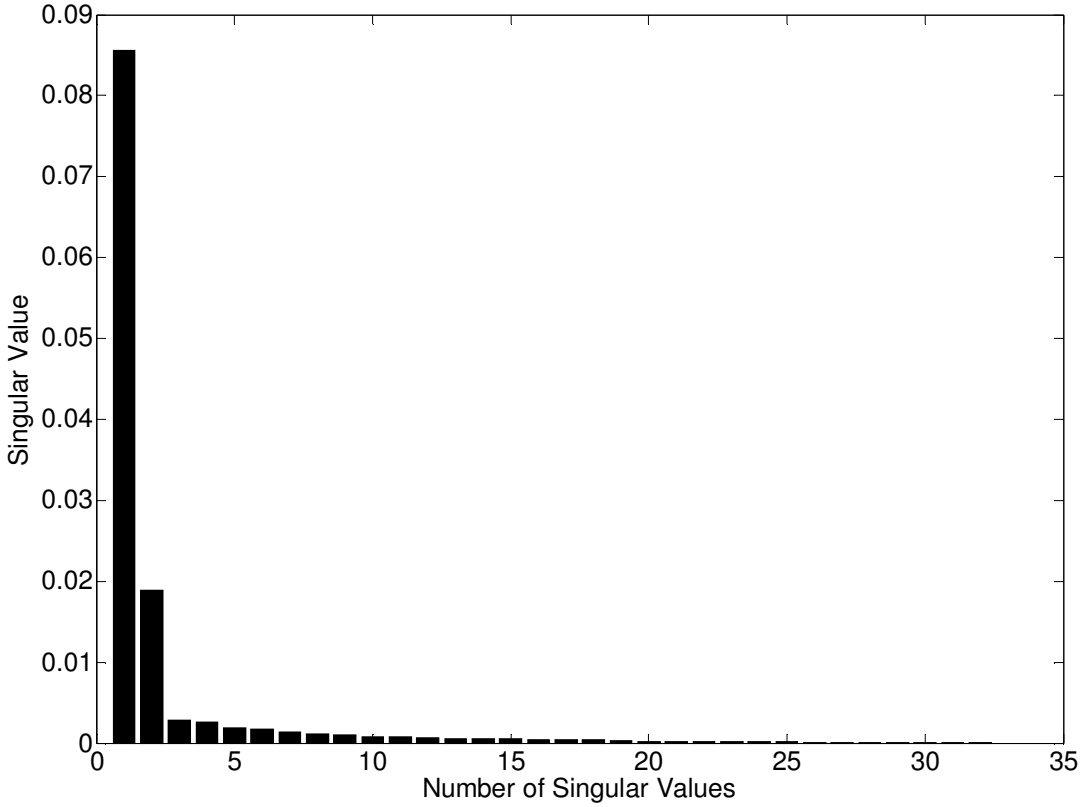

Figure K.25. Singular value plot for prediction of OH.PL.

Table K.16. The relative average and maximum fitting errors in percentage of the surrogate model for OH.PL with increasing active subspace dimension.

Subspace Dimension	In-sample errors (%)		Out-of-sample errors (%)	
	Average	Maximum	Average	Maximum
1	0.35	1.18	0.43	1.16
2	0.08	0.20	0.08	0.18
3	0.06	0.17	0.07	0.21
4	0.04	0.11	0.07	0.21
5	0.04	0.12	0.09	0.27
6	0.02	0.07	0.16	0.48

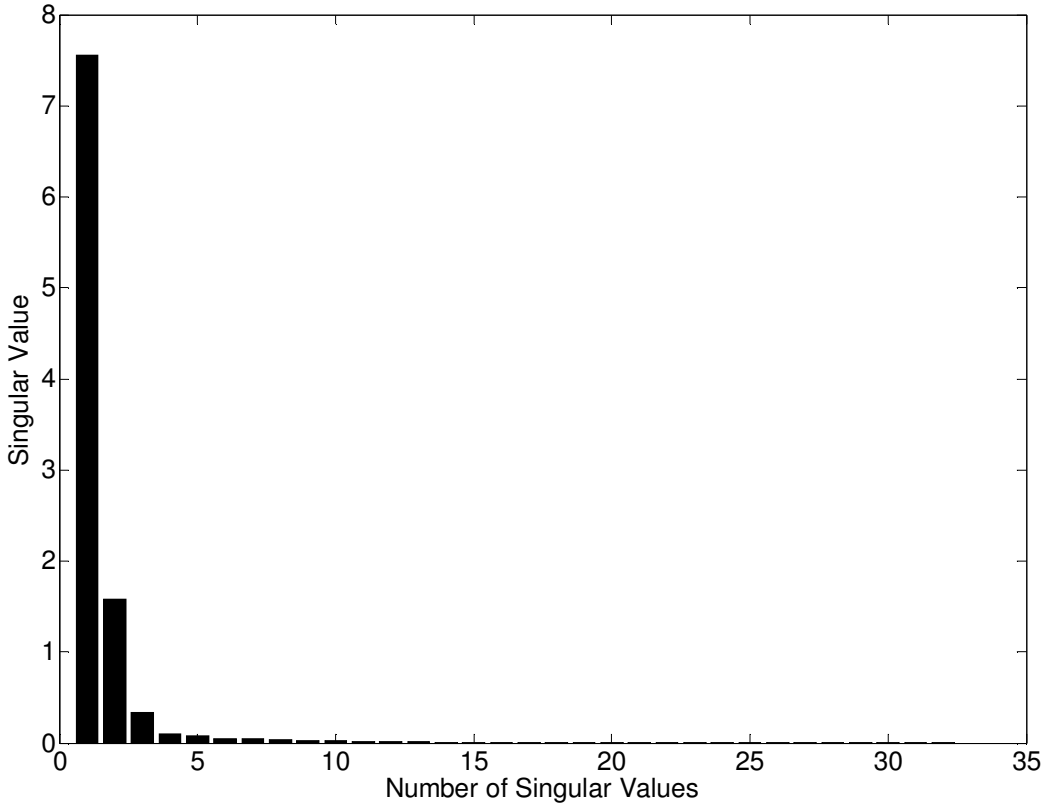

Figure K.26. Singular value plot for prediction of C2H3.PV.

Table K.17. The relative average and maximum fitting errors in percentage of the surrogate model for C2H3.PV with increasing active subspace dimension.

Subspace Dimension	In-sample errors (%)		Out-of-sample errors (%)	
	Average	Maximum	Average	Maximum
1	34.28	136.12	32.69	71.63
2	5.05	20.63	4.65	17.39
3	1.66	5.92	1.52	5.11
4	1.22	4.31	1.71	4.69
5	0.73	2.31	2.27	6.13
6	0.32	1.22	2.97	10.24

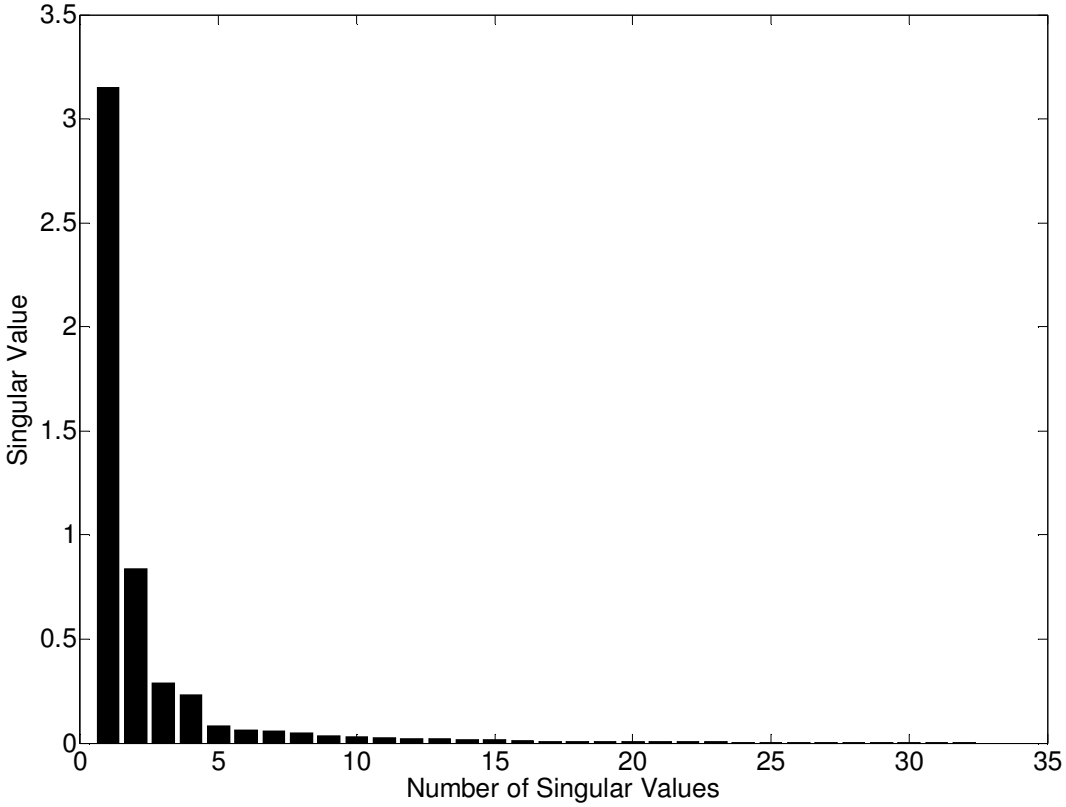

Figure K.27. Singular value plot for prediction of C2H3.PL.

Table K.18. The relative average and maximum fitting errors in percentage of the surrogate model for C2H3.PL with increasing active subspace dimension.

Subspace Dimension	In-sample errors (%)		Out-of-sample errors (%)	
	Average	Maximum	Average	Maximum
1	13.99	54.16	16.81	51.02
2	6.34	28.75	6.77	32.46
3	5.18	15.80	6.80	21.18
4	2.91	7.68	4.76	18.48
5	1.82	6.51	5.81	17.99
6	0.69	2.00	8.90	25.78