# Analysis of a Detailed Kinetic Model of Natural Gas Combustion in IC Engine

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Detailed kinetic models are important to describe the oxidation of hydrocarbon fuels. In the present study, a detailed kinetic models has been developed to simulate the combustion of natural gas in IC engine. The proposed models consists of 208 elementary reactions and 72 species. The rate of the production and sensitivity analysis of the proposed reaction models were carried out to visualize the effect of reactions on the formation of various pollutants. In the rate of production analysis, an absolute rate of production coefficients and the normalized rate of production coefficients were calculated for the reactions involved in the formation of pollutant species (CO, NO, NO<sub>2</sub>, & NH<sub>3</sub>). In sensitivity analysis, normalized logarithmic sensitivity coefficients were determined the reactions of rates affects the output concentrations of the pollutant species. These two analysis were carried out for two temperatures ranges i.e. 1500 °C and 4000 °C under stoichiometric conditions (when  $\varphi = 1.0$ ).

Keywords: Sensitivity Analysis, models, Rate of Production Analysis.

#### INTRODUCTION

Combustion is a very complex phenomenon, characterized by interaction and competition of various physical and chemical processes. The correct description of chemical changes requires the application of reaction models consisting of several hundred or thousand reactions. Detailed combustion models are based on the measurements of the elementary gas phase reaction coefficients. The measurements have provided the temperature and pressure dependencies of the overoverall rate coefficient. The models of Warnatz<sup>1-2</sup> have been used by many people, but were mainly created as illustrations in combustion modeling papers. Another widely used model is of Miller-Bowman NO model<sup>3</sup> which, like the Warnatz model, is now out of-date in many respects. The GRI model is used for the study of the oxidation of methane. This model is based on elementary reactions, where the combinations of the experimental and theoretically determined values are assigned to the rate parameters<sup>4</sup>. Other combustion models are available over the Internet<sup>5</sup>. These models can be used to simulate the combustion methane in internal combustion engines<sup>6</sup>.

The kinetic models development and validation have been investigated by Mansha et al<sup>7</sup>. In the present study, a kinetic model has been developed to simulate the combustion of natural gas (used as CNG in automobile engines) and investigated using Rate of Production Analysis (ROP) and Local Sensitivity Analysis.

The sensitivity analysis methods for chemical kinetics have been reviewed by several researchers. For example; Rabitz et al focused mainly on the interpretation of sensitivity coefficients in reaction-diffusion systems<sup>8</sup>; Turanyi applied the sensitivity analysis methods as tools for investigating the reaction kinetics problems. These studies have an almost complete list of publications on the application of sensitivity analysis in reaction kinetics up to 1989<sup>9</sup>.

The studies on the numerical comparison of the methods for the calculation of local sensitivities have been published by Radhakrishnan<sup>10 – 11</sup>. Tomlin *et al.* have considered sensitivity analysis as one of the mathematical tools applied in combustion chemistry<sup>12</sup>. Several publications on sensitivity analysis are available<sup>8, 12-20</sup>. The rateof-production analysis helps to determine the contribution of each elementary reaction in the kinetic model to the net production or destruction rates of a species.

In the present work, a reaction kinetic model has been developed to simulate the natural gas combustion in IC engine predicting the formation pollutants species. The proposed model was analyzed by Sensitivity Analysis and Rate of Production analysis to identify the reactions involved in the formation of selected pollutants species such as CO, NO,  $NO_2$  and  $NH_3$ .

#### MATERIAL AND METHODS

A detailed reaction model was developed by coupling (i) EXGAS hydrocarbon oxidation mechanism and (ii) Leeds NOx model<sup>5</sup>. The strategy adopted in the coupling of two reaction models is shown in Figure 1. The coupling generated a model consisting of 935 reactions steps and 185 species. The EXGAS<sup>21</sup> model consisted of; (a)  $C_0$ - $C_1$ - $C_2$  reaction base, (b) primary reaction model in which the species in the initial gas mixture are taken as the reactants and (c) secondary model which contains the reactions whose reactants are the molecular products of the primary model. The comprehensive model was reduced by using the chemical lumping techniques. In this model reduction technique, the reactions having similar reactants and product species are omitted.

The types of reactions number of species/radicals are given in Table 1 and Table 2 respectively. This reduction of a resulted model composed of 208 reactions and 72 species as given in Table 3. Thermodynamic data (JANAF format) necessary in CHEMKIN is produced by THERGAS (built-in-module in EXGAS) automatically.

Chemkin 4.1.1 package was used for simulating the natural gas combustion using the proposed reaction model and to carry out the sensitivity analysis and the rate of production analysis. The rate of production analysis of the each kinetic model identified the reactions involved in the

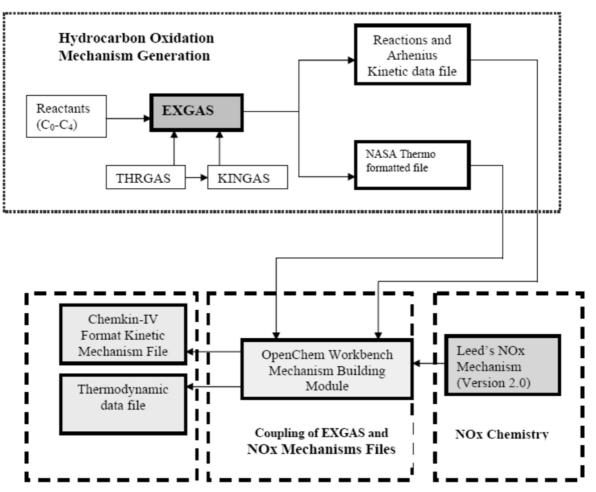


Figure 1. Reaction Mechanisms Coupling Schemes

Table 1. Menu Followed for Generation of Primary Models by EXGAS

Primary Reactions	Options chosen for mechanism		
	generation		
	Yes/No	No. of Reactions	
Unimolecular initiations	Yes	3	
Bimolecular initiations	Yes	3	
Additions with oxygen	No	0	
Isomerizations	No	0	
Beta-scissions	Yes	2	
Decompositions to o-rings	No	2	
Oxidations	Yes	2	
Branching	No	0	
Metatheses	Yes	26	
Combinations	Yes	3	
Dismutations	No	0	
Number of Reactions in Lumped Primary Mechanism generated using EXGAS- I		44	
Number of Reactions in Leeds Mechanism (Version 2.0)-	164		
п			
Total Number of Reactions in Proposed Detailed Kinetic	208		
Mechanism (I+II)			

Table 2. No of Species in Proposed Detailed Kinetic Model

Sr. No	Type of Molecules and Radicals	No of Molecules and Radicals
1	Primary molecules	23
2	Free radicals	22
3	Lumped molecules	34
Total Number of Species		72

formation and consumption of major pollutants. In this analysis, the absolute rate of production (ROP) coefficient and the normalized rate of production coefficients were determined with selected simulation conditions of combustion (as given in Table 4 and Table 5.

Similarly, the normalized (logarithmic) sensitivity coefficients were calculated as defined by the equation (5) using the Local Sensitivity solver in the Chemkin package. The results were plotted by the sensitivity bar charts for CO,  $CO_2$ , NO, NO<sub>2</sub> and NH<sub>3</sub>. The input keywords for the input parameters, solver and outputs for the rate of production and sensitivity analysis are given in Table 3.

#### **RESULTS AND DISCUSSION**

This automatically simplified model consists of 208 elementary reactions and 72 species. Mostly the reactions are of primary type including unimolecular initiations, bimolecular initiations, beta-scissions, oxidations, branching, metatheses and combinations.

The simulation study of natural gas combustion with a proposed kinetic model shows that the maximum peak temperature and pressure was achieved when equivalence ratio (Fuel/air) was  $\approx$ 1.3, compression ratio of  $\approx$ 10.51, engine speed of  $\approx$  3000 rpm and initial inlet temperature of  $\approx$ 1000 °C. The cycle variation in the cylinder pressure and temperature is shown in Figure 2.

The rate of production analysis of the proposed model (Table 3) was carried out using the input variables as given in Table 4 to Table 6 to identify the reactions of the model contributing to the formation of gaseous pollutants (NO, NO<sub>2</sub>, MH<sub>3</sub> and CO). The normalized rate of production coefficients of each reaction contributes to the formation of the pollutants. The total rate of production

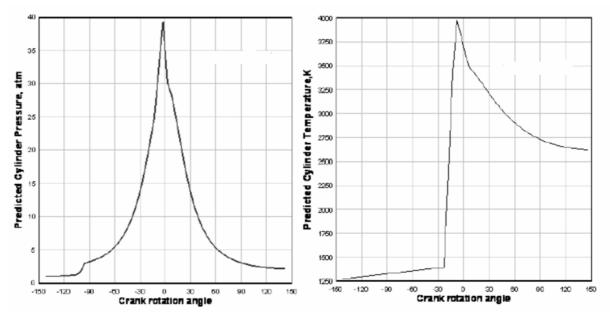


Figure 2. Predicted In-Cylinder Pressure (atm) and Temperature (K)

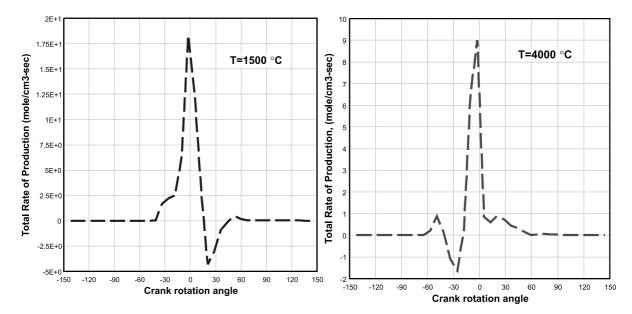


Figure 3. Variation of rate of production of CO at extreme temperatures of T=1500 °C and T=4000 °C in IC engine for equivalence ratio  $\approx 1.0$ 

		0.405.40		00000 5
R-1 R-2	C3H8=>R4CH3+R11C2H5 C4H10=>R11C2H5+R11C2H5	9.40E+16 2.20E+16	0	86903.5 86135.6
R-3	C4H10=>R4CH3+R19C3H7	9.70E+16	0	88015.9
R-4 R-5	C3H8+O2=>R3OOH+R19C3H7 C4H10+O2=>R3OOH+R20C4H9	4.20E+13 4.20E+13	0	54334.2 54334.3
R-6	R19C3H7=>R4CH3+C2H4Z	2.00E+13	0	31000
R-7	R19C3H7=>R1H+C3H6Y	3.00E+13	0	38000
R-8 R-9	R20C4H9=>R11C2H5+C2H4Z R20C4H9=>R1H+C4H8Y	2.00E+13 3.00E+13	0	28700 38000
R-10	R22C4H9=>R4CH3+C3H6Y	2.00E+13	0	31000
R-11	R19C3H7+O2=>C3H6Y+R3OOH	2.80E+12	0	5000
R-12 R-13	R20C4H9+O2=>C4H8Y+R3OOH B1O+C3H8=>R2OH+R19C3H7	1.30E+12 1.00E+14	0	5000 7850
R-14	B10+C4H10=>R2OH+R20C4H9	1.00E+14	0	7850
R-15	C3H8+R1H=>H2+R21C3H7	9.00E+06	2	5000
R-16 R-17	C4H10+R1H=>H2+R20C4H9 C3H8+R2OH=>H2O+R21C3H7	5.70E+07 2.60E+06	2 2	7700 -765
R-17	C4H10+R2OH=>H2O+R20C4H9	5.40E+06	2	450
R-19	C3H8+R3OOH=>H2O2+R21C3H7	4.00E+11	0	15500
R-20 R-21	C4H10+R3OOH=>H2O2+R20C4H9 C3H8+R4CH3=>CH4+R21C3H7	1.20E+12 2.00E+11	0	17000 9600
R-21	C4H10+R4CH3=>CH4+R2IC3H7 C4H10+R4CH3=>CH4+R20C4H9	6.00E-01	4	8200
R-23	C3H8+R5CHO=>HCHO+R21C3H7	1.00E+07	1.9	17000
R-24	C4H10+R5CHO=>HCHO+R20C4H9	2.00E+05	2.5	18500
R-25 R-26	C3H8+R6CH2OH=>CH3OH+R21C3H7 C4H10+R6CH2OH=>CH3OH+R20C4H9	6.00E+01 2.00E+02	3	12000 14000
R-27	C3H8+R7CH3O=>CH3OH+R21C3H7	1.50E+11	0	4500
R-28	C4H10+R7CH3O=>CH3OH+R20C4H9	3.20E+11	0	7300
R-29 R-30	C3H8+R8CH3OO=>CH3OOH+R21C3H7 C4H10+R8CH3OO=>CH3OOH+R20C4H9	3.00E+12 1.20E+13	0	17500 20000
R-31	C3H8+R11C2H5=>C2H6+R21C3H7	2.00E+11	ő	11000
R-32	C4H10+R11C2H5=>C2H6+R20C4H9	6.00E+11	0	13500
R-33 R-34	C3H8+R21C3H7=>C3H8+R19C3H7 C4H10+R21C3H7=>C3H8+R22C4H9	8.40E-03 5.60E-03	4.2	8700 8000
R-35	R1H+R21C3H7=>C3H8	8.30E+12	0	0000
R-36	R2OH+R21C3H7=>C3H7OH	5.90E+12	0	0
R-37 R-38	R3OOH+R21C3H7=>C3H7OOH R4CH3+R21C3H7=>C4H10	4.80E+12 1.50E+13	0	0
R-38 R-39	R5CHO+R21C3H7=>C3H7CHO	5.20E+12	0	0
R-40	R6CH2OH+R21C3H7=>C4H9OH	5.10E+12	0	0
R-41 R-42	R7CH3O+R21C3H7=>C4H10O R8CH3OO+R21C3H7=>C4H10OO	4.90E+12 4.40E+12	0	0
R-42 R-43	R8CH3OO+R21C3H7=>C4H10OO R11C2H5+R21C3H7=>C5H12	4.40E+12 5.20E+12	0	0
R-44	R21C3H7+R21C3H7=>C6H14	2.30E+12	0	0
R-45	H2+CN=HCN+H	1.93E+04	2.9	6.8
R-46 R-47	CH4+N=NH+CH3 CH4+CN=HCN+CH3	1.00E+13 9.03E+04	0 2.6	100.4 -1.2
R-48	O2+N=NO+O	9.03E+09	1	27.2
R-49	O2+NH=HNO+O	3.91E+13	0	74.8
R-50 R-51	02+NH=NO+OH 02+NH2=HNO+OH	7.59E+10 1.51E+12	-0.4	6.4 151
R-52	02+NH2=H2NO+O	1.10E+18	-1.3	140.6
R-53	O2+CN=NCO+O	7.23E+12	0	-1.7
R-54 R-55	02+NCO=NO+CO2 CO+N2O=CO2+N2	1.72E+07 9.77E+10	0	-3.1 73
R-56	CO2+N=NO+CO	1.90E+11	0	14.2
R-57	N2+CH=HCN+N	1.57E+12	0	75.1
R-58 R-59	N2+CH2=HCN+NH NO+N2O=N2+NO2	1.00E+13 1.00E+14	0	309.6 207.8
R-60	NO+N2H2=N2O+NH2	3.00E+12	0	0
R-61	NO+C=CN+O	1.93E+13	0	0
R-62 R-63	NO+C=CO+N NO+H=>N+OH	2.89E+13 2.17E+14	0	0 207.1
R-63	NOHH=>NOHH	2.17E+14 2.83E+13	0	0
R-65	NO+CH=CO+NH	1.20E+13	0	0
R-66	NO+CH=CN+OH	1.20E+13	0	0
R-67 R-68	NO+CH=HCN+O NO+CH2=HOCN+H	9.60E+13 1.39E+12	0	-4.6
R-69	NO+CH2(S)=HCN+OH	9.64E+13	0	0
R-70 R-71	NO+CH3=HCN+H2O	9.28E+11	0	69.9
R-71 R-72	N0+CH3=H2CN+OH N0+H02=N02+OH	9.28E+11 2.09E+12	0	69.9 -2
R-73	NO+HO2=HNO+O2	2.00E+11	Ő	8.3
R-74	NO+HCCO=HOCN+CO	2.00E+13	0	0
R-75 R-76	NO+N=>N2+O N2+O=>NO+N	4.28E+13 1.81E+14	0	6.6 318.4
R-77	NO+NH=N2+OH	3.20E+13	0	53.2
R-78	NO+NH=N2O+H	4.16E+14	-0.5	0
R-79 R-80	NO+NH2=NNH+OH NO+NH2=N2+H2O	2.41E+15 5.48E+15	-1.2	0
R-81	NO+NNH=N2+HNO	5.40E+13	0	0
R-82	N0+HN0=N20+OH	2.95E+05	0	0
R-83 R-84	NO+NCO=N2O+CO NO+M=N+O+M	1.39E+18 3.62E+15	-1.7	3.2 620.6
R-85	N02+N02=N0+N0+02	2.00E+12	0	112.2
R-86	NO2+H=NO+OH	3.47E+14	0	6.2
R-87 R-88	N02+0=N0+02 N02+N=N0+N0	1.00E+13 8.07E+11	0	2.5 0
R-89	NO2+N=NO+NO NO2+N=N2O+O	1.00E+12	0	0
R-90	NO2+NH=HNO+NO	1.00E+11	0.5	16.6
R-91 R-92	N02+NH=N2O+OH N02+NH2=N2O+H2O	<u>9.71E+12</u> 2.03E+17	-1.7	0
R-92 R-93	NO2+NH2=N2O+H2O NO2+CN=NCO+NO	3.00E+13	0	0
R-94	NO2+M=NO+O+M	3.13E+16	0	274.4
R-95 R-96	N2O+C=CN+NO N2O+H=N2+OH	5.12E+12 4.37E+14	0	0 79
R-96 R-97	N2O+H=N2+OH N2O+O=N2+O2	4.3/E+14 1.00E+14	0	117.2
R-98	N2O+O=NO+NO	6.92E+13	0	111.4
R-99 R-100	N2O+OH=N2+HO2 N2O+N=N2+NO	<u>6.31E+11</u> 1.00E+13	0	41.6
N-100	N2O+N=N2+NO N2O+NH=HNO+N2	1.00E+13 2.00E+12	0	83.1 24.9
R-101		1.00E+13	0	0
R-102	N2O+CN=NCO+N2	2.86E+15	0	251
R-102 R-103	N2O+M=N2+O+M			, , , , , , , , , , , , , , , , , , ,
R-102		5.42E+05	2.4	41.5 30.5
R-102 R-103 R-104 R-105 R-106	N2O+M=N2+O+M NH3+H=NH2+H2 NH3+O=>NH2+OH NH3+OH=NH2+H2O	5,42E+05 9,64E+12 3,16E+12	2.4 0 0	30.5 8.4
R-102 R-103 R-104 R-105 R-106 R-107	N2O+M=N2+O+M           NH3+H=NH2+H2           NH3+O=>NH2+OH           NH3+OH=NH2+H2O           NH3+HO2=NH2+H2O2	5.42E+05 9.64E+12 3.16E+12 2.51E+12	2.4 0 0 0	30.5 8.4 99.8
R-102 R-103 R-104 R-105 R-106 R-107 R-108	N2O+M=N2+O-M           NH3+H=NH2+H2           NH3+O=>NH2+OH           NH3+O=>NH2+OH           NH3+OH=NH2+H2O           NH3+OH=NH2+H2O2           NH3+NH2=N2H3+H2	5.42E+05 9.64E+12 3.16E+12 2.51E+12 7.94E+11	2.4 0 0 0 0 0.5	30.5 8.4 99.8 90.2
R-102 R-103 R-104 R-105 R-106 R-107 R-108 R-108 R-109 R-110	N2O+M=N2+O-M           NH3+H=NH2+H2           NH3+O=>NH2+OH           NH3+O=>NH2+OH           NH3+OH=NH2+H2O           NH3+NH2=N2H3+H2           NH3+NH2=N2H3+H2           NH3(+M)=NH2+H(+M)           NH3+M=NH+H2+M	5.42E+05 9.64E+12 3.16E+12 2.51E+12 7.94E+11 8.30E+15 1.80E+15	2.4 0 0 0 0.5 0 0 0	30.5 8.4 99.8 90.2 458.7 390.8
R-102 R-103 R-104 R-105 R-106 R-107 R-108 R-109 R-110 R-111	N2O+M=N2+O-M           NH3+H=NH2+H2           NH3+O=>NH2+OH           NH3+O=>NH2+OH           NH3+O=>NH2+H2           NH3+ND=NH2+H2O2           NH3+NH2=N2H3+H2           NH3+M]=NH2+H(+M)           NH3+M]=NH+H2+H(+M)           NH3+M=NH+H2+M	5.42E+05 9.64E+12 3.16E+12 2.51E+12 7.94E+11 8.30E+15 1.80E+15 1.00E+13	2.4 0 0 0 0.5 0 0 0 0 0	30.5 8.4 99.8 90.2 458.7 390.8 4.2
R-102 R-103 R-104 R-105 R-106 R-107 R-108 R-108 R-109 R-110	N2O+M=N2+O-M           NH3+H=NH2+H2           NH3+O=>NH2+OH           NH3+O=>NH2+OH           NH3+OH=NH2+H2O           NH3+NH2=N2H3+H2           NH3+NH2=N2H3+H2           NH3(+M)=NH2+H(+M)           NH3+M=NH+H2+M	5.42E+05 9.64E+12 3.16E+12 2.51E+12 7.94E+11 8.30E+15 1.80E+15	2.4 0 0 0 0.5 0 0 0	30.5 8.4 99.8 90.2 458.7 390.8

## Table 3. Detailed Kinetic Reaction Model for Natural Gas Combustion in IC Engine

COD         Displayment         Displayment <thdisplayment< th=""> <thdis< th=""><th>D 111</th><th></th><th>1.005.10</th><th><u>^</u></th><th></th></thdis<></thdisplayment<>	D 111		1.005.10	<u>^</u>	
B10         Control         CS         Mode           D11         CONTROL         CONTROL         CONTROL         CONTROL           D11         CONTROL         CONTROL         CONTROL         CONTROL           D10         CONTROL         CONTROL         CONTROL         CONTROL         CONTROL           D10         CONTROL         CONTROL <td>R-114</td> <td>N2H2+OH=NNH+H2O</td> <td>1.00E+13</td> <td>0</td> <td>8.3</td>	R-114	N2H2+OH=NNH+H2O	1.00E+13	0	8.3
Line         Control         Control <thcontrol< th=""> <thcontrol< th=""> <thcont< td=""><td></td><td></td><td></td><td></td><td></td></thcont<></thcontrol<></thcontrol<>					
Phile         Point Martin			1.00E+11	0.5	141.3
Dr.D.         Decisional Anti- anticational Anti- Anticati Anti- Anticational Anti- Anticational Anti- Anticationa	R-117	N2H2+NH2=NH3+NNH	1.00E+13	0	16.6
BAD         CONCRNA         CONCRNA <thconcrna< th=""> <thconcrna< th=""> <thconcr< td=""><td>R-118</td><td>N2H2+M=NNH+H+M</td><td>2.50E+16</td><td>0</td><td>207.8</td></thconcr<></thconcrna<></thconcrna<>	R-118	N2H2+M=NNH+H+M	2.50E+16	0	207.8
BAD         CONCRNA         CONCRNA <thconcrna< th=""> <thconcrna< th=""> <thconcr< td=""><td>R-119</td><td>N2H2+M=NH+NH+M</td><td>7.91E+16</td><td>0</td><td>415.7</td></thconcr<></thconcrna<></thconcrna<>	R-119	N2H2+M=NH+NH+M	7.91E+16	0	415.7
Bog         Cale Control         State Contro	R-120	C2N2+O=NCO+CN			
BODMode of the set					
BODBADOMEDB					
EMB         NEGROSHOM         325/16         31         326           DEG         USCOBINOSAL         300.04         4         40.0           DEG         USCOBINOSAL         300.04         30.0         40.0         40.0           DEG         USCOBINOSAL         300.04         30.0         30.0         40.0         40.0           DEG         USCOBINOSAL         300.04         30.0					
NBS         BDS 05 (000)         C         Add           CF07         470 (000)         400 (000)         400 (000)         400 (000)           CF07         470 (000)         400 (000)         400 (000)         400 (000)           CF07         470 (000)         400 (000)         400 (000)         400 (000)         400 (000)           CF07         470 (000)         400 (000)         400 (000)         400 (000)         400 (000)           CF07         470 (000)         400 (000)         400 (000)         400 (000)         400 (000)           CF07         470 (000)         400 (000)         400 (000)         400 (000)         400 (000)           CF07         470 (000)         400 (000)         400 (000)         400 (000)         400 (000)           CF07         470 (000)         400 (000)         400 (000)         400 (000)         400 (000)           CF07         470 (000)         400 (000)         400 (000)         400 (000)         400 (000)           CF08         470 (000)         400 (000)         400 (000)         400 (000)         400 (000)           CF08         470 (000)         400 (000)         400 (000)         400 (000)         400 (000)         400 (000)         400 (000)					
RDSMEXABADDANAAddAddAddRDSMEXABADDANAMEXABADDANAMEXABADDANAMEXABADDANARDSMEXABADDANAMEXABADDANAMEXABADDANAMEXABADDANARDSMEXABADDANAMEXABADDANAMEXABADDANAMEXABADDANARDSMEXABADDANAMEXABADDANAMEXABADDANAMEXABADDANARDSMEXABADDANAMEXABADDANAMEXABADDANAMEXABADDANARDSMEXABADDANAMEXABADDANAMEXABADDANAMEXABADDANARDSMEXABADDANAMEXABADDANAMEXABADDANAMEXABADDANARDSMEXABADDANAMEXABADDANAMEXABADDANAMEXABADDANARDSMEXABADDANAMEXABADDANAMEXABADDANAMEXABADDANARDSMEXABADDANAMEXABADDANAMEXABADDANAMEXABADDANARDSMEXABADDANAMEXABADDANAMEXABADDANAMEXABADDANARDSMEXABADDANAMEXABADDANAMEXABADDANAMEXABADDANARDSMEXABADDANAMEXABADDANAMEXABADDANAMEXABADDANARDSMEXABADDANAMEXABADDANAMEXABADDANAMEXABADDANARDSMEXABADDANAMEXABADDANAMEXABADDANAMEXABADDANARDSMEXABADDANAMEXABADDANAMEXABADDANAMEXABADDANARDSMEXABADDANAMEXABADDANAMEXABADDANAMEXABADDANARDSMEXABADDANAMEXABADDANAMEXABADDANAMEXABADDANARDSMEXABADDANAMEXABADDANAMEXABADDANAMEXABADDANARDSMEXABADDANAM					
RADE         HERODENBODIM	R-125	HCN+OH=CN+H2O	9.03E+12	0	44.9
RADE         HERODENBODIM	R-126	HCN+OH=HOCN+H	5.85E+04	2.4	52.3
Sold         IBC/01-2001         DD         LB           Sold         ICO11-90-00         ICO10-90-00         ICO10-90-00         ICO10-90-00           Sold         ICO11-90-00         ICO10-90-00         ICO10-90-00         ICO10-90-00           Sold         ICO10-90-00         ICO10-90-00         ICO10-90-00         ICO10-90-00         ICO10-90-00           Sold         ICO10-90-00         ICO10-90-00 <td< td=""><td></td><td></td><td></td><td></td><td></td></td<>					
Bog         HODULHINGON         100/19         0         0           BOG         HODULHINGON         100/19         0         0         0         0           BOG         HODULHINGON         100/19         0         0         0         0         0           BOG         HODULHINGON         100/19         0					
BX0         HCXNN-HQXD         ICXNN-HQXD         G         B           BX3         HX001+HQXD         ICXN1         0.3         SX           BX3         HX001+HQXD         ICXN1         0.3         SX           BX3         HX001+HQXD         ICXN1         0.4         SX           BX4         HX001+HX1         ICXN1         0.4         SX           BX4         HX001+HX1         ICXN1         0.4         SX           BX4         HX001+HX1					
Bh1         Ho0Min MCGui         Doc 11         0         0           B10         HEXD-MARCON         20041         03         00           B10         HEXD-MARCON         20041         03         00           B10         HEXD-MARCON         20041         01         04           B10         HEXD-MARCON         100713         0         00           B10         HEXD-MARCON         100713         0         2005           B10         HEXD-MARCON         100713         0         2005           B10         HEXD-MARCON         100713         0         2005           B10         HEXD-MARCON         200511         0         2005           B10         HEXD-MARCON         200512         0         2005           B10         HEXD-MARCON         200513         0         2005           B10         HE					
BLUP         HECONNECTION         2.88114         C.33         BAD           B131         HECONNECTION         132173         0         333           B131         HECONNECTION         132173         0         333           B138         HECONNECTION         132173         0         333           B138         HECONNECTION         132173         0         332           B138         HECONNECTION         132171         0         332           B138         HECONNECTION         132171         0         332           B138         HECONNECTION         132171         0         332           B140         HECONNECTION         132171         0         342           B141         HECONNECTION         132171         0         342					
BN3         HEGOM-HERGO         1.0014         6         832           BV16         HEGOM-HERGO         2.0017         6         804           BV18         HEGOM-SERGO         3.0017         0         804           BV18         HEGOM-SERGO         3.0017         0         805           BV18					
B34         HBCONGNEG2         0.00000         65.5           C50         HBCONGNEG2         0.00000         0.00000         0.00000         0.00000         0.00000         0.00000         0.000000         0.000000         0.000000         0.0000000         0.00000000000000000000000000000000000	R-132	HNCO+H=NCO+H2	2.05E+14	-0.3	84.7
B34         HBCONGNEG2         0.00000         65.5           C50         HBCONGNEG2         0.00000         0.00000         0.00000         0.00000         0.00000         0.00000         0.000000         0.000000         0.000000         0.0000000         0.00000000000000000000000000000000000	R-133	HNCO+H=NH2+CO	1.10E+14	0	53.2
FIGS         HECOLOGING/O         1961'2         0         6.3.           FIGS         HECOLOGING/A         1061'2         0         602           FIGS         HECOLOGING/A         1061'2         0         602           FIGS         HECOLOGING/ACCOLOGING/A         1061'3         0         1022           FIGS         HECOLOGING/ACCOLOG	R-134	HNCQ+Q=NH+CQ2		0	
Fb58         HCC0-CONKO         200141         8         662           Fb59         HCC0-CONKO         100111         1         0123           Fb59         HCC0-CONKO         306113         1         0123           Fb59         HCC0-CONKO         306113         1         0123           Fb50         HCC0-HCANDERCO         306113         1         0123           Fb51         HCC0-HCANDERCO         306113         1         0123           Fb54         HCC0-HCANDERCO         306113         1         0123           Fb54         HCC0-HCANDERCO         306113         1         0123           Fb54         HCC0-HCANDERCO         306113         1         0         0123           Fb54         HCS0-HCANDERCO         306113         1         0         0           Fb54         HCS0-HCANDERCO         306113         1         0         0           Fb50					
B-B27         H6C004BMECO4DD         0.98413         0.922           B-103         H6C004BMECO4DD         0.88411         0.922           B-103         H6C004BMECO2DD         0.38411         0.922           B-104         H6C004BMECO2DD         0.38411         0.922           B-104         H6C004BMECO2DD         0.38411         0.922           B-104         H6C004BMECO2DD         0.24411         0.923           B-104         H6C004BMECO3DD         0.24411         0.923           B-104         H6C004BMECO3DD         0.24411         0.923           B-104         H6C004BMECO3DD         0.24411         0.923           B-104         H6C004BMECO3DD         0.924517         0.923           B-104         H6C004BMECO3DD         0.924517         0.924517           B-104         H6C004BMECO3DD         0.92517         0.924517           B-104         H6C004BMECO3DD         0.92517         0.924517           B-104         H6C004BMECO3DD         0.92517         0.924517           B-104         H6C004BMECO3DD         0.925117         0.945161           B-104         H6C004BMECO3DD         0.925111         0.945161           B-104         H6C004BMECO3DD					
BASB         HECO-DENE COP         6.562-11         0         122           BASB         HECO-DENE COP         3.361-31         0         122           BASB         HECO-MERINGON         3.361-31         0         123           BASB         HECO-MERINGON         3.361-31         0         432           BASB         HECO-MERINGON         3.361-31         0         432           BASB         HECO-MERINGON         3.361-31         0         435           BASB         HECO-MERINGON         3.361-31         0         435           BASB         HECO-MERINGON         3.361-31         0         450           BASB         CHERON         3.361-31         0					
BA10         HBC0-H02NBC-H020         ADDE-31         O         H212           BA12         HBC0-H02NBC-H020         ADDE-31         O         H212           BA12         HBC0-H02NBC-H020         ADDE-31         O         H212           BA12         HBC0-H02NBC-H020         ADDE-31         O         H213           BA14         HBC0-H02NBC-H020         ADDE-31         O         H214           BA14         HBC0-H02NBC-H020         ADDE-31         O         H214           BA14         HBC2-H02NBC-H020         ADDE-31         O         H214           BA14         HBC2-H02NBC-H020         ADDE-31         O         H216           BA14         HHD0-H7NC         ADDE-31         O         H216           BA14         HHD0-H7NC         ADDE-31         O         H216           BA14         HHD0-H7NC        ADDE-31		HNCO+OH=NCO+H2O			
Field         Higgs Human         386:13         0         480           6142         Higgs Human         240:13         0         240           8143         Higgs Human         240:17         0         450           8143         Higgs Human         240:17         0         450           8144         Higgs Human         260:17         0         450           8146         Higgs Human         260:17         0         450           8147         Higgs Human         260:17         0         0         0           8140         Higgs Human         260:17         0         0         0         0           8140         Higgs Human         260:17         0 <td></td> <td></td> <td></td> <td></td> <td></td>					
Bota         HBCOHMENDATION         ADDED					
Bota         HBCOHMENDATION         ADDED	R-140	HNCO+N=NH+NCO	3.98E+13	0	149.7
Frid2         HNCOMPARITION         1.086-12         0         834           EVAIL         4.027-161         0         4.027-16         0         4.027-16           EVAIL         HWE-MARCA         0.027-12         0         0         4.02           EVAIL         HWE-MARCA         0.027-12         0         0         4.02           EVAIL         HWE-MARCA         0.027-12         0         4.02					
Rid2         INCO-MENCOM         248-19         0         534           Rid4         INCO-MENCOM         200-19         0         0           Rid4         INCO-MENCOM         200-19         0         0           Rid6         INCO-MENCOM         200-19         0         0         0           Rid6         INCO-MENCOM         200-19         0         0         0         0           Rid6         INREGORDARIS         200-19         0					
Fild         HCOMMINKON         2.85(17)         0         4483           Fild         HUBPHIKE         102211         0         10           Fild         HUBPHIKE         309210         0         10           Fild         HUBPHIKE         309210         0         10           Fild         HUBPHIKE         0.02110         0         0         10           Fild         HUBPHIKE         0.02110         0         0         0           Fild         CHUBHIKE         0.02110         0         0         0         0           Fild         CHUBHIKE         0.02110         <					
Rids         Hell-Hell         1.050-11         0         0           Rids         Hell-NH12         0.0021-1         0         0         125           Rids         Hell-NH12         0         0.0021-1         0         0         0           Rids         Hell-NH12         0         0.0021-1         0         0         0           Rids         Hell-NH12         0         0.0021-1         0         0         0           Rids         Hell-NH12         0.0021-1         0					
Ride         Intel_Print         6.051*7         0         0           Rid         Intel_Print         1000*10         0         120           Rid         Intel_Print         0         120         0         120           Rid         Intel_Print         0         120*1         0         120           Rid         Intel_Print         120*1         0         180           Rid         Intel_Print         120*10         0         180           Rid         Intel_Print         120*10         0         0         0           Rid         ChinertChini         120*10         <					
BAT         INNUMPSITE         3388-10         0         1225           BATA         INTOTANDARD         1000-17         0         0         0           BATA         INTOTANDARD         1000-17         0         8.10         0         8.10           BATA         INTOTANDARD         5.262-13         0         8.10         0         8.10           BATA         INTOTANTO         5.262-13         0					
R-140         HH-05-MARCH         1.56±12         0         0           R-140         HH-05-MARCH         1.36±11         0         0         0           R-151         HH-05-MARCH         1.36±13         0         0         0           R-153         HH-05-MARCH         1.36±13         0         0         0         0           R-153         CH-NCH         1.36±13         0         0         0         0           R-154         CH-NCH         1.36±13         0         0         0         0           R-154         CH-NCH         1.36±13         0         0         0         0           R-157         CH-NCH         1.36±13         0         0         0         0           R-157         CH-NCH         1.36±13         0	R-146	H+NH2=NH+H2	6.02E+12	0	0
R-140         HH-05-MARCH         1.56±12         0         0           R-140         HH-05-MARCH         1.36±11         0         0         0           R-151         HH-05-MARCH         1.36±13         0         0         0           R-153         HH-05-MARCH         1.36±13         0         0         0         0           R-153         CH-NCH         1.36±13         0         0         0         0           R-154         CH-NCH         1.36±13         0         0         0         0           R-154         CH-NCH         1.36±13         0         0         0         0           R-157         CH-NCH         1.36±13         0         0         0         0           R-157         CH-NCH         1.36±13         0		H+NNH=N2+H2			
R-16         H-M625-MANNES         1.064-12         0         6.0           R-162         H-M625-MANNES         0.264-12         0         0.0           R-162         H-M625-MANNES         0.264-13         0         0.0           R-162         H-M625-MANNES         0.264-13         0         0         0.0           R-163         CH-M64-KANH         0.264-13         0         0         0         0           R-163         CH-M64-KANH         0.264-13         0         0         0         0           R-163         CH-M64-KANH         0.204-13         0         0         0         0           R-164         CH-M64-KANH         0.204-13         0         0         0         0           R-164         CH-M64-KANH         0.204-13         0					
R-160         H-4635-3020-H2         0         8.8           R-131         H-460-5020-H2         0.264-13         0         16.8           R-131         H-H00-240-0         0.264-13         0         0           R-133         H-H00-240-0         0.264-13         0         0         0           R-135         CH-NBEHCM-H         0.262-13         0         0         0         0           R-135         CH-NBEHCM-H         0.262-13         0         0         0         0           R-136         CH-NBEHCM-H         0.262-13         0					
RH30         HH80C2440         1.28413         0         168           R130         HH80C24410         0.244133         0         0         0           R131         CHM32H00HH         0.062433         0         0         0           R135         CHM32H00HH         0.062433         0         0         0           R135         CHM32H00HH         0.026433         0         0         0           R135         CHM32H00HH         0.026433         0         0         0           R135         CHM32H00HH         0.026433         0         0         0           R136         CHM32H00HG         0.026433         0         0         0           R136         CHM32H00HG         0.026433         0         0         0           R146         OHE24H00H         0.026433         0         0         0           R146         OHE24H00H         0.026433         0         0         0           R146         OHE24H00H         0.026433         0         0         0           R147         OHE34H00H         0.026433         0         0         0           R147         OHE34H00H         0.026433					
R-TE2         IH-NCO-HI+CD         S24E-13         0         0         0           R153         CHN-CDHI         128E-13         0         0         0           R153         CHN-CDHI         328E-13         0         0         0           R154         CHN-SUBRITHI         328E-13         0         0         0           R157         CE-VHACMH         328E-13         0         0         0           R157         CE-VHACMH         228E-13         0         0         33           R151         CE-VHACMH         228E-13         0         0         0           R151         CE-VHACMH         238E-13         0         0         0           R151         CE-VHACMH         328E-13         0         0         0           R151         CE-VHACMH         328E-13         0         0         0           R151         CE-VHACMH         328E-13         0         0         0         0           R151         CE-VHACMH         328E-13         0         0         0         0         0         0         0         0         0         0         0         0         0         0         0					
R-13         CH-NB-LICHH         1.285+13         0         0           R-13         CH-NB-LICHH         1.002+13         0         0           R-13         CH-NB-LICHH         1.002+13         0         0           R-137         CH-NB-LICHH         1.002+13         0         0           R-137         CH-NB-LICHH         1.002+13         0         0           R-137         CH-NB-LICHH         1.002+13         0         0           R-138         CH-NB-LICHH         1.002+13         0         0           R-138         CH-NB-LICHH         1.002+13         0         0         0           R-136         CH-NB-LICHH         1.002+13         0         0         0           R-136         CH-NB-LICHH         0.525+13         0         0         0           R-146         CH-NB-LICHH         0.525+13         0         0         0           R-146         CH-NB-LICHH         0.525+13         0         0         0           R-146         CH-NB-LICHH         0.525+13         0         0         0           R-147         CH-NB-LICHH         0.525+13         0         0         0           R-1					
R-164         CH-NB-HCN-H4         0.006-13         0         0           R-155         CH-NB-HCN-H4H         3.006-13         0         0           R-157         CH-NB-HCN-H4H         2.306-13         0         0           R-156         CH-NB-HCN-H4H         2.306-13         0         0           R-156         CH-NB-HCN-H4H         2.306-13         0         0           R-156         CH-NB-HCN-H4H         2.306-13         0         0           R-157         CH-NB-HCN-H4H         2.306-13         0         0           R-158         CH-NB-HCN-H2H         2.306-13         0         0           R-164         CH-NB-HCN-H2H         0.306-13         0         0           R-164         CH-NB-HCN-H2H         0.306-13         0         0         0           R-164         CH-NB-HAH-H0H         0.306-13         0         0         0         0           R-164         CH-NB-HH1H         0.3         0	R-152	H+NCO=NH+CO	5.24E+13	0	0
R-164         CH-NB-HCN-H4         0.006-13         0         0           R-155         CH-NB-HCN-H4H         3.006-13         0         0           R-157         CH-NB-HCN-H4H         2.306-13         0         0           R-156         CH-NB-HCN-H4H         2.306-13         0         0           R-156         CH-NB-HCN-H4H         2.306-13         0         0           R-156         CH-NB-HCN-H4H         2.306-13         0         0           R-157         CH-NB-HCN-H4H         2.306-13         0         0           R-158         CH-NB-HCN-H2H         2.306-13         0         0           R-164         CH-NB-HCN-H2H         0.306-13         0         0           R-164         CH-NB-HCN-H2H         0.306-13         0         0         0           R-164         CH-NB-HAH-H0H         0.306-13         0         0         0         0           R-164         CH-NB-HH1H         0.3         0	R-153	CH+N=CN+H	1.26E+13	0	0
R-55         OH-MBCHNHHH         300E-13         0         0           R-55         OC2N-HICMH         500E-13         0         0           R-55         OC2N-HICMH         300E-13         0         0           R-56         OC2N-HICMH         300E-13         0         0           R-59         C2N-HICM-CH2         200E-13         0         0           R-50         OC2N-HICM-CH2         302E-13         0         0         0           R-50         ONHEA-CH2         302E-13         0         0         0           R-50         ONHEA-CH2         302E-13         0         0         0           R-56         ONHEA-CH4         8.50E-11         0         0         0.00           R-56         ONHEA-CH4         8.50E-11         0         0         0.02           R-56         ONHEA-CH4         1.00E-13         0         0.02           R-56         ONHEA-CH4         1.00E-13         0         0.02           R-57         ONHEA-CH4         1.00E-13         0         0.02           R-56         ONHEA-CH4         1.00E-13         0         0           R-57         OHHACHACH4         1.00E-13 <td></td> <td></td> <td></td> <td></td> <td></td>					
R18         CH2NHCNHH         5.00E13         0         0           R157         CH2NHCNHH         3.00E13         0         3.0           R158         CH2NHCNHH         3.00E13         0         3.0           R161         CH2NHCNHH         2.00E13         0         3.0           R161         CH2NHCNHH         2.00E13         0         0         0           R161         CH2CHHNHCH2CAPL         3.72E13         0         0         0           R163         CH2CHHNHCH2CAPL         5.00E13         0         0         0           R163         CHRCHNHCH2CH         5.00E13         0         2.0         2.0           R164         CHRCHNHCH2CH         5.00E13         0         2.0         2.0           R165         CHNHCH2CH         5.00E13         0         2.2         2.0           R165         CHNHCH2CH         5.00E13         0         2.2         2.4           R167         CHNHCH2CH         5.00E13         0         2.2         4.2           R167         CHNHCH2CH         5.00E13         0         0         0           R167         CHNHCH2CH         5.00E13         0         0					
R-167         OE2NH=NCM+HH         300E+13         0         10           R-169         OE3NN=H2CM+H         2,05E+14         0         3.5           R-169         OE3NN=H2CM+H2CM+C2P2         1220E+13         0         0         0           R-161         DE3NN=H2CM+C3P2         1272H-13         0         0         0         0           R-162         ONH-HOH         6.55E+13         0         0         0         0           R-164         ONH2=NH-OH         6.55E+13         0         0         2.0           R-164         ONH2=NH-OH         6.05E+14         -0.5         1.4           R-164         ONH2=NH-OH         0.05E+14         -0.5         1.4           R-166         ONH2=NH-OH         1.05E+14         -0.2         -0.2           R-167         ONH2=NH-OH         1.05E+13         0         0         0           R-168         OHHO-OH-NO         1.05E+13         0         0         0         0           R-170         ON-MCO-HO-CO         3.16E+13         0         0         0         0         0         0         0         0         0         0         0         0         0         0         <					
Resist         CH3N+B2CNH         2.568+14         0         3.5           Resist         C203+H4ECN-CH22         2.002+13         0         0           Resist         C203+H4ECN-CH22         1.002+13         0         0           Resist         C203+H4ECN-CH22         0.025+13         0         0         0           Resist         C305+13         0         0         0         0           Resist         CM3D-WHC         6.002+11         0.3         0.68           Resist         CM4D-HMC-HMC         1.002+13         0         2.028           Resist         CM4D-HMC-HMC         1.002+13         0         2.028           Resist         CM4NH-HACH         1.002+13         0         2.028           Resist         CM4NH-HACH         1.002+13         0         0         0           Resist         CM4NH-HACH         1.002+13         0         0         0         0           Resist         CM4NH-HACH         1.002+13         0         0         0         0           Resist         CM4NH-HACH         1.002+13         0         0         0         0         0         0         0         0         0					
R-150         C244+HCM-CH2         2.00E+13         0         0           R-150         C4CCH+HA/CH2/24         1.02E+13         0         0         0           R-151         C-HB-NOH         0.372E+13         0         0         0           R-151         C-HB-NOH         0.372E+13         0         0         0           R-164         O+HB2-NHOH         0.82E+14         -0.5         1.4           R-164         O+HB2-NHOH         0.02E+13         0         2.02           R-165         O+HB2-NHOH         1.02E+13         0         2.02           R-168         O+HB2-NHOH         0.02E+11         0.5         2.4           R-169         O+HNO-CH4         1.02E+13         0         0         0           R-169         O+HOO-CH4         1.02E+13         0         0         0         0           R-170         O+HNO-CO         3.0E+11         0.4         0.5         8.3           R-171         OH-HNO+HO         0.0E+10         0.4         0.5         8.3           R-170         OHHNO-HO         0.0E+10         0.4         0.5         8.3           R-170         OHHNO+HO         0.0E+10         0.4			3.00E+13	0	
R-160         H2CCHN+ICM-CB2         1.06E+13         0         0           R-161         O-MHEN-OH         3.72E+13         0         0         0           R-162         O-MHEN-OH         6.56E+13         0         0         0           R-163         O-MHEN-OH         6.56E+13         0         0         0           R-163         O-MHEN-OH         0.02E+14         0.3         2.04           R-164         O-MNEN-ROCH         1.02E+13         0         1.02           R-167         O-MNEN-ROCH         1.02E+13         0         1.02           R-167         O-MNEN-ROCH         1.02E+13         0         0         0           R-167         O-MNEN-ROCH         1.02E+13         0         0         0           R-170         O-MONO-MO         1.02E+13         0         0         0           R-171         O-MEN-NOCH         1.02E+13         0         0         0           R-172         O-MEN-NOCH         1.02E+13         0         0         0           R-173         O-MEN-NOCH         5.0E+11         0.5         8.3           R-173         O-MEN-NOCH         5.0E+13         0         0 <t< td=""><td>R-158</td><td>CH3+N=H2CN+H</td><td>2.59E+14</td><td>0</td><td>3.5</td></t<>	R-158	CH3+N=H2CN+H	2.59E+14	0	3.5
R-160         H2CCHN+ICM-CB2         1.06E+13         0         0           R-161         O-MHEN-OH         3.72E+13         0         0         0           R-162         O-MHEN-OH         6.56E+13         0         0         0           R-163         O-MHEN-OH         6.56E+13         0         0         0           R-163         O-MHEN-OH         0.02E+14         0.3         2.04           R-164         O-MNEN-ROCH         1.02E+13         0         1.02           R-167         O-MNEN-ROCH         1.02E+13         0         1.02           R-167         O-MNEN-ROCH         1.02E+13         0         0         0           R-167         O-MNEN-ROCH         1.02E+13         0         0         0           R-170         O-MONO-MO         1.02E+13         0         0         0           R-171         O-MEN-NOCH         1.02E+13         0         0         0           R-172         O-MEN-NOCH         1.02E+13         0         0         0           R-173         O-MEN-NOCH         5.0E+11         0.5         8.3           R-173         O-MEN-NOCH         5.0E+13         0         0 <t< td=""><td>R-159</td><td>C2H3+N=HCN+CH2</td><td>2.00E+13</td><td>0</td><td>0</td></t<>	R-159	C2H3+N=HCN+CH2	2.00E+13	0	0
R-161         O-MHENOH         3.72E-13         0         0           R-162         O-MHENOH         6.50E+13         0         0           R-163         O-MHEZ-MH-OH         6.50E+11         0.3         0.4           R-164         O-MHEZ-MH-OH         6.50E+11         0.3         0.4           R-164         O-MHEZ-MH-OH         6.50E+13         0         1.6           R-165         O-MHEX-MH-OH         1.50E+13         0         0         2.4           R-166         O-MHEX-MH-OH         5.51E+11         0.6         8.3           R-167         O-MONCOH-NO         5.51E+11         0.6         0         0           R-177         O-MEX-OFN         1.10E+13         0					
R-R22         O-HNRCHMCH         5.50E-13         0         0           R-R43         O-HNRCHMCH         6.50E-11         0.3         0.5           R-R46         O-HNRCHMCH         6.80E-11         0.3         0.6           R-R46         O-HNRCHMCH         6.80E-11         0.3         0.2           R-R46         O-HNRCHACH         1.02E-13         0         0.2           R-R47         O-HNRCHACH         1.02E-13         0         0         0           R-R48         O-HNRCHACH         1.02E-13         0         0         0           R-R49         O-HNRCHACH         1.02E-13         0         0         0           R-R47         O-HNRCHACHACH         1.02E-13         0         0         0           R-77         O-HNRCHACHACH         1.02E-13         0         0         0           R-77         O-HNRCHACHACH         1.02E-13         0         0         0           R-77         O-HNRCHACHACHACHACHACHACHACHACHACHACHACHACHAC					
R-163         O+M22HNCH         0.3         0.3           R-164         O+M22HNCH         0.50E+13         0         20.5           R-165         O+MNHA2CH         1.00E+13         0         12.5           R-166         O+MNHA2CH         1.00E+13         0         12.5           R-167         O+MNHA2CH         1.00E+13         0         12.5           R-167         O+MNHA2CH         1.00E+13         0         0           R-167         O+MNHA2CH         1.00E+12         0.5         0.5           R-170         O+NO-ONO-ONO-ONO         1.00E+13         0         0         0           R-171         O+NNHANCH         1.00E+12         0.5         0.8         8           R-172         O+NNHANCH         5.01E+11         0.5         8.3           R-173         O+NNHANCH         5.01E+11         0.5         8.3           R-173         O+NNHANCH         5.01E+11         0.5         8.3           R-175         O+NNHANCH         5.01E+11         0.5         0         0           R-175         O+NNOHONOHON         5.01E+11         0.5         0         0         0           R-175         O+NNOHONOHONOHONOHO					
R-164         O-NN2=NNO-H         6.53         1.4           R-165         O-NNHH-N2O-H         1.00E+13         0         20.8           R-166         O-NNHH-N2O-H         1.00E+13         0         20.8           R-167         O-NNHH-N2O-H         1.00E+13         0         20.8           R-169         O-NNHH-N2O-H         1.05E+14         4.2         4.2           R-169         O-NNHH-N2O-H         0.0         0         0         0           R-170         O-HNHH-NAO-H         1.00E+12         0.5         8.5           R-171         O-HNHH-NAO-H         1.00E+12         0.5         6.3           R-172         O-HNH2=O-MH3         0.90E+11         0.5         6.3           R-173         O-HNH2=O-MH3         0.90E+11         0.5         6.3           R-174         O-HNH2=O-MH3         0         0         0         0           R-175         O-HNH2=O-MH3         0 <td></td> <td></td> <td></td> <td></td> <td></td>					
R-165         O+NNH-R2-OH         1.00E+13         0         20.8           R-166         O+NNH-R2-OH         1.00E+13         0         20.8           R-167         O+NNH-NH-NO         1.00E+13         0         20.8           R-168         O+NNO-OHNO         5.01E+11         0.5         8.3           R-169         O+NNO-ONN-CO         1.01E+11         0.5         8.3           R-170         O+NNO-ONN-CO         1.02E+12         0.5         8.3           R-172         O+HNH-NH-ON         1.02E+12         0.5         8.3           R-172         O+HNH-NH-ON         1.02E+12         0.5         8.3           R-173         OH-HND2-NH-NH-20         3.02E+13         0         0         0           R-174         OH-HND2-NH-H20         3.02E+13         0         0         0         0         0           R-175         OH-HND2-NH-H20         3.02E+13         0         0         0         0         0         0           R-175         OH-HND2-NH-H20         0.02E+13         0         0         0         0         0         0           R-175         OHHND2-NH-H20         0.02E+13         0         0         0	R-163				
R-166         O-NNH-N2O-H         1.00E+13         0         12.5           R-167         O-NNH-N4NO         1.65E+14         -0.2         -4.2           R-168         O-HNO-OH+NO         5.01E+11         0.5         6.3           R-168         O-HOC-ON         1.02E+13         0         0           R-170         O-HOC-ON-N         1.02E+13         0         0           R-171         O-HOME-NHO-OH         1.02E+13         0         0           R-172         O-HHME-NHO-OH         1.02E+13         0         0           R-173         O-HHME-NHO-OH         5.01E+11         0.5         8.3           R-174         O-HHME-NHHO         5.01E+11         0.5         8.3           R-175         O-HHME-NHHO         1.06E+13         0         0         0           R-176         O-HHMO-NHO         1.06E+13         0         0         0         0           R-176         O-HHMO-NHO         1.06E+13         0         0         0         0           R-176         O-HHMO-NHO         1.06E+13         0         0         0         0           R-176         O-HHMO-NHO         0         0         0         0	R-164		8.93E+14	-0.5	
R-167         O-NNH-NH-NO         1.65E+14         -0.2         -4.2           R-168         O-HNO-OH+NO         5.01E+11         0.5         8.3           R-169         O-HNO-CH-CO         3.16E+13         0         0           R-171         OH-HANEHNOHH         1.00E+12         0.5         8.3           R-172         OH-HANEHNOHH         0.501E+11         0.5         8.3           R-173         OH-HANEHNALGO         5.01E+11         0.5         8.3           R-173         OH-HANE-AD-NH33         0.30E+12         0.5         8.3           R-174         OH-HANE-AD-NH30         5.01E+11         0.5         8.3           R-175         OH-HANE-AD-NH420         5.01E+11         0.5         8.3           R-176         OH-HANE-AD-NH420         5.02E+13         0         0         0           R-177         OH-HOCANO-CO-H         1.00E+13         0         0         0         0         0           R-177         OH-HOCANO-CO-H         1.02E+13         0         0         0         0         0         0           R-178         OH-HOCANO-CO-H         1.02E+13         0         0         0         0         0         0	R-165	O+NNH=N2+OH	1.00E+13	0	20.8
R-167         O-NNH-NH-NO         1.65E+14         -0.2         -4.2           R-168         O-HNO-OH+NO         5.01E+11         0.5         8.3           R-169         O-HNO-CH-CO         3.16E+13         0         0           R-171         OH-HANEHNOHH         1.00E+12         0.5         8.3           R-172         OH-HANEHNOHH         0.501E+11         0.5         8.3           R-173         OH-HANEHNALGO         5.01E+11         0.5         8.3           R-173         OH-HANE-AD-NH33         0.30E+12         0.5         8.3           R-174         OH-HANE-AD-NH30         5.01E+11         0.5         8.3           R-175         OH-HANE-AD-NH420         5.01E+11         0.5         8.3           R-176         OH-HANE-AD-NH420         5.02E+13         0         0         0           R-177         OH-HOCANO-CO-H         1.00E+13         0         0         0         0         0           R-177         OH-HOCANO-CO-H         1.02E+13         0         0         0         0         0         0           R-178         OH-HOCANO-CO-H         1.02E+13         0         0         0         0         0         0	R-166	O+NNH=N2O+H	1.00E+13	0	12.5
R-168         O+HNO-OH+NO         5.01E+11         0.5         8.3           R-169         O+CN-CO-N         1.02E+13         0         0           R-170         O+CN-CO-N         3.16E+13         0         0           R-171         O+HNN+HNO+H         1.00E+12         0.5         8.3           R-172         O+HNN+N+HZO         5.01E+11         0.5         8.3           R-173         O+HNR2-NH-N2O         5.01E+11         0.5         6.3           R-174         O+HNR2-NH-N2O         3.16E+13         0         0         0           R-174         O+HNR2-NH-N2O         3.16E+13         0         0         0           R-177         O+HNR2-NH-N2O         3.16E+13         0         0         0           R-177         O+HNR2-ND-NO-H2O         3.02E+13         0         0         0           R-177         O+HACD-NO-H2O         3.02E+13         0         0         0           R-177         O+HACD-NO-H2O         3.02E+13         0         0         0           R-178         O+HACD-NO-H2O         3.02E+13         0         0         0           R-180         N-NNMARCM         6.32E+15         0         0					
R-169         O+CN-CO+N         1.02E+13         0         0           R-170         O+NCG-NO+CO         3.16E+13         0         0           R-171         OH+NN=HNO+H         1.00E+12         0.5         8.3           R-172         OH+NN=HNO+H         0.5         8.3           R-173         OH+NN=HN2>O+NH3         5.01E+11         0.5         8.3           R-173         OH+NN=HN2>O+NH3         5.01E+11         0.5         8.3           R-174         OH+NN=HN2+O         5.01E+11         0.5         8.3           R-175         OH+NN=HN2+O+NH2O         5.01E+11         0.5         0.0         0           R-177         OH+NO=NO+OH         1.00E+13         0         0         0           R-178         OH+NO=NO+OCH         5.00E+13         0         0         0           R-180         HO2+NH2=HNO+H2O         5.00E+13         0         0         0           R-181         HCO-N+NHON+OCH         5.00E+13         0         0         0           R-184         N+NH=N2+H         6.31E+11         0.5         0         0           R-184         N+NH=N2+H         6.31E+13         0         0         0 <t< td=""><td></td><td></td><td></td><td></td><td></td></t<>					
R-170         O*NGC=NO-CO         3.16E+13         0         0         0           R-171         OH+NN=NO+H         1.00E+12         0.5         8.3           R-172         OH+NN=NO+H         0.5         8.3           R-173         OH+NN=2-NH-H20         5.01E+11         0.5         8.3           R-174         OH+NNE2-NH-H20         5.01E+11         0.5         8.3           R-174         OH+NNE2-NH-H20         3.16E+13         0         0         0           R-176         OH+NNE-NCH-QCH         6.02E+13         0         0         0           R-177         OH+NCO-NCH-QCH         6.02E+13         0         0         0         0           R-177         OH+NCO-NCH-H20         1.00E+13         0         0         0         0           R-178         OH+NCO-NCH-H20         1.00E+13         0         0         0         0           R-178         OH+NCO-NCO-H20         1.00E+13         0         0         0         0           R-1818         NHMENTHH         6.02E+13         0         0         0         0           R-182         NHMENTHH         6.31E+11         0.5         0         0         0					
R-171         OH-NH-HNO-H         0.00E+12         0.5         8.3           R-172         OH-NH-HH2O         5.01E+11         0.5         8.3           R-173         OH-NH2->O+NH3         1.99E+10         0.4         2.1           R-174         OH-NH2->O+NH3         1.99E+10         0.4         2.1           R-175         OH+NNE-NH2+QD         5.01E+11         0.5         8.3           R-175         OH+NNE-N2+H2D         3.16E+13         0         0           R-176         OH-NCN-NO-H2D         1.05E+13         0         0           R-177         OH-NCNO-NHCO         5.00E+13         0         0           R-178         OH-NCO-NO-HCO         1.05E+13         0         0           R-178         OH-NCO-NO-HCO         1.05E+13         0         0         0           R-181         HO2-NNE-HO+H2O         1.57E+13         0         0         0         0         0         0           R-182         N+NHA-R2+M         6.50E+13         0         0         0         0         0         0           R-184         N+NHA-R2+M         6.31E+11         0.5         0         0         0         0         0      <					
R-172         OH-NH=N+H2D         5.01E+11         0.5         8.3           R-173         OH-NH2=OHH3         5.01E+11         0.5         8.3           R-174         OH-NH2=OHH3         0         0         0           R-175         OH-NN=NH2H0         3.16E+13         0         0         0           R-176         OH-NN=NH2H0         6.02E+13         0         0         0           R-177         OH-NOCO-H         6.02E+13         0         0         0           R-178         OH-NOCO-H         6.00E+12         0         62.8           R-179         OH-NOCO-NO-GO+H         1.00E+13         0         0         0           R-180         H02-NH2=NNCH20         1.57E+13         0         0         0           R-181         HCCO-NH2H0         5.32E+15         0         0         0           R-182         N+NH4P2H         6.52E+15         0         0         0         0           R-184         N+H02=N2+HH         6.33E+11         0.5         0         0         0         0           R-185         N+NH2=N2+H         3.16E+13         0         0         0         0         0         0					
R-173         OH+NH2>20+NH3         1.98E+10         0.4         2.1           R-174         OH+NH2>HH2O         5.01E+11         0.5         8.3           R-175         OH+NNH=N2+H2O         3.16E+13         0         0           R-176         OH+NNE+N2+H2O         1.08E+13         0         0           R-177         OH+CN=NCO+H         6.02E+13         0         0           R-178         OH+NCO=NO+OCO-H         1.00E+12         0         6.22           R-179         OH+NCO=NO+OCO-H         1.00E+13         0         0         0           R-180         HO2*NEP-NO+H2O         1.57E+13         0         0         0           R-181         HCOCO+N=HCA+CO         5.00E+12         0         0         0           R-182         N+NH-NEPAH         6.31E+13         0         0         0           R-183         N+NH=NEPAH         6.31E+13         0         0         0           R-184         N+NH=NEPAH         6.31E+13         0         0         0           R-186         N+NH=NEPAH         0         0         0         0           R-186         N+NH=NEPAH         0         0         0         0					
R-174         OH+NH2=NH+H2D         5.0TE+11         0.5         8.3           R-175         OH+NNE-NE42D         3.0EE+13         0         0         0           R-176         OH+NND-NOCH2D         1.0EE+13         0         0         0           R-177         OH+CNENCOH         6.0ZE+13         0         0         0           R-178         OH+NCO-NO+HCO         5.0DE+12         0         6.2Z           R-179         OH+NCO-NO+CO+H         1.0DE+13         0         0         0           R-180         HO2 <nh22hno+h2d< td="">         5.0DE+13         0         0         0           R-181         HCCO-NH-NO-NCO         6.52E+15         0         0         0           R-182         N=NHAP2H         6.52E+15         0         0         0           R-183         N=NHAP2H         6.31E+11         0.5         0         0           R-184         N=NH2P2H         1.31E+14         0         0         0         0           R-186         N=NCN=O-N2         2.20E+13         0         0         0         0           R-186         N=NCN=O-N2         2.27E+13         0         0         0         0         0</nh22hno+h2d<>	R-172	OH+NH=N+H2O	5.01E+11	0.5	8.3
R-174         OH+NH-2N+H2D         5.01E+11         0.5         6.3.           R-175         OH+NNE-N2H2D         3.16E+13         0         0         0           R-176         OH+NNC-NOCH4D         1.06E+13         0         0         0           R-177         OH+CN-NOCH4         6.02E+13         0         0         0           R-178         OH+NCO-NO+FCO-H         1.00E+13         0         0         0           R-180         HO2-NN2=HNO+H2D         1.57E+13         0         0         0           R-181         HCCO-NH-HCN+CO         5.00E+13         0         0         0           R-181         HCCO-NH-HCN+CO         6.51E+11         0.5         0         0           R-182         N=NH=N2+H         6.51E+11         0.5         0         0         0           R-184         N=NH2-N2+HH         6.31E+11         0.5         0	R-173	OH+NH2=>O+NH3	1.99E+10	0.4	2.1
R-175         OH+NNI=N2+H2O         3.16E+13         0         0         0           R-176         OH+NOPOH+D2O         1.08E+13         0         0         0           R-177         OH+NCO-NH2CO+H         6.02E+13         0         0         6.28           R-179         OH+NCO-NO+HCO         5.00E+12         0         6.28           R-179         OH+NCO-NO+CO+H         1.00E+13         0         0         0           R-180         HO2C+ND+CO         5.00E+13         0         0         0           R-181         HCCO+N=HCN+CO         5.00E+13         0         0         0           R-181         N=NME-N2+H         6.31E+11         0.5         0         0           R-183         N=NH=N2+H         6.31E+11         0.5         0					
R-176         OH+HNO-NO+H2O         1,08E+13         0         0         0           R-177         OH+CN-NO+HCO+         6,02E+13         0         0         0           R-178         OH+NCO-NO+HCO         1,00E+13         0         0         0           R-190         H-DCO-NO+HCO         1,07E+13         0         0         0           R-181         HCO-NH-HCO+HZO         5,00E+13         0         0         0           R-181         HCO-NH-HCHCHCO         5,00E+13         0         0         0           R-182         N+NH-NEX-M         6,52E+15         0         0         0           R-183         N-NHI-NZ+H         6,52E+13         0         0         0           R-184         N-NHI-NZ+H         6,52E+13         0         0         0           R-185         N-NHN-NH+NH-NZ         3,16E+13         0         10         0           R-186         N-NHO-SC+NZ         1,81E+14         0         0         0         0           R-187         C-N2>N+CN         2,206E+13         0         0         0         0           R-188         N+H2CN-N2+CH2         2,206E+13         0         0         0 <td></td> <td></td> <td></td> <td></td> <td></td>					
R:177         OH+CN=NCO+H         6,02E+13         0         0         0           R:179         OH+NCO=NO+COCH         1,00E+13         0         0         0           R:190         HO2+ND+ZPNO+HZO         1,07E+13         0         0         0           R:181         HCCO=NN+ICN=CO         5,00E+13         0         0         0           R:182         N=NH=N2+M         6,32E+15         0         0         0           R:183         N=NH=N2+H         6,32E+15         0         0         0           R:183         N=NH=N2+H         6,32E+13         0         0         0           R:185         N=NNN=NENX=CH2         3,16E+13         0         8,3         0         0         0           R:186         N=NNN=NENX=CH2         3,16E+13         0         10         <					
R-178         OH+NCO=NO+CO+HC         5.00E+12         0         62.8           R-179         OH+NCO=NO+CO+H         1.00E+13         0         0         0           R-180         H02+NH2=HNO+H2O         1.57E+13         0         0         0           R-181         H0CO+N+HCN+CO         5.00E+13         0         0         0           R-182         N+HMEN2+M         6.52E+15         0         0         0           R-183         N+HEN2+H         6.33E+13         0         0         0           R-184         N+HH2+N2+H         6.33E+13         0         0         0           R-185         N+HNH=NE+H4         0         0         0         0         0           R-186         N+HNH=NE+H4         0         0         0         0         0         0           R-186         N+CN=NE-CH2         2.00E+13         0         0         0         0         0         0           R-186         N+H2C=NE2CH2         2.00E+13         0         0         0         0         0         0           R-180         N+H2C=NE2CH2         2.00E+13         0         0         0         0         0         0					
R-199         OH+NCO=N0+CO+H         1.00E+13         0         0           R-180         HO2+NH2HN0+RO         1.57E+13         0         0         0           R-181         HCCO+N+CO         5.00E+13         0         0         0           R-182         N+NH=N2+M         6.52E+15         0         0         0           R-183         N+NH=N2+H         6.31E+11         0.5         0         0           R-184         N+NH=Z+H         6.31E+11         0.5         0         0         0           R-185         N+NNE=N2+N+H         3.16E+13         0         8.3         3         0         8.3           R-186         N+NCN=SC+N2         1.81E+14         0         0         0         167.9           R-188         N+H2CN=N2-CH2         2.00E+13         0         177.2         2.00E         1.99E+13         0 </td <td></td> <td></td> <td></td> <td></td> <td></td>					
R-180         H02+NH2=ND+H20         1.57E+13         0         0         0           R-181         H020+NH2-NH20         5.00E+13         0         0         0           R-182         N+NH=N2+M         6.52E+15         0         0         0           R-183         N+NH=N2+H         6.31E+11         0.5         0         0           R-184         N+NH=N2+H         6.31E+11         0.5         0         0           R-184         N+NNH=N2+H         6.31E+11         0.5         0         0           R-185         N+NNH=N2+H         0         3.16E+13         0         8.3           R-186         N+CO=N2+CN2         1.81E+14         0         0         0           R-187         C+N2=N+CN         5.24E+13         0         167.9           R-188         N+CO=N0+CN         2.00E+13         0         0         0           R-189         N+NCO=N2+CP         2.00E+13         0         0         0           R-190         N+NCO=N2+CO         1.99E+13         0         0         0           R-191         N+HNH=N2+NH2+H         5.3E+13         0         4.9         0         4.9           R-192 <td></td> <td></td> <td></td> <td></td> <td></td>					
R-181         HCC0+N=HCN+CO         0         0         0         0           R-182         N+NH=N2+M         6.32E+15         0         0           R-183         N+NH=N2+M         6.31E+11         0.5         0           R-184         N+NH=N2+M         6.31E+13         0         0         0           R-185         N+NH=NH+N2         3.16E+13         0         0         0           R-185         N+NH=NH+N2         3.16E+13         0         0         0           R-186         N+CN=>C+N2         1.81E+14         0         0         0           R-187         C+N2=N+CN         2.00E+13         0         0         0           R-188         N+H2CN=N2+CH2         2.00E+13         0         0         0           R-190         N+NCO=N2+CO         1.99E+13         0         0         0           R-191         N+H+N2=N2H+H         5.13E+15         -0.5         0         0           R-192         N+H+NH=N2+N2H+H         5.13E+13         0         0         0           R-192         N+H+NH=N2+N2+N2+N2         2.00E+11         0.5         8.3         3.3           R-194         N+H+N2=N2H2+H					
R-182         N+N-M=N2+M         0         0         0           R-183         N+NH=N2+H         6.31E+11         0.6         0           R-184         N+NH=N2+N2+H+H         6.31E+11         0.6         0           R-185         N+NNH=N1+N2         3.16E+13         0         8.3           R-186         N=NN=N=N+N2         3.16E+13         0         8.3           R-186         N=CN=N2+CN2         1.31E+14         0         0         0           R-188         N=CO=N2+CN2         2.20E+13         0         167.9           R-189         N=NCO=N2+CO2         2.20E+13         0         0         0           R-190         N=NCO=N2+CO2         1.99E+13         0         0         0           R-191         NH+NH=N2+H+H         5.13E+13         0         0         0           R-192         N=HAN2=N2H2+H         2.20E+11         0.5         6.3           R-193         NH+NH=N2+NH2         2.20E+11         0.5         6.3           R-194         N=H+NH=N2+NH2         2.20E+11         0.5         4.5           R-195         NH2+NH2=NH2+NH2         3.39E+13         0         41.8           R-196         NH					
R-182         N+N-MA=N2+M         0         0         0           R-183         N+NH=N2+H         6.31E+11         0.5         0           R-184         N+NH=N2+N2+H+H         6.31E+11         0.5         0           R-185         N+NN=N1+N2         3.16E+13         0         8.3           R-186         N+NN=N1+N4         0         8.3           R-186         N-CN>2-CM2         1.31E+14         0         0         8.3           R-187         C+N2=>N+CN         5.24E+13         0         167.9           R-188         N+NCO=N0+CN2         2.00E+13         0         0         0           R-199         N+NCO=N0+CN         2.00E+13         0         0         0           R-191         N+H+N=N2+H+H         5.13E+13         0         0         0           R-192         N+H+N=N2+NH2         2.00E+11         0.5         6.3           R-194         N+H+M=N2+NH2         2.00E+11         0.5         0           R-194         N+H=N=N+H+M         7.57E+14         0         315.9           R-196         NH2+NH2=NH3+NH         7.57E+14         0         41.8           R-197         NH2+NH2=NH3+NH         5.00	R-181	HCCO+N=HCN+CO	5.00E+13	0	0
R+183         N+NH=N2+H         0.5         0           R-184         N+NH2N2+H         6.93E+13         0         0         0           R-185         N+NNH=N+H+N2         3.16E+13         0         8.3           R-185         N+NNH=N+H+N2         3.16E+13         0         8.3           R-186         N+CN=>C+N2         1.81E+14         0         0         0           R-187         C+N2=>N+CN         5.24E+13         0         187.9           R-188         N+H2CN=N2+CH2         2.00E+13         0         0         0           R-189         N+NCO=N0+CN         2.77E+18         -1         72.2           R-190         N+NC=N2+CO         1.99E+13         0         0         0           R-192         N+H=N2+H+H         5.13E+13         0         0         0           R-193         NH=NNE=N2+NH2         1.51E+15         -0.5         0           R-193         NH=NNE=N2+NH2         2.00E+11         0.5         8.3           R-195         NH2+NH2=NH3+NH         7.57E+14         0         315.9           R-196         NH2+NH2=NH3+NH         0         41.8         7.91E+23         -2         382.4					
R-184         N+NH2=N2+H+H         0         0         0           R-185         N+NNH=NH+N2         3.16E+13         0         8.3           R-186         N+CN=>C+N2         1.81E+14         0         0           R-187         C+N2=>N+CN         5.24E+13         0         167.9           R-188         N+H2CN=N2+CH2         2.00E+13         0         0         0           R-189         N+NCO=N0+CN         2.77E+18         -1         7.22           R-190         N+NCO=N0+CO         1.99E+13         0         0         0           R-191         NH+NH=N2+H+H         0         1.51E+15         -0.5         0           R-192         NH+NH=N2+H+H         1.51E+15         -0.5         0         0           R-192         NH+NN=N2+NH2         2.00E+11         0.5         8.3           R-193         NH=NN=N=N2+H2         3.98E+13         0         44.9           R-194         NH=N=N2+H2         0         345.9         0           R-195         NH2+NH2=N2H2+H2         3.98E+13         0         44.9           R-196         NH2+NH2=N2H3+NH         0         44.9           R-197         NH2+NH=N2+NH3+NH					
R+185         N+NNH=NH+N2         3.16E+13         0         8.3           R+186         N+CN=>C+N2         1.81E+14         0         0         0           R+187         C+N2=>N+CN         5.24E+13         0         187.9           R+188         N+H2CN=N2+CH2         2.00E+13         0         0         0           R+189         N+H2CN=N2+CH2         2.00E+13         0         0         0           R+190         N+NCO=N0+CN         2.77E+18         -1         772.2           R+190         N+NCO=N0+CN         2.00E+13         0         0         0           R+192         N+H+N12=N2H+1H         5.13E+13         0         0         0         0           R+192         N+H+N1=N2+1H+         2.00E+11         0.5         8.3         0         0         0         0         15.9           R+193         NH+NNH=N2+NH2         3.38E+13         0         49.9         7.37E+14         0         315.9           R+196         NH2+NH2=NH3+NH         5.00E+13         0         49.9           R+197         NH2+NH=N2+NH3         0         40.9         3.00E+13         0         42.4           R+198         NH2+NH=N2+NH3					
R+186         N+CN=>C+N2         1.81E+14         0         0         0           R+187         C+N2=>N+CN         5.24E+13         0         187.9           R+188         N+H2CN=N2+CH2         2.00E+13         0         0         0           R+189         N+NCO=N0+CN         2.77E+18         -1         72.2           R+190         N+NCO=N0+CN         2.77E+18         -1         72.2           R+191         N+H+NI=N2+H+H         0         0         0         0           R+192         NH+NH=N2+H+H         5.13E+13         0         0         0         0           R+192         NH+NH=N2+NH2         2.00E+11         0.5         8.3         3.3         0         0         315.9           R+194         NH+M2=N2H2+H         2.00E+11         0.5         44.9         3.96E+13         0         44.9           R+196         NH2+NH2=NH2NH3+NH         5.00E+13         0         44.9         44.9           R+197         NH2+MN=N2+NH3         0         44.9         0         0         0         44.8           R+198         NH2+NH=N2+NH3         0         0         0         0         0         0         0 <td< td=""><td></td><td></td><td></td><td></td><td></td></td<>					
$\begin{array}{c c c c c c c c c c c c c c c c c c c $					
R+188         N+H2CN=N2+CH2         0         0         0           R+189         N+NCO=N2+CO         2.77E+18         -1         72.2           R+190         N+NCO=N2+CO         1.99E+13         0         0         0           R+191         NH+NC=N2H2+H         5.13E+13         0         0         0           R+192         NH+NH=N2+H1+         5.13E+13         0.         0         0           R+192         NH+NNH=N2+NH2         2.00E+11         0.5         8.3           R+193         NH+NNH=N2+NH2         2.00E+11         0.5         8.3           R+194         NH+M=N+H+M         7.57E+14         0         315.9           R+195         NH2+NH2=N2H3+NH         5.00E+13         0         41.8           R+196         NH2+NH2=N2H3+NH         5.00E+13         0         41.8           R+197         NH2+NH=N2+NH3         0         0         0         0           R+198         NH2+NNH=N2+NH3         0					
R+189         N+NCO=N0+CN         2.77E+18         -1         72.2           R+190         N+NCO=N2+CO         1.99E+13         0         0         0           R-191         NH+NH=N2+H+H         5.13E+13         0         0         0           R-192         NH+NH=N2+H2H         1.51E+15         -0.5         0           R-193         NH+NH=N2+NH2         2.00E+11         0.5         8.33           R-194         NH+M=N2+NH2         2.00E+11         0.5         8.33           R-195         NH2+NH2=N2H22H         3.98E+13         0         49.9           R-196         NH2+NH2=N2H2H4         0         315.9           R-197         NH2+NH2=NH3*NH         0         44.9           R-198         NH2+NH2=NH3*NH         0         44.8           R-197         NH2+MN=N2+NH3         0         0         0           R-198         NH2+NN=N2+NH3         0         0         0         0           R-199         NH2+NN=N2+NH3         0         0         0         0           R-200         NNH=N2+H         0.50E+11         0.5         1.2.8           R-201         NNH=N2+H         3.00E+08         0         0					187.9
R+189         N+NCO=N0+CN         2.77E+18         -1         72.2           R+190         N+NCO=N2+CO         1.99E+13         0         0         0           R-191         NH+NH=N2+H+H         5.13E+13         0         0         0           R-192         NH+NH=N2+H2H         1.51E+15         -0.5         0           R-193         NH+NH=N2+NH2         2.00E+11         0.5         8.33           R-194         NH+M=N2+NH2         2.00E+11         0.5         8.33           R-195         NH2+NH2=N2H22H         3.98E+13         0         49.9           R-196         NH2+NH2=N2H2H4         0         315.9           R-197         NH2+NH2=NH3*NH         0         44.9           R-198         NH2+NH2=NH3*NH         0         44.8           R-197         NH2+MN=N2+NH3         0         0         0           R-198         NH2+NN=N2+NH3         0         0         0         0           R-199         NH2+NN=N2+NH3         0         0         0         0           R-200         NNH=N2+H         0.50E+11         0.5         1.2.8           R-201         NNH=N2+H         3.00E+08         0         0			2.00E+13		
R+190         N+NC0=N2+CO         1.99E+13         0         0         0           R-191         NH+NH=N2+HH         5.13E+13         0         0         0           R-192         NH+NH=N2+HH         5.13E+13         0         0         0           R-193         NH+NNE=N2+NH2         1.51E+15         -0.5         0           R-194         NH+NN=N+N+M         0         315.9         8.3           R-195         NH2+NH2NH2NH2         3.38E+13         0         49.9           R-196         NH2+NH2=NH3+NH         0         41.9           R-197         NH2+MN=N2+H14         0         41.9           R-196         NH2+NH2=NH3+NH         5.00E+13         0         43.9           R-197         NH2+MN=N2+NH3         0         0         43.9           R-198         NH2+NN=N2+NH3         0         0         0         0           R-198         NH2+NN=N2+NH3         0 <td>R-189</td> <td>N+NCO=NO+CN</td> <td>2.77E+18</td> <td>-1</td> <td></td>	R-189	N+NCO=NO+CN	2.77E+18	-1	
R-191         NH+NH=N2+H+H         5.13E+13         0         0         0           R-192         NH+NH=N2+HH         1.51E+15         -0.5         0           R-193         NH+NN=N2+NH2         2.00E+11         0.5         8.3           R-194         NH+NN=N2+NH2         2.00E+11         0.5         8.3           R-195         NH2+NH2=N2H2H2         3.98E+13         0         49.9           R-196         NH2+NH2=N2H2H2         3.98E+13         0         49.9           R-196         NH2+NH2=NH3NH         0         41.8           R-197         NH2+NH=N2+NH3         0         41.8           R-198         NH2+NN=N2+NH3         0         0           R-199         NH2+NN=N2+NH3         0         0         0           R-199         NH2+NN=N2+NH3         0         0         0         0           R-200         NNH=N2+H         0.5         1.00E+13         0         0         0           R-201         NNH=N2+H         0.5         0         0         0         0         0           R-201         NNH=N2+H         0.5         0         0         0         0         0         0         0					
R-192         NH+NH2=N2H2+H         1.51E+15         -0.5         0           R-193         NH+NH=N2+NH2         2.00E+11         0.5         8.3           R-194         NH+M=N2+NH2         0         315.9           R-195         NH2+NH2=N2H2+H2         3.39E+13         0         49.9           R-196         NH2+NH2=NAHANH         0         315.9           R-197         NH2+NH2=NH3+NH         0         41.8           R-197         NH2+NN=NH2+NH3         0         41.8           R-198         NH2+NN=NH4+M         0         0         0           R-198         NH2+NN=NAS+NO         5.01E+11         0.5         4.2           R-200         NNH=N2+H         0         0         0         0           R-201         NNH=N2+H         0.5.01E+11         0.5         4.2           R-200         NNH=N2+H         3.00E+08         0         0         0           R-201         NNH+M=N2+H+M         0.5.01E+11         0.5         1.02           R-202         NNH+N2=N2+M3         0.5         1.02         0         0         0         0         0         0         0         0         0         0         0					
R-193         NH+NNH=N2+NH2         2.00E+11         0.5         8.3           R-194         NH+M=N+H+M         7.57E+14         0         315.9           R-195         NH2+NH2=N2H2+H2         3.38E+13         0         449.9           R-196         NH2+NH2=N2H3+NH         0         449.9           R-197         NH2+NH3=NH4+M         0         0         41.8           R-197         NH2+NH=NH+H+M         7.91E+23         -2         382.4           R-198         NH2+NN=N2+NH3         0         0         0         0           R-199         NH2+NN=N2+NH3         0         0         0         0         0           R-199         NH2+HNO=NH3+NO         5.01E+13         0.5         4.2           R-200         NNH=N2+H         3.00E+08         0         0         0           R-201         NNH=N2+H         0.5.00E+13         0.5         12.8           R-202         NNH=N2+H+M         2.50E+13         0.5         12.8           R-203         N2H3+M=N2/2+H+M         0         0         0           R-204         NHH=N2+H+M         2.50E+16         0         174.6           R-205         HNO+M=H>N2+H+M					
R-194         NH+M=N+H+M         7.57E+14         0         315.9           R-195         NH2+NH2=N2H2H42         3.98E+13         0         49.9           R-196         NH2+NH2=N2H2+H2         0         49.9           R-197         NH2+NH2=NH3+NH         0         49.9           R-197         NH2+NN=N2+NH3         0         49.9           R-198         NH2+NN=N2+NH3         0         0           R-198         NH2+NN=N2+NH3         0         0           R-199         NH2+NN=N2+NH3         0         0         0           R-199         NH2+NN=N2+NH3         0.5         0         0           R-200         NNH=N2+H         0.5         0.5         12.8           R-201         NNH=N2+H         0.5         0         0           R-202         NNH=N2+H02         0.00E+08         0         0           R-203         N2H3+M=N22+H02         5.00E+13         0.5         12.8           R-204         NH1+02=N2+H02         0         0         0           R-203         N2H3+M=N22+HH4         2.50E+16         0         127.6           R-204         N2H3+M=N22+NH+M         2.50E+16         0         127.6					
R+195         NH2+NH2=N2H2+H2         3.98E+13         0         49.9           R-196         NH2+NH2=NH3+NH         5.00E+13         0         41.8           R-197         NH2+MN=NH2=NH3+NH         5.00E+13         0         41.8           R-198         NH2+NN=NQ2+NH3         -2         382.4           R-199         NH2+HNO=NR3+NO         0         0         0           R-200         NNH=N2+H         0.5         4.2           R-201         NNH+N0=NR3+NO         5.01E+11         0.5         4.2           R-202         NNH+N2+H         3.00E+08         0         0         0           R-202         NNH+O2=N2+HO2         5.00E+12         0         0         0           R-203         N2H3+M=N2H+HM         2.50E+16         0         207.8           R-204         N2H3+M=N2H2+H+M         2.50E+16         0         174.6           R-203         N2H3+M=N2H+H+M         2.50E+16         0         207.8           R-204         N2H3+M=N2H+H+M         2.50E+16         0         203.7           R-205         HNO+M=H+NO+M         5.00E+14         0         203.7           R-206         H2CN+M=HCN+H+M         5.00E+15         0					
R-196         NH2+NH2=NH3+NH         0         41.8           R-197         NH2+ME-NH3+NH+M         7.91E+23         -2         382.4           R-198         NH2+NNH=M2×NH3         0         0         0         0           R-198         NH2+NNH=M2×NH3         0         0         0         0         0         0         0           R-198         NH2+NN=M2×NH3         0.501E+11         0.5         4.2         2         3.02         0					
R-197         NH2+M=NH+H+M         7.91E+23         -2         382.4           R-198         NH2+NNH=N2+NH3         0         0         0           R-199         NH2+NN=N2+NH3         0.0E+13         0         0         0           R-199         NH2+NN=N2+NH3         0.5         4.2         3.00E+11         0.5         4.2           R-200         NNH=N2+H         3.00E+08         0         0         0           R-201         NNH=N2+H         3.00E+13         0.5         12.8           R-202         NNH+0=N2+H+M         2.50E+13         0.5         12.8           R-203         N2H3+M=N2H2+H+M         2.50E+16         0         207.8           R-204         N2H3+M=N2H2+H+M         2.50E+16         0         174.6           R-205         HNO+M=H+NO+M         5.90E+16         0         1203.7           R-206         H2CN+M=HCN+H+M         5.90E+16         0         203.7           R-206         H2CN+M=HCN+H+M         0         92.37.7           R-206         H2CN+M=HCN+H+M         0         195.4					
R-197         NH2+M=NH+H+M         7.91E+23         -2         382.4           R-198         NH2+NNH=N2+NH3         0         0         0           R-199         NH2+NN=N2+NH3         0.0E+13         0         0         0           R-199         NH2+NN=N2+NH3         0.5         4.2         3.00E+11         0.5         4.2           R-200         NNH=N2+H         3.00E+08         0         0         0           R-201         NNH=N2+H         3.00E+13         0.5         12.8           R-202         NNH+0=N2+H+M         2.50E+13         0.5         12.8           R-203         N2H3+M=N2H2+H+M         2.50E+16         0         207.8           R-204         N2H3+M=N2H2+H+M         2.50E+16         0         174.6           R-205         HNO+M=H+NO+M         5.90E+16         0         1203.7           R-206         H2CN+M=HCN+H+M         5.90E+16         0         203.7           R-206         H2CN+M=HCN+H+M         0         92.37.7           R-206         H2CN+M=HCN+H+M         0         195.4					
R-198         NH2+NNH=N2+NH3         1.00E+13         0         0         0           R-199         NH2+HN0=NH3+NO         5.01E+11         0.5         4.2           R-200         NNH=N2+H         3.00E+08         0         0           R-201         NNH+M=N2+H+M         2.50E+13         0.5         12.8           R-202         NNH=N2+HO         5.00E+12         0         0         0           R-203         N2H3+M=N2H2+H+M         2.50E+16         0         207.8           R-204         N2H3+M=N2H+H         2.50E+16         0         174.6           R-205         HNO+M=H+NO+M         5.90E+16         0         203.7           R-206         H2CN+M=HCN+H+M         7.50E+14         0         92           R-207         NCO-M=N+CO+M         2.91E+15         0         195.4					
R+199         NH2+HNO=NH3+NO         5.01E+11         0.5         4.2           R-200         NNH=N2+H         3.00E+08         0         0         0           R-201         NNH=N2+H         0.50E+13         0.5         12.8           R-202         NNH=N2+H+M         0.50E+13         0.5         12.8           R-203         N2H3+M=N2P2+H2M         0         0         0           R-204         N2H3+M=N2P2+H1+M         2.50E+16         0         207.8           R-205         HNO+M=H+NO+M         2.50E+16         0         174.6           R-206         H2CN+M=HCN+H+M         0         203.7           R-206         H2CN+M=HCN+H+M         0         92.9           R-207         NCO-M=N+CO+M         2.91E+15         0         195.4					
R-200         NNH=N2+H         3.00E+08         0         0           R-201         NNH+M=N2+H+M         2.50E+13         0.5         12.8           R-202         NNH+O2=N2+HO2         5.00E+12         0         0         0           R-203         N2H3+M=N2H2+H+M         2.50E+16         0         207.8           R-204         N2H3+M=N2H1H+M         2.50E+16         0         174.6           R-205         HNO+M=H+NO+M         5.00E+16         0         203.7           R-206         H2CN+M=HCN+H+M         7.50E+14         0         92.9           R-207         NCO+M=N+CO+M         2.91E+15         0         195.4					
R-201         NNH+M=N2+H+M         2.50E+13         0,5         12.8           R-202         NNH+O2=N2+HO2         0         0         0         0           R-203         N2H3+M=N2H2+H+M         2.50E+16         0         207.8           R-204         N2H3+M=NH2+NH+M         2.50E+16         0         174.6           R-205         HNO+M=H+NO+M         5.09E+16         0         203.7           R-206         H2CN+M=HCN+H+M         7.50E+14         0         92           R-207         NCO-M=N+CO+M         2.91E+15         0         195.4					
R-202         NNH+02=N2+H02         5.00E+12         0         0           R-203         N2H3+M=N2H2+H+M         2.50E+16         0         207.8           R-204         N2H3+M=NH2+NH+M         2.50E+16         0         174.6           R-205         HNO+M=H+NO+M         5.90E+16         0         203.7           R-206         H2CN+M=HCN+H+M         7.50E+14         0         92.9           R-207         NCO-M=N+CO+M         2.91E+15         0         195.4					
R-203         N2H3+M=N2H2+H+M         2.50E+16         0         207.8           R-204         N2H3+M=NH2+NH+M         2.50E+16         0         174.6           R-205         HNO+M=H+NO+M         5.09E+16         0         203.7           R-206         H2CN+M=HCN+H         0         92           R-207         NCO+M=N+CO+M         2.91E+15         0         195.4					
R-204         N2H3+M=NH2+NH+M         2.50E+16         0         174.6           R-205         HNO+M=H+NO+M         5.09E+16         0         203.7           R-206         H2CN+M=HCN+H+M         7.50E+14         0         92           R-207         NCO+M=H+CO+M         2.91E+15         0         195.4					
R-204         N2H3+M=NH2+NH+M         2.50E+16         0         174.6           R-205         HNO+M=H+NO+M         5.09E+16         0         203.7           R-206         H2CN+M=HCN+H+M         7.50E+14         0         92           R-207         NCO+M=H+CO+M         2.91E+15         0         195.4	R-203	N2H3+M=N2H2+H+M	2.50E+16	0	207.8
R-205         HNO+M=H+NO+M         5.09E+16         0         203.7           R-206         H2CN+M=HCN+H+M         7.50E+14         0         92           R-207         NCO+M=N+CO+M         2.91E+15         0         195.4					
R-206         H2CN+M=HCN+H+M         7.50E+14         0         92           R-207         NCO+M=N+CO+M         2.91E+15         0         195.4					
R-207 NCO+M=N+CO+M 2.91E+15 0 195.4					
k-208 H2O+CH=CH2O+H 5.72E+12 0 -3.2					
	R-208	H2O+CH=CH2O+H	5.72E+12	0	-3.2

(net value of the absolute rate of production or consumption) of each selected pollutants during the engine cycle and plotted versus crank rotation angle as shown in Figure 3 to Figure 6 for CO, NO,  $NO_2$  and  $NH_3$ , respectively.

The total rate of production (mole/cm<sup>3</sup>-sec) was calculated at two ranges of temperature of 1500°C and 4000 °C. The effect of temperature variation on the contribution of each reaction in emissions is clear (from the values of Normalized ROP coefficients) from the formation and consumption profiles (Figure 3 to 6) for each pollutant. The variation in the pattern of each profile of both of the temperature ranges is correlated with the reactions and their contribution to the total rate of production. It is clear from each profile that the formation of each pollutant occurs during the combustion process after the compression stroke.

 
 Table 4. Common Input Variables for Rate of Production Analysis and Sensitivity Analysis (Local) of Kinetic Models

Sr. No	Operating Parameter	Value
1	Equivalence Ratio (F/A)	1.0
2	Initial Inlet Temperature	1500 °C & 4000 °C
3	Initial Inlet Pressure	1.0 atm
4	Engine Speed	3000 rpm
5	Starting Crank Angle	-142°

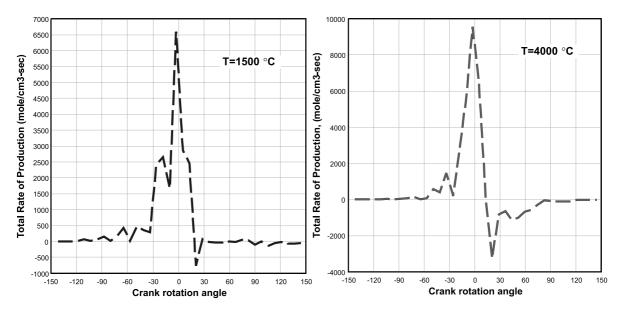


Figure 4. Variation of rate of production of NO at extreme temperatures of T=1500 °C and T=4000 °C in IC engine for equivalence ratio ≈1.0

Table 5. Typical Engine Geometrical	Input Parameters and
Gas Mixture Composition	

Engine Geometrical Input Parameters		ameters Initial Gas Mixture (CNG composition), Mole Fraction	
Parameter (unit)	Value	Component	Mole Fraction
Cylinder volume (cm <sup>3</sup> )	63	Methane (CH4)	0.8903
Displaced Volume (cm <sup>3</sup> )	56.52	Ethane (C <sub>2</sub> H <sub>6</sub> )	0.0105
Clearance Volume (cm <sup>3</sup> )	6.48	Propane (C <sub>3</sub> H <sub>8</sub> )	0.027
Cylinder Diameters (cm)	14.67	Butane (C <sub>4</sub> H <sub>10</sub> )	0.0017
Crank to Connecting rod ratio	1.632	Nitrogen (N2)	0.072
Combustion Starting Crank Angle	-142°	Carbon Dioxide (CO <sub>2</sub> )	0.026
	Parameter (unit)         Cylinder volume (cm³)         Displaced Volume (cm³)         Clearance Volume (cm³)         Cylinder Diameters (cm)         Crank to Connecting rod ratio         Combustion Starting Crank	Parameter (unit)         Value           Cylinder volume (cm <sup>3</sup> )         63           Displaced Volume (cm <sup>3</sup> )         56.52           Clearance Volume (cm <sup>3</sup> )         6.48           Cylinder Diameters (cm)         14.67           Crank to Connecting rod ratio         1.632           Combustion Starting Crank         -142°	composition). M           Parameter (unit)         Value         Component           Cylinder volume (cm <sup>3</sup> )         63         Methane (CH4)           Displaced Volume (cm <sup>3</sup> )         56.52         Ethane (C2H6)           Clearance Volume (cm <sup>3</sup> )         6.48         Propane (C3H8)           Cylinder Diameters (cm)         14.67         Butane (C4H10)           Crank to Connecting rod ratio         1.632         Nitrogen (N2)           Combustion Starting Crank         -142°         Carbon Dioxide

Table 7 shows the reactions involved in the formation or consumption of each pollutant at 1500 °C and 4000 °C and their normalized rate of production coefficients and the absolute rate of production coefficients. In the last column of Table 6 the reference number of the reaction designated in the model shows. According to the data, it predicted that the reaction is  $HNCO+M \le NH+CO+M$  (0.98) significantly contributes to the formation of CO at 1500 °C and the reaction NCO+M<=>N+CO+M (0.907) produces more CO at 4000 °C. Similarly nitric oxide (NO) is formed from reactions  $NO+M \le N+O+M$  (0.905) and N+OH=>NO+H (0.712) of the model at 1500 °C and 4000 °C, respectively in the IC engine simulated under the given conditions. The only reaction  $NO_2+H \le NO+OH$  take part in the formation of other important component of NO<sub>x</sub> at 1500 °C and 4000 °C.

When the local sensitivity analysis of this automatically simplified kinetic model (Table 3) was carried out, we were able to identify that the reactions of the rates have influence on the formation of gaseous pollutants including nitrogen, containing compounds (NO, NO<sub>2</sub> and NH<sub>3</sub>)

Table 6. Key words Input for Rate of Production and Sensitivity Analysis of Kinetic Mechanisms

For Rate of Production Analysis	For Local Sensitivity Analysis	
ICEN ! Internal Combustion Engine	ICEN ! Internal Combustion Engine	
TRAN ! Transient Solver	TRAN ! Transient Solver	
EQUI 1.0 ! Equivalence Ratio	EQUI 1.0 ! Equivalence Ratio	
PRES 2.24551668 ! Pressure (atm)	PRES 2.24551668 ! Pressure (atm)	
TEMP 1573.15 ! Temperature (K)	TEMP 1573.15 ! Temperature (K)	
CMPR 10.51 ! Engine Compression Ratio	CMPR 10.51 ! Engine Compression Ratio	
DEG0 -142.0 ! Starting Crank Angle (degrees)	DEG0 -142.0 ! Starting Crank Angle (degrees)	
LOLR 1.632 ! Engine Connecting Rod to Crank Radius Ratio	LOLR 1.632 ! Engine Connecting Rod to Crank Radius Ratio	
RPM 2000.0 ! Engine Speed (rpm)	RPM 2000.0 ! Engine Speed (rpm)	
VOLD 63.0 ! Engine Cylinder	VOLD 63.0 ! Engine Cylinder	
Displacement Volume (cm3)	Displacement Volume (cm3)	
CPROD CO2 ! Complete-Combustion Products	CPROD CO2 ! Complete-Combustion Products	
CPROD H2O ! Complete-Combustion Products	CPROD H2O ! Complete-Combustion Products	
CPROD N2 ! Complete-Combustion Products	CPROD N2 ! Complete-Combustion Products	
	TIME 0.043 ! End Time (sec)	
	DELT 0.01 ! Time Interval for Printing (sec)	
	LSEN ! Local Sensitivity Method	
	ASEN CO ! A - factor Sensitivity	
SDIR ! Staggered Direct Method	ASEN CO2 ! A -factor Sensitivity	
	ASEN H2O ! A -factor Sensitivity	
	ASEN NO ! A - factor Sensitivity	
	ASEN NO2 ! A -factor	
	END	

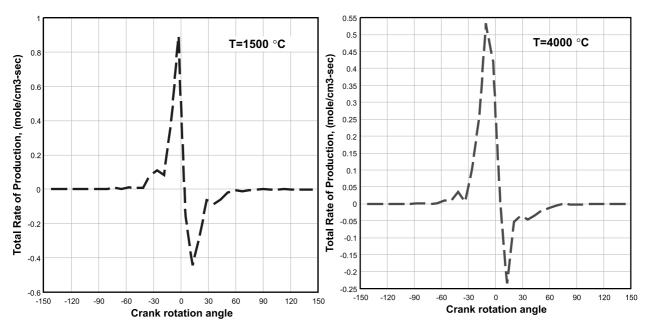


Figure 5. Variation of rate of production of NO<sub>2</sub> at extreme temperatures of T=1500 °C and T=4000 °C in IC engine for equivalence ratio ≈1.0

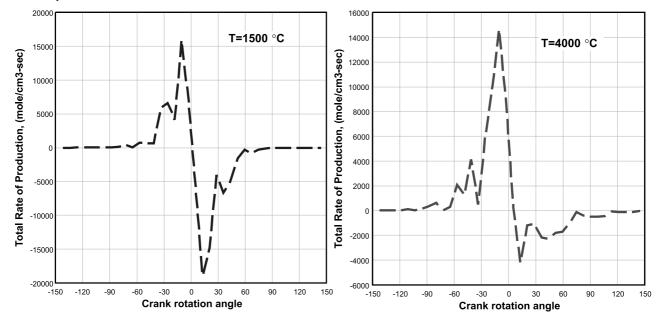


Figure 6. Variation of rate of production of NH<sub>3</sub> at extreme temperatures of T=1500 °C and T=4000 °C in IC engine for equivalence ratio  $\approx 1.0$ 

and carbon oxides (CO & CO<sub>2</sub>). The sensitivity bar-plot for each of the said pollutants is shown in Figure 7 to 11 respectively for CO, CO<sub>2</sub>, NO, NO<sub>2</sub> and NH<sub>3</sub>. In these plots, normalized logarithmic sensitivity coefficients were calculated at the condition mentioned for the each of the reaction step.

In Figure 7, the sensitivity of CO concentrations towards some important reaction rates is shown. This plot illustrates that the dominant reactions are  $O2+N \le NO+O O_2+CN \le NCO+O$  for the formation of carbon monoxide in the combustion chamber of IC engine at 1500 °C and 4000 °C. These reactions show positive sensitivity in the forwards direction. Similarly, the CO<sub>2</sub> sensitivity bar-plot predicts that sensitivity of CO<sub>2</sub> concentrations (Figure 8) are greatly affected by the reactions at the; AT T=1500 °C;

$$NO+N=>N_2+O$$
 (R-73)

$$HNCO+OH <=>NH_2+CO_2$$
(R-136)  
And at T=4000 °C

$$And at I = 4000 C$$

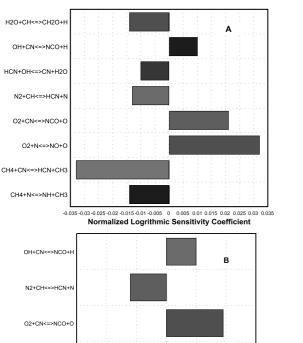
$$N+OH=>NO+H$$
(R-62)

$$HNCO+OH <=> NH_2 + CO_2$$
(R-136)

From the NO and NO<sub>2</sub> sensitivity bar-plots (Figure 9 & Figure 10), it is predicted that NO & NO<sub>2</sub> concentrations are dominantly affected by the rates of the following reactions at 1500 °C and 4000 °C;

- For Nitric Oxide (NO); the important reactions are; N+OH=>NO+H (R-62) and  $N_2+O=>NO+N$  (R-74) which greatly affects the NO concentrations.

- For Nitric Oxide (NO<sub>2</sub>); the NO<sub>2</sub> concentrations show sensitivity towards the following reaction; N+OH=>NO+H (R-62) CH<sub>4</sub>+CN<=>HCN+CH<sub>3</sub> (R-45) and NO<sub>2</sub>+H<=>NO+OH (R-84) at 1500 °C and N+OH=>NO+H (R-62), NO<sub>2</sub>+H<=>NO+OH (R-84) and NO+NH<=>N<sub>2</sub>O+H (R-75) at 4000 °C during the combustion of natural gas in IC engine.



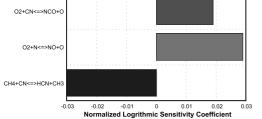


Figure 7. CO sensitivity bar plot for natural gas combustion with proposed kinetic model in IC engine at equivalence ratio =1.0 when (A) T=1500 °C and (B) T=4000 °C

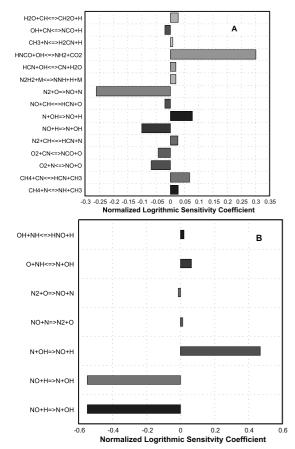


Figure 8.  $CO_2$  sensitivity bar plot for natural gas combustion with proposed kinetic model in IC engine at equivalence ratio =1.0 when (A) T=1500 °C and (B) T=4000 °C

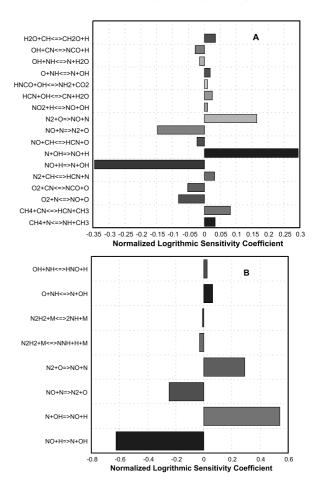


Figure 9. NO sensitivity bar Plot for natural gas combustion with proposed kinetic model in IC engine at equivalence ratio =1.0 when (A) T=1500 °C and (B) T=4000 °C

Similarly, in Figure 11 sensitivity of NH<sub>3</sub> concentrations towards the most important reactions are shown at temperature of 1500 °C and 4000 °C. This sensitivity barplot shows that N<sub>2</sub>+O=>NO+N, N+OH=>NO+H and O<sub>2</sub>+N<=>NO+O

#### CONCLUSION

The rate of production analysis and sensitivity analysis of the proposed reaction model was carried out using Chemkin 4.1.1. The two analyses were carried out for stoichiometric conditions ( $\varphi$ =1.0) at 1500 °C and 4000 °C to identify the reactions contributing the formation of pollutant species of NO, NO<sub>2</sub>, NH<sub>3</sub>, CO and CO<sub>2</sub>. The rate of production analysis revealed that different types of reactions are involved at both temperatures. The sensitivity analysis of the detailed kinetic model identified the reactions of pollutants species. The rate of production analysis and sensitivity analysis indicate that the proposed reaction model is the representative reaction schemes of natural gas combustion in IC engines predict the pollutants species.

#### ACKNOWLEDGEMENT

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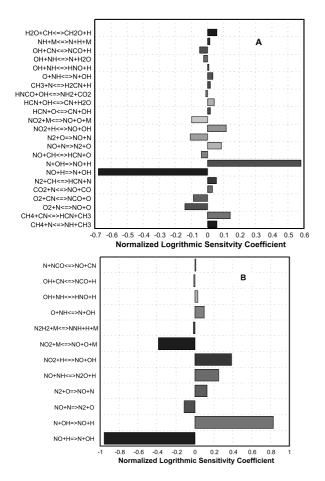


Figure 10. NO<sub>2</sub> sensitivity bar plot for natural gas combustion with proposed kinetic model in IC engine at equivalence ratio =1.0 when (A) T=1500 °C and (B) T=4000 °C

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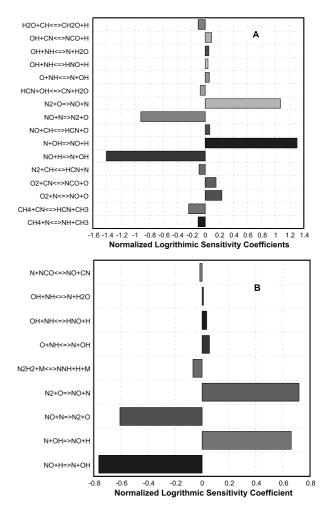
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**Figure 11.** NH<sub>3</sub> sensitivity bar plot for natural gas combustion with proposed kinetic model in IC engine at equivalence ratio =1.0 when (A) T=1500 °C and (B) T=4000 °C

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