

## Computing Equilibrium Constants of Chemical Reactions – A New Approach

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**Abstract:** Exponential curves of the form:  $10^a T^b \exp(c/T)$  have been fitted to the published data of equilibrium constants of formation of chemical species, available at regular temperature intervals. A method of evaluating the equilibrium constants of chemical reactions as a function of temperature, from the curve fit coefficients of the equilibrium constants of formation of the involved chemical species, is presented.

**Keywords:** Chemical thermodynamics, reaction equilibrium constants.

### Introduction:

The equilibrium constants of the chemical reactions based on partial pressures ( $K_{pi}$ ) and on mole concentrations ( $K_{ci}$ ) are very much needed for the analysis of the oxidation mechanisms of fuels and for the calculation of equilibrium compositions and flame temperatures of fuel-oxidiser mixtures. The value of the equilibrium constant of a chemical reaction indicates whether a reaction will proceed to completion or not. Generally a reaction with an equilibrium constant value greater than 1000 is assumed to proceed to completion. A reaction with an equilibrium constant value less than 0.001 is assumed not to occur at all. Small values of equilibrium constants indicate that a reaction will not proceed to any appreciable degree. It is also known that the equilibrium constant of an endothermic reaction increases with increase in temperature and that of an exothermic reaction decreases with increase in temperature. Using the values of equilibrium constants of a chemical reaction at two different temperatures, it possible to find the enthalpy of reaction applicable for that temperature range.

Generally equilibrium constants of chemical reactions are evaluated assuming ideal gas behavior for all constituent species. The equilibrium constant of a reaction involving ideal gases depends only on the reaction temperature and is independent of the pressure. It depends only on the stoichiometric relation between the reactants and the products and it is independent of the amount of various constituents initially present in the mixture.

This paper presents a method of an obtaining an expression for the equilibrium constants of chemical reactions as a function of temperature from the curve fit coefficients of equilibrium constants of formation of the chemical species involved.

### Equilibrium Constants of Formation of Chemical Species

The equilibrium constants of formation of chemical species ( $K_{pi}$ ) are available in Thermo Chemical Tables [1] but only at regular temperature intervals. Log  $K_{pi}$  values have been published for most of the chemical species in the temperature range 100-6000 K at 100 degree intervals. Such tables are most useful for quick hand calculations carried out at the tabulated temperatures or with linear interpolation, at intermediate temperatures.

Log  $K_{pi}$  values stand for the logarithms of the thermodynamic equilibrium constants based on partial pressures ( $K_{pi}$ ) for the reaction in which the given species is formed from its elements in their most stable form

at the indicated temperature [2]. The equilibrium constants of formation of chemical species based on mole concentrations ( $K_{ci}$ ) can be obtained using  $K_{pi}$  and the change in the number of moles of species as the transformation takes place from reactants to products for the reaction in which the given species is formed from its elements in their most stable form.

### Nomenclature

$K_p$	Equilibrium constant based on partial pressures (atm)
$K_c$	Equilibrium constant based on mole concentrations (mol/cc)
$i$	Species index
$j$	Reaction index
$\sum_p$	Summation over products
$\sum_r$	Summation over reactants
$\Delta G_R^\circ$	Standard state Gibbs function change of the reaction (kJ/kmol)
$\Delta H_R^\circ$	Standard state enthalpy change of the reaction (kJ/kmol)
$\Delta S_R^\circ$	Standard state entropy change of the reaction (kJ/kmol K)
$T$	Absolute temperature (K)
$\Delta G_R^\circ$	Universal gas constant (kJ/kmol K)
$\Delta H_R^\circ$	Universal gas constant (cc atm/mol K)
$\Delta S_R^\circ$	stoichiometric coefficient
$T$	$a, b, c$
$\bar{R}$	$m, n, s$
$\bar{R}_p$	$\bar{a}, \bar{b}, \bar{c}$
$\gamma$	$\bar{m}, \bar{n}, \bar{s}$
	constants
$\gamma$	A, B, C, D chemical species

### Equilibrium Constants of Chemical Reactions

The equilibrium constant of a chemical reaction based on partial pressures ( $K_{pj}$ ) can easily be calculated from the equilibrium constants of formation of the species ( $K_{pi}$ ) involved, as given below:

$$\log K_{pj} = \sum_p \gamma_i \log K_{pi} - \sum_r \gamma_i \log K_{pi} \quad \dots\dots\dots (1)$$

When the  $\log K_{pi}$  values of the species are not readily available, the reaction equilibrium constants based on partial pressures ( $K_{pj}$ ) can be computed from the standard state Gibbs function change for the reaction using the expression:

$$\ln K_{pj} = -\Delta G_R^\circ / \bar{R}T$$

$$= -(\Delta H_R^\circ - T\Delta S_R^\circ) / \bar{R}T \quad \dots\dots\dots (2)$$

The reaction equilibrium constant based on mole concentrations ( $K_{cj}$ ) can be computed using  $K_{pj}$  and the change in the number of moles of species as the transformation takes place from reactants to products. The reaction equilibrium constants  $K_{pj}$  and  $K_{cj}$  are related by the expression:

$$K_{cj} = K_{pj} \left( \bar{R}_p T \right)^{-\left( \sum_p \nu_i - \sum_c \nu_i \right)}$$

..... (3)

Hence, the reaction equilibrium constant  $K_{cj}$  will be equal to  $K_{pi}$  when the number of moles of the product species are equal to the number of moles of the reactant species.

The reaction equilibrium constants based on partial pressures ( $K_{pj}$ ) and on mole concentrations ( $K_{cj}$ ) are not readily available in literature for most of the chemical reactions. They have to be computed as stated earlier using the equilibrium constants of formation of the species involved or the standard state Gibbs function change for the reaction. A continuous representation of the reaction equilibrium constant as a function of temperature will be more useful than the values at regular temperature intervals. Such approximations are more accurate and efficient, both as regards speed and computer storage, than methods of interpolation between tabulated values.

### Continuous Representation of Equilibrium Constants

A method of obtaining expressions for the reaction equilibrium constants  $K_{pj}$  and  $K_{cj}$  as a function of temperature from the equilibrium constants of formation of the chemical species involved has been devised. This involves the fitting of exponential curves of the form:  $10^a T^b \exp(c/T)$  to the equilibrium constants of formation of the species which are available at regular temperature intervals in Thermo Chemical Tables [1]. Table I gives the curve fit coefficients a, b and c of the equilibrium constants of formation based on partial pressures ( $K_{pi}$ ) for 48 C-H-O-N-S chemical species for two different temperature ranges, 1000-3000K and 3000-6000K. These constants were obtained by applying the method of Least Squares to the published data available at regular temperature intervals. Tables II gives, similarly obtained, curve fit coefficients m, n and s of the equilibrium constants of formation based on mole concentrations ( $K_{ci}$ ) for the same chemical species and for the same temperature ranges. It is to be noted that the curve fit coefficient c for  $K_{pi}$  has the same value as the curve fit coefficient s for  $K_{ci}$  for any chemical species for a given temperature range.

**Table I Curve Fit Coefficients for the Equilibrium Constants of Formation of Chemical Species Based on Partial Pressures ( $K_{pi}$ ) for the Temperature Ranges 1000–3000 K and 3000–6000 K  $K_{pi} = 10^a T^b \exp(c/T)$**

S. N o.	Chemical Species	Temperature Range 1000 – 3000 K			Temperature Range 3000 – 6000 K		
		a	b	c	a	b	c
1	C <sub>2</sub> H <sub>4</sub>	-3.9749	-0.0965	-4475	-3.2034	-0.2780	-5434
2	C <sub>2</sub> H <sub>2</sub>	3.8304	-0.3013	-27125	3.2224	-0.1381	-26833
3	C <sub>2</sub> N <sub>2</sub>	2.8618	-0.1405	-37718	4.0745	-0.4492	-38692
4	C <sub>2</sub> H	9.7175	-0.8780	-57955	8.7116	-0.6147	-57324
5	CH <sub>4</sub>	-5.6173	-0.0524	10982	-5.3799	-0.0971	10432
6	CH <sub>3</sub>	-0.0057	-0.3534	-16740	1.0215	-0.6091	-17698
7	CH <sub>2</sub> O	-0.8549	-0.3249	14799	0.4806	-0.6589	13595
8	CH <sub>2</sub>	2.6300	-0.2090	-45963	3.4990	-0.4252	-46774
9	CHO	4.9931	-0.7922	1236	6.5273	-1.1819	-11
10	CO <sub>2</sub>	0.8905	-0.2399	47224	2.1213	-0.5535	46248
11	COS	0.7463	-0.0622	24305	1.2786	-0.1977	23879
12	CS <sub>2</sub>	0.5809	-0.0663	-1215	1.2547	-0.2387	695
13	CH	6.9943	-0.3427	-71649	7.6244	-0.4975	-72284
14	CO	7.5207	-0.8445	12598	8.6178	-1.1248	11742
15	CN	7.3329	-0.5981	-52837	4.9749	0.0088	-51112
16	CS	7.1731	-0.7126	-20548	7.8577	-0.8880	-21070
17	C	9.6076	-0.3776	-86753	9.8707	-0.4473	-86903
18	C(solid)	0.0000	0.0000	0	0.0000	0.0000	0
19	H <sub>2</sub> O	-1.7700	-0.3365	29574	-2.0438	-0.2597	29629
20	H <sub>2</sub> S	-2.9799	0.1124	11043	-3.0565	0.1360	11013
21	H <sub>2</sub>	0.0000	0.0000	0.0000	0.0000	0.0000	0
22	HCN	2.3634	-0.2048	-16207	2.6223	-0.2665	-16510

23	HNO <sub>3</sub>	-14.7981	1.1468	17501	-12.7165	0.6178	15819
24	HNO	-2.7376	0.0469	-11547	-1.4973	-0.2688	-12536
25	HS	0.7252	0.0232	-9546	0.9271	-0.0269	-9738
26	H	1.2980	0.4907	-26290	2.7447	0.1181	-27347
27	O <sub>3</sub>	-4.3048	0.2195	-17069	-2.2871	-0.2986	-18578
28	O <sub>2</sub>	0.0000	0.0000	0	0.0000	0.0000	0
29	O	2.4878	0.2675	-30160	3.2390	0.0723	-30667
30	N <sub>2</sub> H <sub>4</sub>	-17.2380	1.4591	-8849	-17.1606	1.4543	-9253
31	N <sub>2</sub> O <sub>5</sub>	-25.3228	2.1889	-618	-20.0002	0.8215	-4588
32	N <sub>2</sub> O <sub>4</sub>	-22.3888	2.1099	271	-19.1575	1.2841	-2237
33	N <sub>2</sub> H <sub>2</sub>	-7.8695	0.4917	-24225	-7.7119	0.4588	-24515
34	N <sub>2</sub> O	-5.9403	0.6177	-9403	-5.0069	0.3792	-10130
35	N <sub>2</sub>	0.0000	0.0000	0	0.0000	0.0000	0
36	NH <sub>3</sub>	-6.8142	0.1855	6976	-9.4266	0.8601	8847
37	NO <sub>3</sub>	-10.7105	0.8492	-7992	-7.9408	0.1386	-10078
38	NH <sub>2</sub>	-1.7246	-0.1309	-19633	-1.2861	-0.2376	-20097
39	NO <sub>2</sub>	-3.6245	0.0889	-3784	-1.9436	-0.3414	-5070
40	NH	0.9414	0.0277	-40706	1.0283	0.0068	-40805
41	NO	0.7178	-0.0148	-10906	1.4961	-0.2148	-11484
42	NS	0.4238	0.0832	-23967	0.6094	0.0351	-24097
43	N	2.0965	0.3722	-56972	1.8552	0.4288	-56665
44	S <sub>2</sub> O	-3.7317	0.1152	22400	-2.6593	-0.1597	21589
45	S <sub>2</sub>	0.0000	0.0000	0	0.0000	0.0000	0
46	SO <sub>3</sub>	-10.9731	0.6745	55961	-8.6626	0.0839	54175
47	SO <sub>2</sub>	-4.4810	0.1918	43751	-3.5263	-0.0532	43035
48	S	2.1022	0.2972	-25889	1.6259	0.4186	-25512

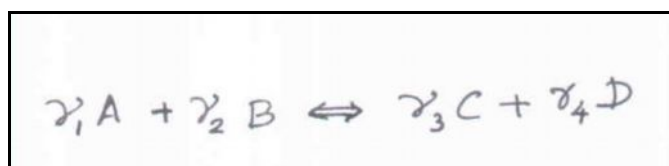
**Table II Curve Fit Coefficients for the Equilibrium Constants of Formation of Chemical Species Based on Mole Concentration ( $K_{ci}$ ) for the Temperature Ranges 1000–3000 K and 3000–6000 K  $K_{ci} = 10^m T^n \exp(s/T)$**

S. N o.	Chemical Species	Temperature Range 1000 – 3000 K			Temperature Range 3000 – 6000 K		
		m	n	s	m	n	s
1	C <sub>2</sub> H <sub>4</sub>	1.7675	2.9035	-4475	2.5390	2.7220	-5434
2	C <sub>2</sub> H <sub>2</sub>	7.6587	1.6987	-27125	7.0507	1.8619	-26833
3	C <sub>2</sub> N <sub>2</sub>	6.6900	1.8600	-37718	7.9028	1.5508	-38692
4	C <sub>2</sub> H	12.5886	0.6220	-57955	11.5828	0.8853	-57324
5	CH <sub>4</sub>	-1.7890	1.9476	10982	-1.5516	1.9029	10432
6	CH <sub>3</sub>	2.8655	1.1466	-16740	3.8927	0.8909	-17698
7	CH <sub>2</sub> O	2.0163	1.1751	14799	3.3517	0.8411	13595
8	CH <sub>2</sub>	4.5441	0.7910	-45963	5.4131	0.5748	-46774
9	CHO	6.9072	0.2078	1236	8.4414	-0.1819	-11
10	CO <sub>2</sub>	2.8046	0.7601	47224	4.0354	0.4465	46248
11	COS	2.6604	0.9378	24305	3.1928	0.8023	23879
12	CS <sub>2</sub>	2.4951	0.9337	-1215	3.1689	0.7613	695
13	CH	7.9514	0.1573	-71649	8.5815	-0.0025	-72284
14	CO	8.4778	-0.3445	12598	9.5749	-0.6248	11742
15	CN	8.2899	-0.0981	-52837	5.9320	0.5088	-51112
16	CS	8.1302	-0.2126	-20548	8.8147	-0.3880	-21070
17	C	9.6076	-0.3776	-86753	9.8707	-0.4473	-86903
18	C(solid)	0.0000	0.0000	0	0.0000	0.0000	0
19	H <sub>2</sub> O	-0.8130	0.1635	29574	-1.0867	0.2403	29629
20	H <sub>2</sub> S	-2.0229	0.6124	11043	-2.0994	0.6360	11013
21	H <sub>2</sub>	0.0000	0.0000	0	0.0000	0.0000	0

22	HCN	4.2776	0.7952	-16207	4.5364	0.7335	-16510
23	HNO <sub>3</sub>	-11.9269	2.6468	17501	-9.8453	2.1178	15819
24	HNO	-1.7805	0.5469	-11547	-0.5402	0.2312	-12536
25	HS	0.7252	0.0232	-9546	0.9271	-0.0269	-9738
26	H	0.3409	-0.0093	-26290	1.7876	-0.3819	-27347
27	O <sub>3</sub>	-3.3477	0.7195	-17069	-1.3301	0.2014	-18578
28	O <sub>2</sub>	0.0000	0.0000	0	0.0000	0.0000	0
29	O	1.5307	-0.2325	-30160	2.2819	-0.4277	-30667
30	N <sub>2</sub> H <sub>4</sub>	-13.4097	3.4591	-8849	-13.3323	3.4543	-9253
31	N <sub>2</sub> O <sub>5</sub>	-20.5374	4.6889	-618	-15.2149	3.3215	-4588
32	N <sub>2</sub> O <sub>4</sub>	-18.5605	4.1099	271	-15.3293	3.2841	-2237
33	N <sub>2</sub> H <sub>2</sub>	-5.9553	1.4917	-24225	-5.7978	1.4588	-24515
34	N <sub>2</sub> O	-4.9833	1.1177	-9403	-4.0498	0.8792	-10130
35	N <sub>2</sub>	0.0000	0.0000	0	0.0000	0.0000	0
36	NH <sub>3</sub>	-4.9000	1.1855	6976	-7.5124	1.8601	8847
37	NO <sub>3</sub>	-8.7964	1.8492	-7992	-6.0266	1.1386	-10078
38	NH <sub>2</sub>	-0.7675	0.3691	-19633	-0.3291	0.2624	-20097
39	NO <sub>2</sub>	-2.6674	0.5889	-3784	-0.9865	0.1586	-5070
40	NH	0.9414	0.0277	-40706	1.0283	0.0068	-40805
41	NO	0.7178	-0.0148	-10906	1.4961	-0.2148	-11484
42	NS	0.4238	0.0832	-23967	0.6094	0.0351	-24097
43	N	1.1395	-0.1278	-56972	0.8981	-0.0712	-56665
44	S <sub>2</sub> O	-2.7746	0.6152	22400	-1.7022	0.3403	21589
45	S <sub>2</sub>	0.0000	0.0000	0	0.0000	0.0000	0
46	SO <sub>3</sub>	-9.0590	1.6745	55961	-6.7485	1.0839	54175
47	SO <sub>2</sub>	-3.5240	0.6918	43751	-2.5692	0.4468	43035
48	S	1.1451	-0.2028	-25889	0.6688	-0.0814	-25512

The exponential curves of the form used are found to fit to the published data excellently well. The equilibrium constants of formation of the species given in published thermochemical tables [1] can be readily obtained with the help these curve fit coefficients with an error less than 3%. The curve fit coefficients a,b and c or m,n and s of the equilibrium constants of formation of the chemical species are used to compute the reaction equilibrium constants  $K_{pj}$  and  $K_{cj}$  as indicated below:

Considering the chemical reaction of the form:



..... (4)

the equilibrium constants of formation based on partial pressures, of the chemical species A,B,C and D are expressed as:

$$\begin{aligned}
 K_p(A) &= 10^{a_1} T^{b_1} \exp(C_1/T) \\
 K_p(B) &= 10^{a_2} T^{b_2} \exp(C_2/T) \\
 K_p(C) &= 10^{a_3} T^{b_3} \exp(C_3/T) \\
 K_p(D) &= 10^{a_4} T^{b_4} \exp(C_4/T)
 \end{aligned}$$

.....(5)

Similarly the equilibrium constants of formation based on mole concentrations, of the species A, B, C and D are expressed as:

$$\begin{aligned}
 K_c(A) &= 10^{m_1} T^{n_1} \exp(s_1/T) \\
 K_c(B) &= 10^{m_2} T^{n_2} \exp(s_2/T) \\
 K_c(C) &= 10^{m_3} T^{n_3} \exp(s_3/T) \\
 K_c(D) &= 10^{m_4} T^{n_4} \exp(s_4/T)
 \end{aligned}$$

..... (6)

Then the reaction equilibrium constants  $K_{pj}$  and  $K_{cj}$  for the reaction (4) can be obtained from these curve fit coefficients of the equilibrium constants of formation of the species as given below. The reaction equilibrium constant based on partial pressures ( $K_{pj}$ ) can be computed as:

$$\begin{aligned}
 K_{pj} &= 10^{\bar{a}} T^{\bar{b}} \exp(\bar{c}/T) \quad \text{where} \\
 \bar{a} &= \sum_p \nu_i a_i - \sum_r \nu_i a_i = \nu_3 a_3 + \nu_4 a_4 - \nu_1 a_1 - \nu_2 a_2 \\
 \bar{b} &= \sum_p \nu_i b_i - \sum_r \nu_i b_i = \nu_3 b_3 + \nu_4 b_4 - \nu_1 b_1 - \nu_2 b_2 \\
 \bar{c} &= \sum_p \nu_i c_i - \sum_r \nu_i c_i = \nu_3 c_3 + \nu_4 c_4 - \nu_1 c_1 - \nu_2 c_2
 \end{aligned}$$

..... (7)

Similarly, the reaction equilibrium constant based on mole concentration ( $K_{cj}$ ) of the reaction (4) can be computed as:

$$\begin{aligned}
 K_{cj} &= 10^{\bar{m}} T^{\bar{n}} \exp(\bar{s}/T) \quad \text{where} \\
 \bar{m} &= \sum_p \nu_i m_i - \sum_r \nu_i m_i = \nu_3 m_3 + \nu_4 m_4 - \nu_1 m_1 - \nu_2 m_2 \\
 \bar{n} &= \sum_p \nu_i n_i - \sum_r \nu_i n_i = \nu_3 n_3 + \nu_4 n_4 - \nu_1 n_1 - \nu_2 n_2 \\
 \bar{s} &= \sum_p \nu_i s_i - \sum_r \nu_i s_i = \nu_3 s_3 + \nu_4 s_4 - \nu_1 s_1 - \nu_2 s_2
 \end{aligned}$$

..... (8)



The coefficients  $\bar{a}$ ,  $\bar{b}$  and  $\bar{c}$  or  $\bar{m}$ ,  $\bar{n}$  and  $\bar{s}$  of the reaction equilibrium constants can thus be readily computed for any reaction involving the particular

species. The units of  $\bar{a}$  is (atm) raised to the power  $(\sum_p \nu_i - \sum_r \nu_i)$  and that of  $\bar{m}$  is (mol/cc) raised to the power  $(\sum_p \nu_i - \sum_r \nu_i)$ . The units of  $\bar{b}$  and  $\bar{n}$  is dimensionless and that of  $\bar{c}$  and  $\bar{s}$  is Kelvin.

The equilibrium constants of any number of chemical reactions (both in forward and reverse directions) can thus be evaluated with the help of these curve fit coefficients of equilibrium constant formation of chemical species involved. The comparison of the values of reaction equilibrium constants  $K_{pj}$  and  $K_{cj}$  computed using these curve fit coefficients  $a$ ,  $b$ ,  $c$ ,  $m$ ,  $n$  and  $s$  with the values obtained using the specific temperature  $\log K_{pi}$  data of JANAF thermochemical tables [1] is found to be in very good agreement, with a deviation less than 5%. Table 3 shows the comparison of  $K_{pj}$  values obtained using the above two methods for three different temperatures for 15 chemical reactions normally encountered in reaction mechanisms.

**Table III Comparison of Computed Reaction Equilibrium Constant ( $K_{pj}$ ) Values**

S.No.	Chemical Reaction	Reaction Equilibrium constants ( $K_{pj}$ ) obtained using curve fit coefficients of $K_{pi}$ of species			Reaction Equilibrium constants ( $K_{pj}$ ) obtained using the specific temperature (Janaf table) data of $\log K_{pi}$ of species		
		1000K	3000K	6000K	1100K	3000K	6000K
1.	$\text{CO}_2 + \text{H}_2 \leftrightarrow \text{CO} + \text{H}_2\text{O}$	0.696	7.187	9.121	0.695	7.278	9.268
2.	$\text{CO}_2 + \text{H}_2 \leftrightarrow \text{CO} + \frac{1}{2} \text{O}_2$	$6.00 \times 10^{-11}$	0.328	69.249	$6.05 \times 10^{-11}$	0.345	69.823
3.	$\text{CO} + \text{O}_2 \leftrightarrow \text{CO}_2 + \text{O}$	2.591	0.344	0.284	2.600	0.344	0.283
4.	$\text{C(s)} + 2\text{H}_2 \leftrightarrow \text{CH}_4$	0.098	$6.17 \times 10^{-5}$	$1.02 \times 10^{-5}$	0.096	$6.04 \times 10^{-5}$	$1.0 \times 10^{-5}$
5.	$\text{C(s)} + \frac{1}{2} \text{O}_2 \leftrightarrow \text{CO}$	$2.87 \times 10^{11}$	$2.56 \times 10^6$	$1.65 \times 10^5$	$2.89 \times 10^{10}$	$2.53 \times 10^6$	$1.59 \times 10^5$
6.	$\text{CH}_4 + \text{H}_2\text{O} \leftrightarrow 3\text{H}_2 + \text{CO}$	25.07	$1.88 \times 10^9$	$1.23 \times 10^{11}$	26.24	$1.90 \times 10^9$	$1.25 \times 10^{11}$
7.	$\text{O}_2 \leftrightarrow \text{O} + \text{O}$	$2.42 \times 10^{-20}$	0.013	384.510	$2.48 \times 10^{-20}$	0.013	390.840
8.	$\text{H}_2\text{O} \leftrightarrow \text{H}_2 + \frac{1}{2} \text{O}_2$	$8.62 \times 10^{-11}$	0.046	7.592	$8.71 \times 10^{-11}$	0.045	7.534
9.	$\text{H}_2 \leftrightarrow \text{H} + \text{H}$	$5.07 \times 10^{-18}$	0.025	264.780	$5.15 \times 10^{-18}$	0.025	266.680
10.	$\text{N}_2 \leftrightarrow \text{N} + \text{N}$	$8.73 \times 10^{-44}$	$1.93 \times 10^{-10}$	0.056	$8.71 \times 10^{-44}$	$1.93 \times 10^{-10}$	0.056
11.	$\frac{1}{2} \text{N}_2 + \frac{1}{2} \text{O}_2 \leftrightarrow \text{NO}$	$8.65 \times 10^{-5}$	0.122	0.713	$8.65 \times 10^{-5}$	0.122	0.715
12.	$\text{N} + \text{O}_2 \leftrightarrow \text{NO} + \text{O}$	$4.55 \times 10^7$	991.230	59.160	$4.61 \times 10^7$	995.410	59.570
13.	$\text{NO} + \text{N} \leftrightarrow \text{N}_2 + \text{O}$	$6.08 \times 10^{15}$	$6.62 \times 10^4$	116.240	$6.17 \times 10^{15}$	$6.66 \times 10^4$	116.680
14.	$\text{N} + \text{O}_3 \leftrightarrow \text{NO}_2 + \text{O}$	$6.02 \times 10^{17}$	$1.14 \times 10^6$	$1.20 \times 10^3$	$6.09 \times 10^{17}$	$1.15 \times 10^6$	$1.20 \times 10^3$
15.	$\text{SO}_2 + \text{O}_2 \leftrightarrow \text{SO}_3 + \text{O}$	$2.82 \times 10^{-10}$	$1.01 \times 10^{-4}$	$3.03 \times 10^{-3}$	$2.84 \times 10^{-10}$	$1.01 \times 10^{-4}$	$3.02 \times 10^{-3}$

## Conclusion:

A new method of computing equilibrium constants of chemical reactions as a function of temperature from the curve fit coefficients of equilibrium constants of formation of the chemical species involved, is presented. It is more accurate and useful than the methods of interpolation between tabulated values.

The combustion mechanism of many fuels are now theoretically analyzed by simulating the oxidation reactions in a high speed computer. An oxidation mechanism of a fuel may involve a large number of chemical reactions, but the chemical species involved will be relatively smaller in number. Hence, for ease of computation, it is suggested that the equilibrium constants of formation of the species be expressed as a function of temperature from which the reaction equilibrium constant can be computed using the method presented here. This method is more efficient in the computer analyses, both as regards speed and storage.

## References

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