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THERMODYNAMIC ESTIMATE OF THE REACTION
OF HYDROGEN WITH OXYGEN-BEARING
IMPURITIES IN SALADO SALT AT
ELEVATED TEMPERATURES

W. D. Bond
W. E. Clark

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CHEMICAL TECHNOLOGY DIVISION
Chemical Development Section B

THEMODYNAMIC ESTIMATE OF THE REACTION OF HYDROGEN WITH
OXYGEN-BEARING IMPURITIES IN SALADO SALT AT ELEVATED
TEMPERATURES

W. D. Bond
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ABSTRACT

Thermodynamic estimates indicate that materials produced by a contained nuclear explosion in bedded rock salt which are as efficient reducing agents as hydrogen will be converted to their oxides by oxygen-bearing impurities in the salt. Since all combustible gases are reductants, the results indicate that the production of fuels by a nuclear event in this environment is not likely. The thermodynamic estimates were made considering reactions between hydrogen and calcium sulfate (anhydrite), iron oxides, carbonaceous materials, and silicates.

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1.0 INTRODUCTION

The purpose of this report is to present thermodynamic estimates of the nature and stability of some chemical states of hydrogen which can co-exist in equilibrium with rock salt. Salt from the beds of the Salado formation was chosen since it is expected to be the containment medium for the GNOME event. The results of these calculations can be used to predict the stable species which will result from other elements whose reactivities relative to hydrogen are known. A knowledge of the chemical species of isotopes, which are of interest for recovery, serves to indicate the magnitude and nature of chemical problems associated with the recovery of those isotopes. Also, the chemical species of hydrogen in this environment is of interest since it represents a possible chemical fuel. Production of hydrogen from water or CO from carbon may be a way to convert the tremendous energy from a contained event to a useful form.

The temperature range from 298-1500°K was considered to be the most important, since the system exists for the longest time in this temperature environment following a nuclear detonation. Above 1500°K, heat is rapidly transferred by radiation. Equilibrium constants were calculated for the reaction of H₂ and H₂O with each constituent of the system, and prediction of the most stable post-explosion hydrogen products was then made from these equilibrium constants considering all constituents of the system.

2.0 EQUILIBRIUM CONSTANT CALCULATIONS

2.1 Definition of the System

Salado salt is sodium chloride (rock salt) containing various impurities. The most consistent impurities are reported to be CaSO₄ (anhydrite), iron oxides, carbonates, silicates, and carbonaceous material, which may include CH₄ in pockets of the salt matrix. Potassium and magnesium salts may also be present. Thus, the system with which we are concerned is one which contains all of these constituents plus elemental hydrogen gas. All constituents are assumed to be intimately mixed.

2.2 Method and Limitations

The nature and extent of the various reactions were estimated from standard free energy data using the relation

$$\Delta F^{\circ} = -RT \ln K$$

where ΔF° = standard free energy, cal/mole at temperature T
R = gas constant per mole, cal/deg·mole
K = equilibrium constant
T = absolute temperature, °K

Where available, equilibrium constants were taken directly from the literature. Free energy temperature equations, the reference states employed, and the calculated free energies for each compound used in the calculations in this text are given in the appendix.

Thermodynamics determines the extent to which a given reaction will occur under equilibrium conditions but not the rate at which it will occur. However, it is most probable that all reactions thermodynamically possible will take place at reasonable rates at the temperatures expected ($\sim 1100^\circ\text{K}$). Most reactions possess activation energies of 20-100 kcal, and such reactions are usually perceptible at temperatures in the expected range.

Of particular interest from a rate standpoint is the sudden quenching of the system to the melting point of NaCl (1074°K) by roof cave-in immediately following the detonation.¹ Such rapid cooling is very likely to produce metastable products which may then exist for indefinite periods of time. However, calculations of equilibrium constants a few hundred degrees above the final quench temperature give good indications as to what the metastable products might be. Metastable states are observed much more frequently on rapid cooling than on rapid heating since the metastable state reverts to the stable state much more rapidly at higher temperature.

3.0 DISCUSSION

Free energies and equilibrium constants for some reactions of H_2 , CH_4 , and CO with CaSO_4 and of H_2 and H_2O with FeO , Fe_2O_3 , Fe_3O_4 , C, CO, CO_2 , CH_4 , and silicates were calculated. Included with these calculations are thermal decomposition data for CaSO_4 , CaCO_3 , and the alkali metal carbonates and calculation of the equilibrium constant for the reaction between NaCl and CaSO_4 .

3.1 Calcium Sulfate

Calcium sulfate is reduced to CaS by H_2 (Table 1). The magnitude of the equilibrium constants shows that H_2 will be converted to H_2O . CaSO_3 need not be considered as a reduction product since it would be further reduced to the sulfide;² thus under equilibrium conditions the production of H_2 as a burnable fuel is not possible.

There is little likelihood that appreciable quantities of H_2S can be produced (Table 2). CaSO_4 does not react with NaCl nor does it thermally decompose at the temperature of interest (Tables 3 and 4).

3.2 Iron Oxides

Dushman³ has tabulated equilibrium constants for reactions between H_2 and iron oxides from 800 to 1400°K (Table 5). It is seen that iron oxides readily oxidize hydrogen although not so readily as CaSO_4 (Table 1). In any event the combined effect of CaSO_4 and iron oxides is to convert H_2 to H_2O .

3.3 Carbon, Carbon Monoxide, Carbon Dioxide, and Methane

Equilibrium constants for reactions between CO, CH_4 , CO_2 , C, and O_2 have been calculated by Rossini et al.⁴ (Table 6). Equilibrium constants for the reaction between CaSO_4 with CH_4 and with CO were calculated using the data of Rossini et al.⁴ and Kelly⁵ (Table 7). Carbon dioxide presumably will result from thermal decomposition of carbonates present

(Table 8). In general, the data show that at the melting point of NaCl, H_2 is a more stable product than H_2O with respect to CH_4 , CO, CO_2 , and C (Table 6). However, the presence of excess $CaSO_4$ in the system would convert H_2 to H_2O (Table 1) and also CH_4 and CO to CO_2 and H_2O and to CO_2 , respectively (Tables 6 and 7). Thus, considering the system as a whole, the most stable hydrogen-containing product is H_2O . The extreme instability of CO and CH_4 in the presence of $CaSO_4$ would prevent their existence in the final gas products (Table 7).

It is to be emphasized that the above conclusions are drawn from equilibrium calculations. A sample of gaseous products obtained a few seconds after detonation and rapidly cooled to ambient conditions would probably contain metastable products from the entire series of reactions.

3.4 Silicates

Thermodynamic data are not available to allow calculation of equilibrium constants for reactions between H_2 and various types of silicates. However, calculations of the extent of reaction between H_2 and some typical metal oxides of which silicates are composed will give the maximum extent of reaction that can be postulated in a system containing silicates composed of these oxides.

Equilibrium constants were calculated for the reactions between H_2 and SiO_2 , CaO, Al_2O_3 , and Na_2O (Table 9). The equilibrium constants are too low to be of any significance.

Table 1. The Reduction of CaSO₄(anh) by H₂(g)
See also Fig. 1

Temp., °K	CaSO ₄ (anh) + H ₂ (g) ⇌ CaO(s) + SO ₂ (g) + H ₂ O(g)		CaSO ₄ (anh) + 4H ₂ (g) ⇌ CaS(s) + 4H ₂ O(g)	
	-ΔF, kcal	K ^a	-ΔF, kcal	K ^b
298.1	-41.175	6.54 x 10 ⁻³¹	16.660	1.63 x 10 ¹²
300	-41.752	3.86 x 10 ⁻³¹	16.671	1.56 x 10 ¹²
400	-36.072	1.96 x 10 ⁻²⁰	21.018	3.04 x 10 ¹¹
500	-30.416	4.57 x 10 ⁻¹⁴	25.602	1.69 x 10 ¹¹
600	-24.905	8.00 x 10 ⁻¹⁰	28.549	2.68 x 10 ¹⁰
700	-19.576	7.47 x 10 ⁻⁷	32.179	1.18 x 10 ¹⁰
800	-14.259	8.06 x 10 ⁻⁴	35.547	5.39 x 10 ⁹
900	-10.043	3.61 x 10 ⁻³	38.742	2.66 x 10 ⁹
1000	- 3.908	1.40 x 10 ⁻¹	41.765	1.34 x 10 ⁹
1100	1.211	1.78	45.310	1.00 x 10 ⁹
1200	6.024	1.25 x 10 ¹	48.485	6.78 x 10 ⁸
1300	10.827	6.61 x 10 ¹	49.916	2.47 x 10 ⁸
1400	15.525	2.65 x 10 ²	52.537	1.59 x 10 ⁸
1500	20.076	8.42 x 10 ²	54.627	9.11 x 10 ⁷

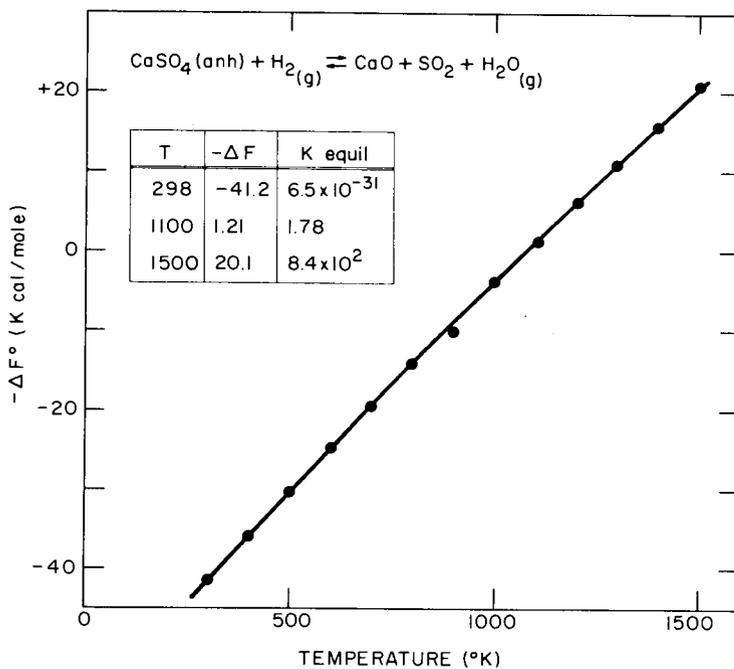
a.

$$K = \frac{[P_{SO_2}] [P_{H_2O}]}{[P_{H_2}]}$$

b.

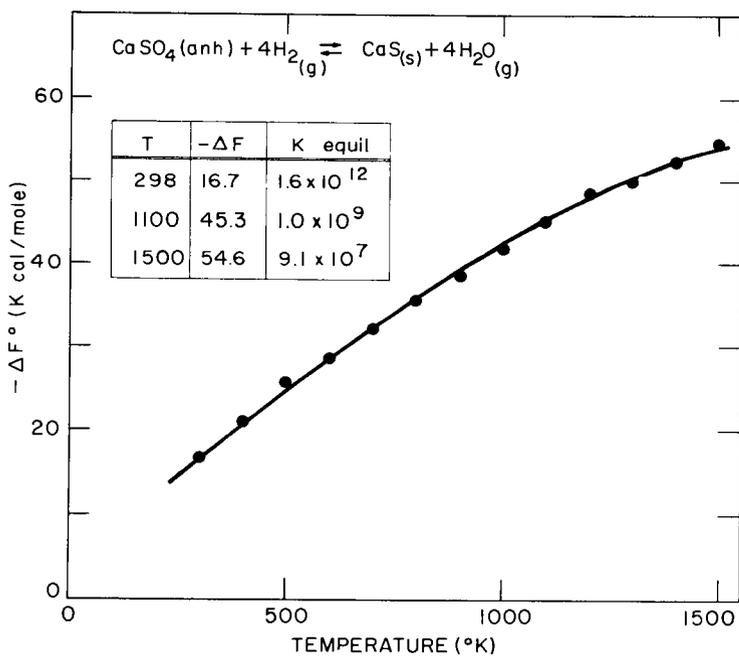
$$K = \frac{[P_{H_2O}]^4}{[P_{H_2}]^4}$$

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(a) The Reaction $\text{CaSO}_4 + \text{H}_2 \rightleftharpoons \text{CaO}(\text{s}) + \text{SO}_2 + \text{H}_2\text{O}(\text{g})$

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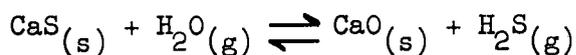


(b) The Reaction $\text{CaSO}_4 + 4\text{H}_2 \rightleftharpoons \text{CaS}(\text{s}) + 4\text{H}_2\text{O}(\text{g})$

Fig. 1. The Reduction of $\text{CaSO}_4(\text{anh})$ by H_2 .

Table 2. Reaction of CaS(s) with H₂O(g)

See also Fig. 2



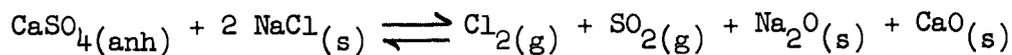
Temp., °K	-ΔF, kcal	K ^a
298.1	-12.41	7.99 x 10 ⁻¹⁰
500	-13.09	1.81 x 10 ⁻⁶
1000	-13.11	1.37 x 10 ⁻³
1500	-12.93	1.31 x 10 ⁻²

a.

$$K = \frac{[\text{P}_{\text{H}_2\text{S}}]}{[\text{P}_{\text{H}_2\text{O}}]}$$

Table 3. Reaction of NaCl(s) with CaSO₄(anh)

See also Fig. 3



Temp., °K	-ΔF, kcal	K ^a
298.1	-199.8	3.39 x 10 ⁻¹⁴⁷
500	-173.8	5.91 x 10 ⁻⁷⁷
1000	-137.9	7.32 x 10 ⁻³¹
1500	-108.2	1.72 x 10 ⁻¹⁶

a.

$$K = \frac{[\text{P}_{\text{Cl}_2}][\text{P}_{\text{SO}_2}]}{[\text{P}_{\text{NaCl}}]^2}$$

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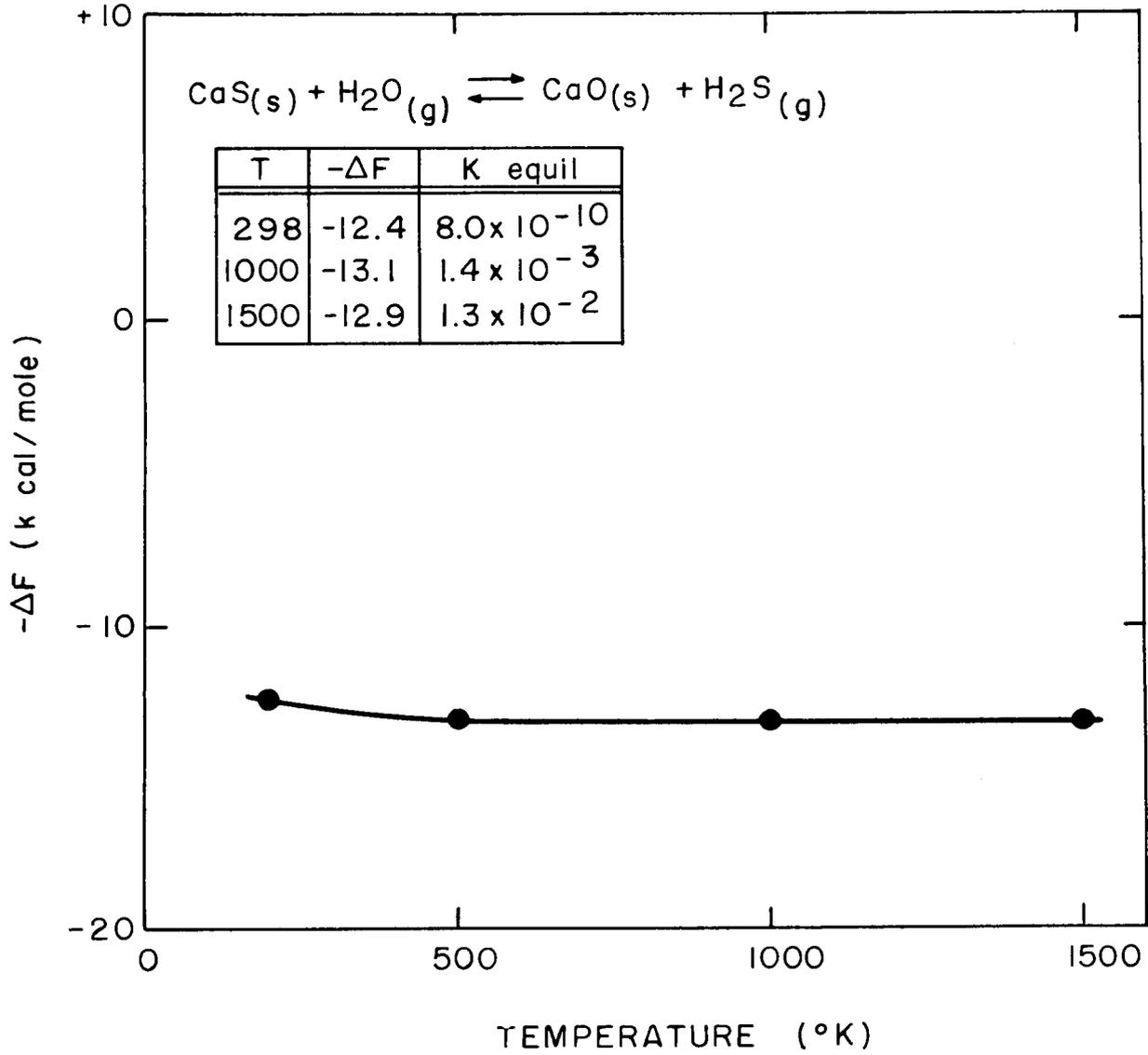


Fig. 2. The Reaction of CaS with H_2O .

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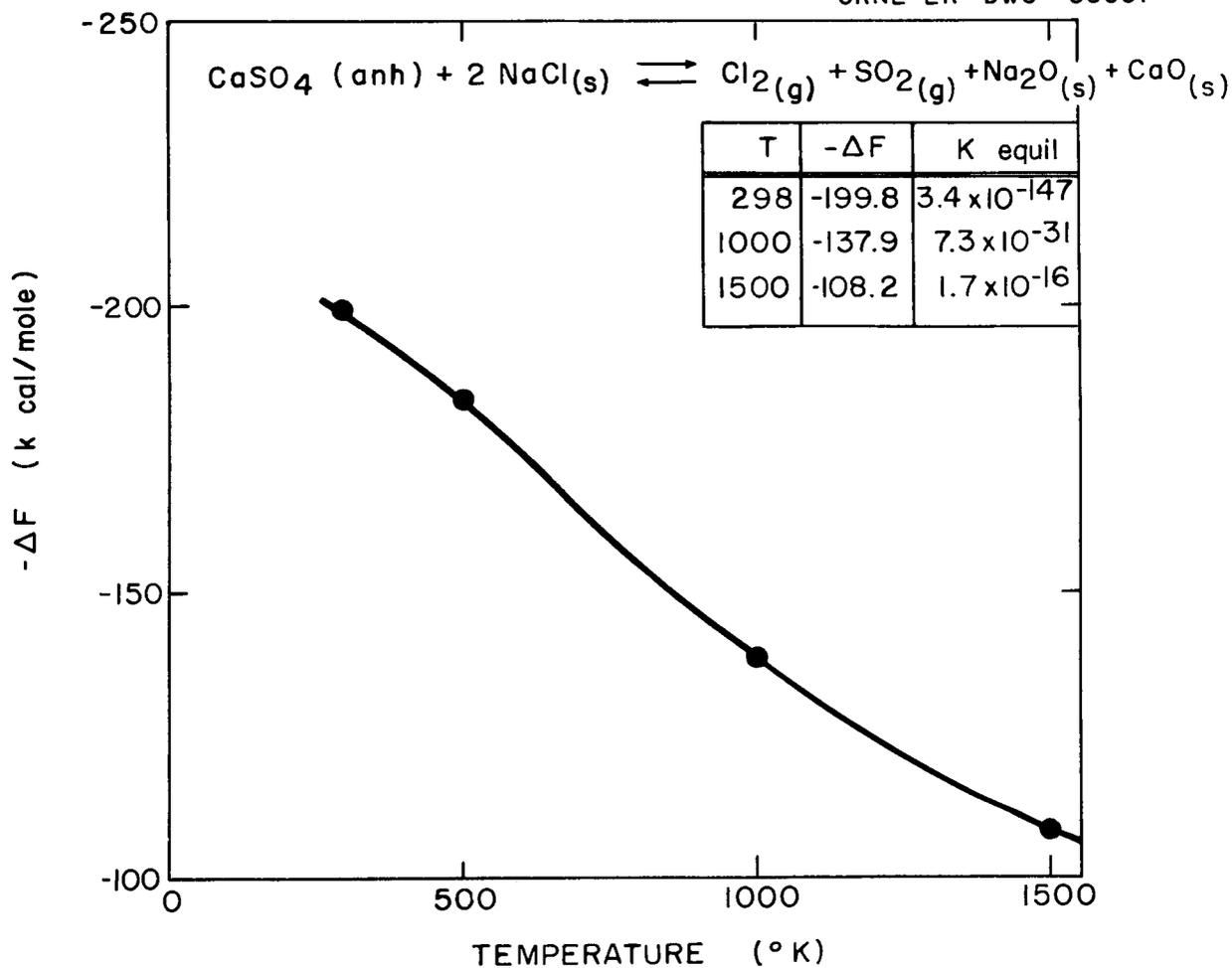
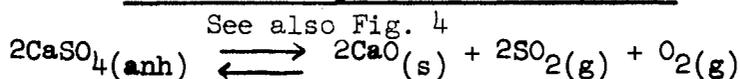


Fig. 3. The Reaction of NaCl with CaSO_4 .

Table 4. Thermal Decomposition of Anhydrite^a



Temp., °K	K ^b
1473	9.13 x 10 ⁻⁹
1501	5.93 x 10 ⁻⁸
1608	8.00 x 10 ⁻⁶
1646	3.79 x 10 ⁻⁵

a. Experimental data of Zawadski²

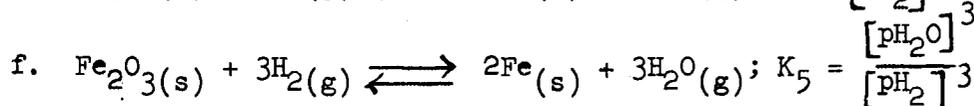
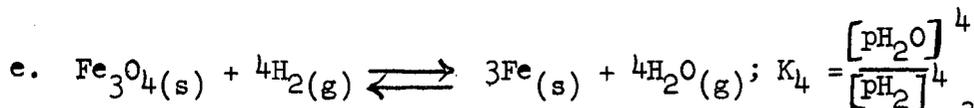
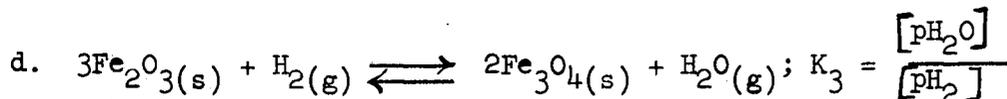
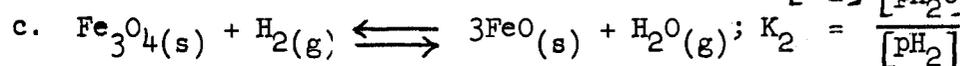
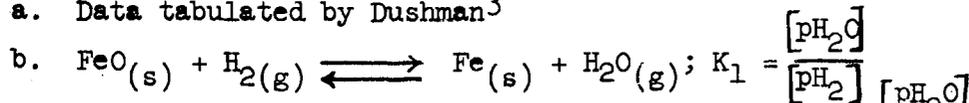
b. $K = \frac{[\text{p}_{\text{SO}_2}]^2}{[\text{p}_{\text{O}_2}]}$

Table 5. Reduction of FeO, Fe₃O₄, and Fe₂O₃ by H₂^a

See also Fig. 5

Temp., °K	K ₁ ^b	K ₂ ^c	K ₃ ^d	K ₄ ^e	K ₅ ^f
700	---	---	---	0.159	---
800	---	---	18.8	0.275	1.45
823	0.283	---	---	---	---
873	0.340	---	---	---	---
900	---	0.66	16.8	0.398	1.78
923	0.376	---	---	---	---
973	0.422	---	---	---	---
1000	---	1.27	15.7	0.603	2.70
1073	0.499	---	---	---	---
1100	---	2.16	14.4	0.785	3.90
1173	0.582	---	---	---	---
1200	---	3.33	12.9	0.984	5.30
1273	0.662	---	---	---	---
1300	---	4.92	---	---	---
1373	0.743	---	---	---	---
1400	---	6.71	11.4	1.340	8.00

a. Data tabulated by Dushman³



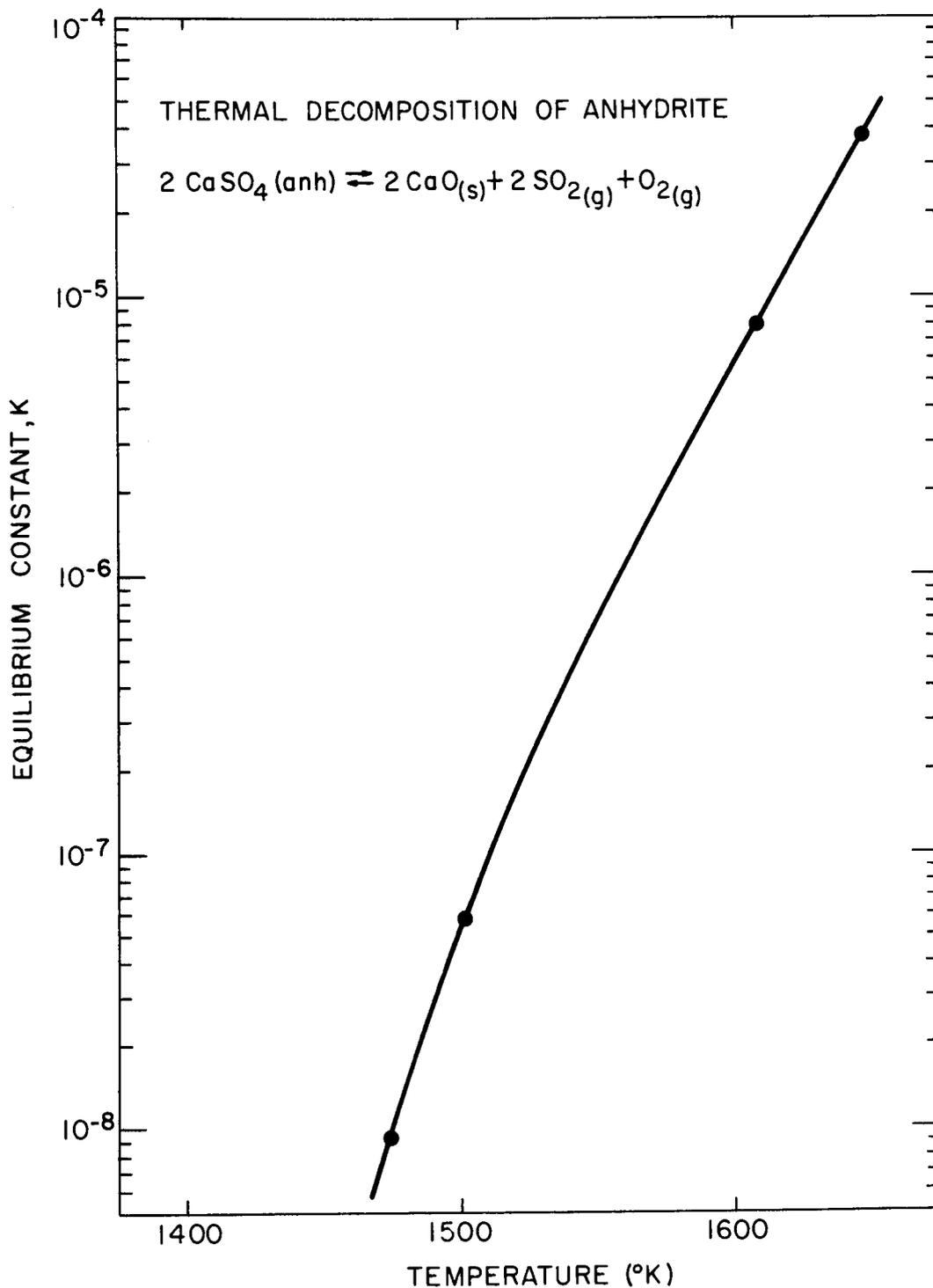


Fig. 4. The Thermal Decomposition of Anhydrite.

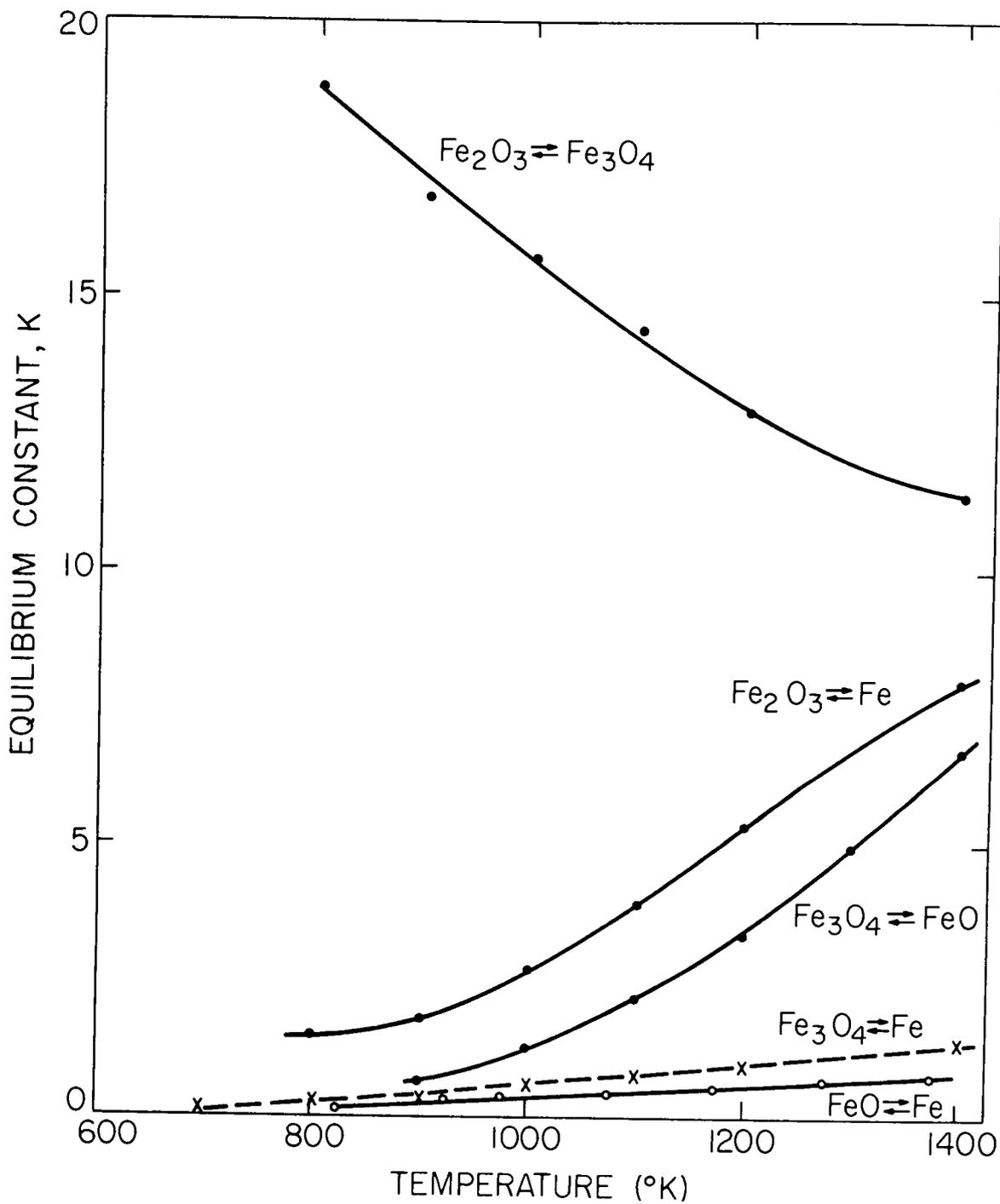


Fig. 5. The Reduction of Iron Oxides by H_2 .

Table 6. Equilibrium Constants of Some Reactions Involving O₂, H₂, H₂O, C, CO, CO₂, and CH₄^a

Reaction	Equilibrium Constant, K ^b												
	298.16°K	400°K	500°K	600°K	700°K	800°K	900°K	1000°K	1100°K	1200°K	1300°K	1400°K	1500°K
CO _(g) + 1/2 O _{2(g)} ⇌ CO _{2(g)}	1.1x10 ⁴⁵	2.6x10 ³²	1.0x10 ²⁵	1.2x10 ²⁰	3.5x10 ¹⁶	7.8x10 ¹³	6.9x10 ¹¹	1.6x10 ¹⁰	7.2x10 ⁸	5.5x10 ⁷	6.3x10 ⁶	9.9x10 ⁵	2.0x10 ⁵
CO _(g) + H ₂ O _(g) ⇌ CO _{2(g)} + H _{2(g)}	9.9x10 ⁴	1.5x10 ³	1.3x10 ³	27	9.0	4.0	2.2	1.4	0.94	0.70	0.54	0.44	0.37
CH _{4(g)} + 1/2 O _{2(g)} ⇌ CO _(g) + 2H _{2(g)}	1.4x10 ¹⁵	4.3x10 ¹³	6.7x10 ¹²	2.2x10 ¹²	1.0x10 ¹²	6.1x10 ¹¹	4.1x10 ¹¹	3.1x10 ¹¹	2.4x10 ¹¹	2.0x10 ¹¹	1.7x10 ¹¹	1.4x10 ¹¹	1.3x10 ¹¹
CH _{4(g)} + CO _{2(g)} ⇌ 2CO _(g) + 2H _{2(g)}	1.3x10 ⁻³⁰	1.7x10 ⁻¹⁹	6.6x10 ⁻¹³	1.9x10 ⁻⁸	3.0x10 ⁻⁵	7.7x10 ⁻³	0.52	19	3.3x10 ²	3.5x10 ³	2.6x10 ⁴	1.5x10 ⁵	6.4x10 ⁵
CH _{4(g)} + H ₂ O _(g) ⇌ CO _(g) + 3H _{2(g)}	1.3x10 ⁻²⁵	2.4x10 ⁻¹⁶	8.7x10 ⁻¹¹	5.1x10 ⁻⁷	2.7x10 ⁻⁴	3.1x10 ⁻²	1.3	26	3.1x10 ²	2.5x10 ³	1.4x10 ⁴	6.4x10 ⁴	2.4x10 ⁵
CH _{4(g)} + 2H ₂ O _(g) ⇌ CO _{2(g)} + 4H _{2(g)}	1.3x10 ⁻²⁰	3.6x10 ⁻¹³	1.2x10 ⁻⁸	1.4x10 ⁻⁵	2.4x10 ⁻³	0.13	2.9	36	3.0x10 ²	1.7x10 ³	7.8x10 ³	2.8x10 ⁴	8.7x10 ⁴
C(s; graphite) + CO _{2(g)} ⇌ 2CO _(g)	1.0x10 ⁻²¹	5.2x10 ⁻¹⁴	1.8x10 ⁻⁹	1.9x10 ⁻⁶	2.7x10 ⁻⁴	1.1x10 ⁻²	0.19	1.9	12	57	2.1x10 ²	6.3x10 ²	1.6x10 ³
C(s; graphite) + H ₂ O _(g) ⇌ CO _(g) + H _{2(g)}	1.0x10 ⁻¹⁶	7.7x10 ⁻¹¹	2.2x10 ⁻⁷	5.1x10 ⁻⁵	2.4x10 ⁻³	4.4x10 ⁻²	0.42	2.6	12	40	1.1x10 ²	2.8x10 ²	6.0x10 ²
H _{2(g)} + 1/2 C _{2(g)} ⇌ H ₂ O _(g)	1.1x10 ⁴⁰	1.7x10 ²⁹	7.7x10 ²²	4.3x10 ¹⁸	3.8x10 ¹⁵	1.9x10 ¹³	3.1x10 ¹¹	1.2x10 ¹⁰	7.7x10 ⁸	7.9x10 ⁷	1.2x10 ⁷	2.2x10 ⁶	5.3x10 ⁵

a. Calculated by Rossini et al.⁴ Listed here only to two significant figures.

b. K is defined as the product of the partial pressure of the gaseous substances on the right side of each equation divided by the product of the partial pressures of the gaseous substances on the left side of each equation, each partial pressure being raised to the proper power as indicated by its coefficient.

Table 7. Reduction of CaSO₄ by CH₄ and by CO

See also Figs. 6 and 7

Temp., °K	CaSO ₄ (anh) + CH ₄ (g) \rightleftharpoons CaS(s) + CO ₂ (g) + 2H ₂ O(g)		CaSO ₄ (anh) + 4CO(g) \rightleftharpoons CaS(s) + 4CO ₂ (g)	
	-ΔF, kcal	K ^a	-ΔF, kcal	K ^b
298.1	-10.390	2.42 x 10 ⁻⁸	43.928	1.60 x 10 ³²
300	-10.333	2.97 x 10 ⁻⁸	43.937	1.01 x 10 ³²
400	1.737	8.889	43.956	1.00 x 10 ²⁵
500	7.082	1.28 x 10 ³	44.292	2.67 x 10 ¹⁹
600	15.195	3.55 x 10 ⁵	44.277	1.49 x 10 ¹⁶
700	23.082	2.81 x 10 ⁷	44.415	7.95 x 10 ¹³
800	32.250	6.74 x 10 ⁸	44.423	1.45 x 10 ¹²
900	40.632	7.68 x 10 ⁹	44.390	6.30 x 10 ¹⁰
1000	48.913	4.89 x 10 ¹⁰	44.294	2.06 x 10 ⁹
1100	57.767	2.99 x 10 ¹¹	44.826	8.04 x 10 ⁸
1200	66.256	1.17 x 10 ¹²	45.041	1.60 x 10 ⁸
1300	73.049	1.91 x 10 ¹²	43.616	2.15 x 10 ⁷
1400	79.892	2.97 x 10 ¹²	43.256	5.66 x 10 ⁶
1500	88.432	7.67 x 10 ¹²	42.795	1.72 x 10 ⁶

a.

$$K = \frac{[P_{CO_2}][P_{H_2O}]^2}{[P_{CH_4}]}$$

b.

$$K = \frac{[P_{CO_2}]^4}{[P_{CO}]^4}$$

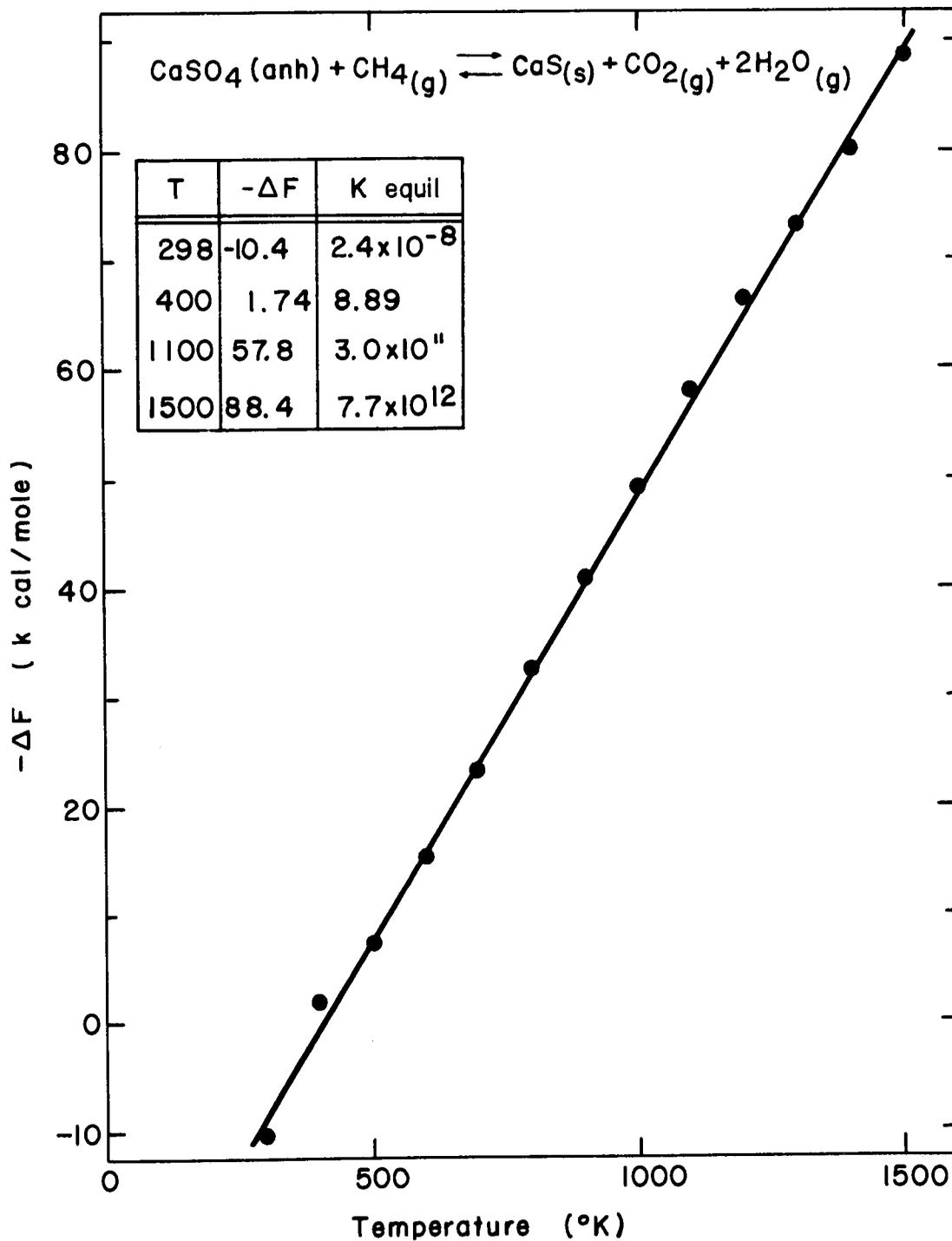


Fig. 6. The Reduction of CaSO_4 by CH_4 .

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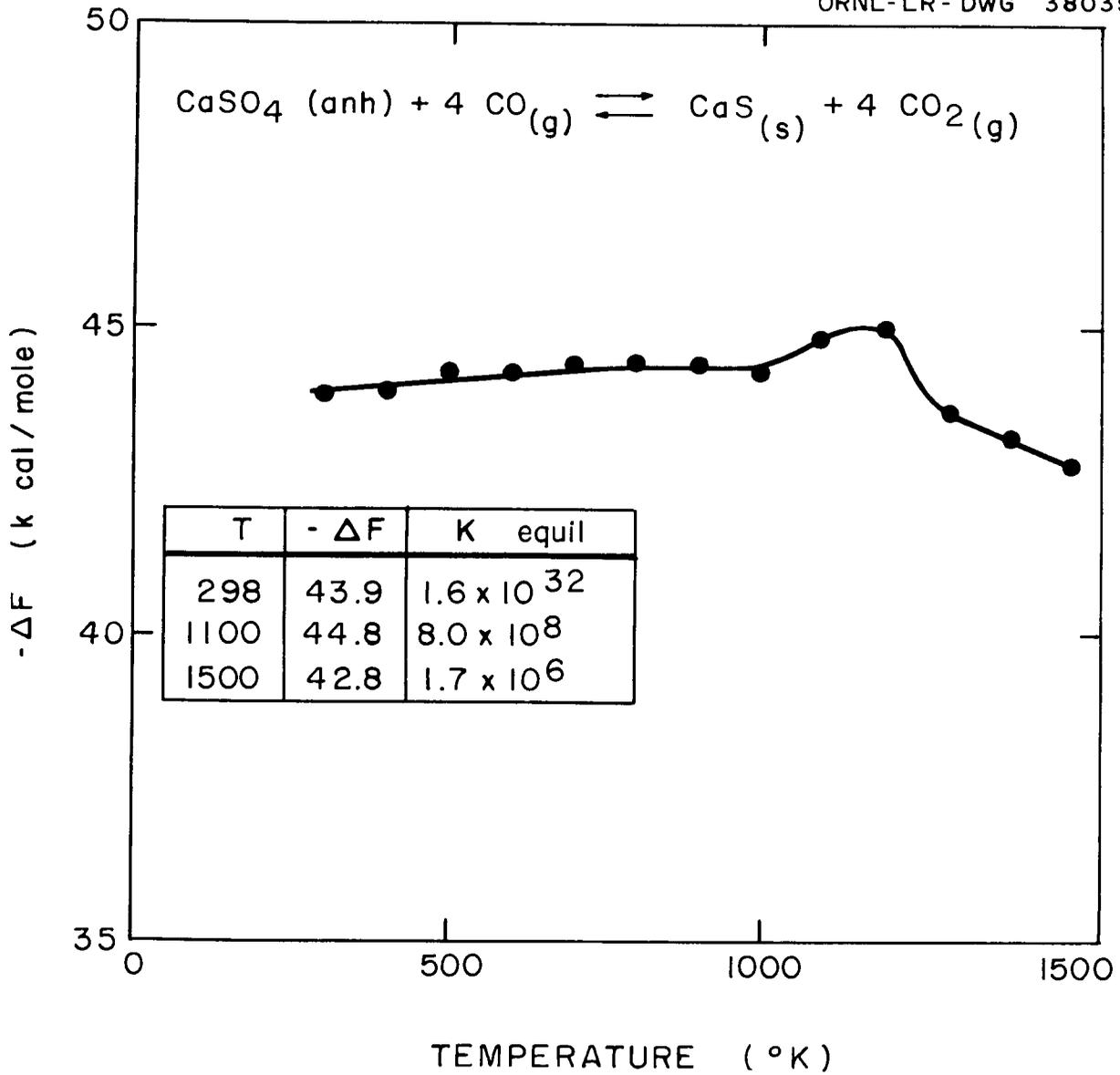


Fig. 7. The Reduction of CaSO_4 by CO .

Table 8. Dissociation Pressure of Carbonates

See also Fig. 8

Temp., °K	P_{CO_2} , mm of Hg					
	$CaCO_3^a$	$Li_2CO_3^b$	$Na_2CO_3^b$	$K_2CO_3^b$	$MgCO_3^e$	
					T	P
773	0.733	c	c	c	763.1	0.983
873	1.84	c	c	c	843.1	1.763 3.67 ^d
973	22.4	c	c	c		
1073	167	c	c	c	873.1	13.9 ^d
1173	793	17.4	c	c	973.1	473.4 ^d
1223	c	32.7	0.00	1.2		
1273	2943	56.2	1.5	2.1		
1373	c	134.4	5.5	7.4		
1473	c	c	14.0	10.3		
1573	c	c	29.0	15.1		
1673	c	c	66.0	35.6		

a. Tabulated by S. Glasstone.⁶

b. Tabulated by J. Suttle.⁷

c. No data reported.

d. Calculated from: $\log kP_1 - kP_2 = \Delta H(T_1 - T_2) / 4.571(T_1 \times T_2)$.

e. International Critical Tables.⁹

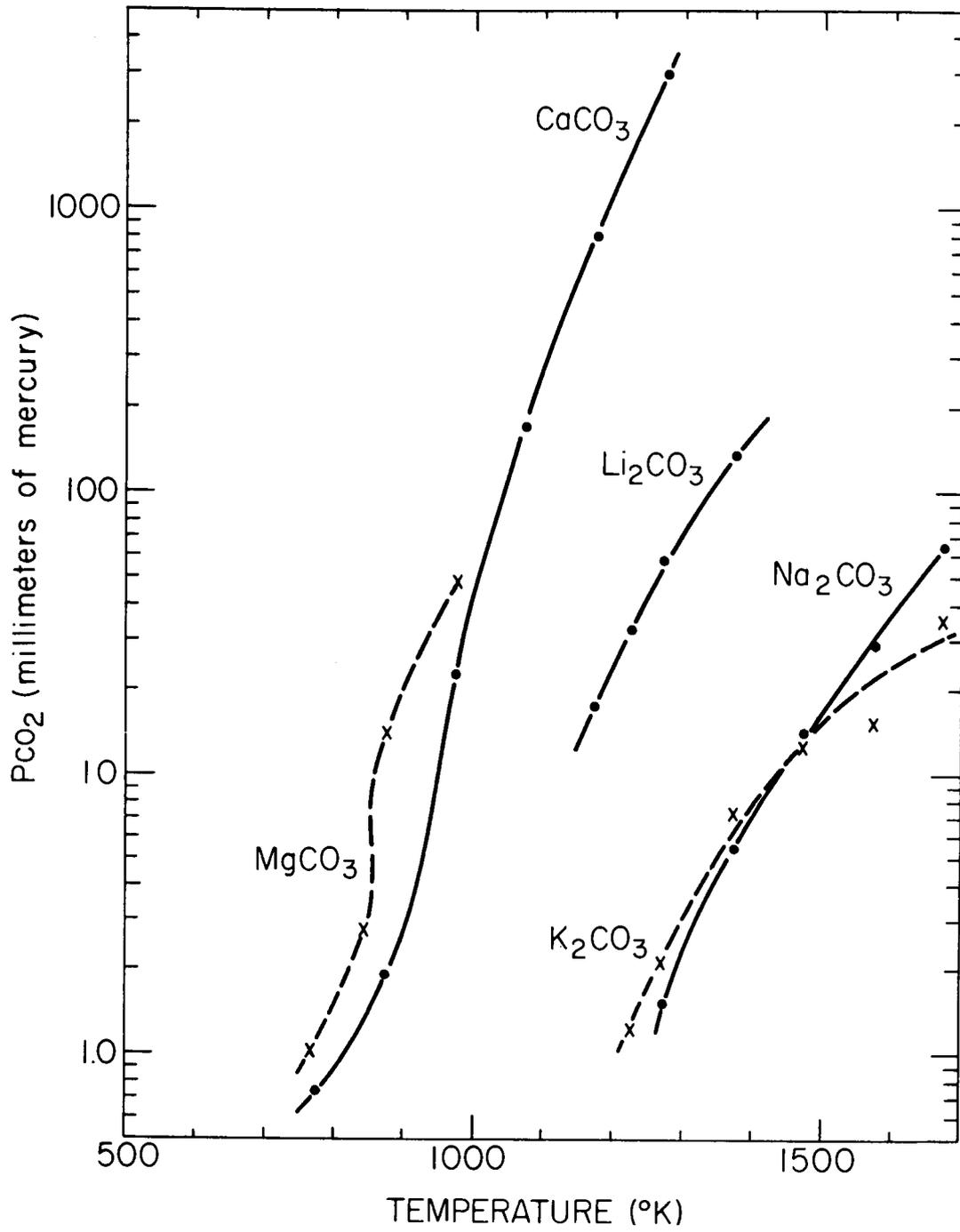


Fig. 8. Dissociation Pressure of Carbonates.

Table 9. Reaction of SiO_2 , CaO , Al_2O_3 , and Na_2O with H_2

Reaction	300°K		500°K		1000°K		1500°K	
	$-\Delta F$, kcal	K^a	$-\Delta F$, kcal	K^a	$-\Delta F$, kcal	K^a	$-\Delta F$, kcal	K^a
$\text{SiO}_2(\text{quartz}) + 2\text{H}_2(\text{g}) \rightleftharpoons \text{Si}(\text{s}) + 2\text{H}_2\text{O}(\text{g})$	-88	7.90×10^{-65}	-83	3.95×10^{-37}	-74	6.74×10^{-17}	-67	1.73×10^{-10}
$\text{CaO}(\text{s}) + \text{H}_2(\text{g}) \rightleftharpoons \text{Ca}(\alpha) + \text{H}_2\text{O}(\text{g})$	-90.0	2.69×10^{-38}	-86.1	1.73×10^{-38}	-80.7	2.32×10^{-18}	-75.8	9.02×10^{-12}
$\text{Al}_2\text{O}_3(\text{s}) + 3\text{H}_2(\text{g}) \rightleftharpoons 2\text{Al}(\text{s}) + 3\text{H}_2\text{O}(\text{g})$	-211	1.99×10^{-154}	-203	9.22×10^{-90}	-189	4.98×10^{-42}	-173	6.20×10^{-26}
$\text{Na}_2\text{O}(\text{s}) + \text{H}_2(\text{g}) \rightleftharpoons 2\text{Na}(\text{s}) + \text{H}_2\text{O}(\text{g})$	-35.4	1.63×10^{-26}	-30.5	4.20×10^{-14}	-20.0	4.26×10^{-5}	1.3	1.55

a. K for each reaction is $\frac{[\text{P}_{\text{H}_2\text{O}}]^x}{[\text{P}_{\text{H}_2}]^x}$, where x is the coefficient of H_2 and H_2O in the chemical equation.

Table 10. Free Energy Values Used in Calculations

Temp., °K	- Δ F, kcal/mole												
	CaSO ₄ (anh)	CaS(s)	SO ₂ (g)	H ₂ S(g)	CaO(s)	H ₂ O(g)	CH ₄ (g)	CO(g)	CO ₂	NaCl(s)	Na ₂ O	SiO ₂ (quartz)	Al ₂ O ₃ (s)
298.1	311.860	109.980	77.750	7.865	144.30	54.635	12.140	32.808	94.260				
300	311.690	109.971	71.753		144.57	54.615	12.104	32.846	94.260	92	90	196	375
400	309.677	109.631	71.989		141.10	53.516	10.048	35.007	94.235				
500	293.643	109.103	72.159	9.965	138.58	52.538	7.840	37.184	94.392	87	83	188	361
600	284.617	108.550	72.268		136.29	51.154	5.49	39.358	94.444				
700	275.586	108.117	72.318		133.78	49.912	3.05	41.526	94.497				
800	266.592	107.567	72.310		131.38	48.643	0.55	43.677	94.539				
900	257.638	106.984	72.246		128.00	47.349	-2.01	45.816	94.578				
1000	248.719	106.340	72.125	12.620	126.65	46.036	-4.61	47.942	94.610	77	66	166	327
1100	239.757	106.227	71.948		124.31	44.710	-7.22	50.053	94.637				
1200	231.053	106.058	71.717		121.99	43.370	-9.85	52.151	94.661				
1300	222.310	104.158	71.430		119.68	42.017	-12.50	54.235	94.667				
1400	213.616	103.344	71.090		117.39	40.661	-15.14	56.308	94.692				
1500	205.035	102.478	70.695	13.795	115.12	39.296	-17.80	58.370	94.707	63	38	146	291

Table 11. Reference States and Free Energy-Temperature Equations Employed

Compound	Reference State	Free Energy-Temperature Dependence
$\text{CaSO}_4(\text{anh})$	$\text{Ca}(\alpha); \text{S}(\text{rh}); 2\text{O}_2(\text{g})$	$\Delta F^\circ = -336,420 + 15.91 T \log T - 5.94 \times 10^{-3} T^2 - 1.091 \times 10^{-5} T^{-1} + 46.02 T$
$\text{CaS}(\text{s})$	$\text{Ca}(\alpha); \text{S}(\text{rh})$	$\Delta F^\circ = -111,340 - 3.02 T \log T + 2.88 \times 10^{-3} T^2 + 11.18 T$
$\text{SO}_2(\text{g})$	$\text{S}(\text{rh}); \text{O}_2(\text{g})$	$\Delta F^\circ = -70,635 + 1.04 T \log T + 2.542 \times 10^{-3} T^2 + 0.084 \times 10^5 T^{-1}$
$\text{H}_2\text{S}(\text{g})$	$\text{H}_2(\text{g}); \text{S}(\text{rh})$	$\Delta F^\circ = -3,725 + 7.02 T \log T + 1.865 \times 10^{-3} T^2 - 31.82 T$
$\text{CaO}(\text{s})$	$\text{Ca}(\alpha); 1/2 \text{O}_2(\text{g})$	$\Delta F^\circ = -151,700 - 1.428 T \log T - 6.0 \times 10^{-4} T^2 + 29.6 T + 338$
$\text{H}_2\text{O}(\text{g})$	$\text{H}_2(\text{g}); 1/2 \text{O}_2(\text{g})$	Tabulated in 100° increments by Rossini et al. ⁴
$\text{CH}_4(\text{g})$	$\text{C}(\text{s}; \text{graphite}); 2\text{H}_2(\text{g})$	Tabulated in 100° increments by Rossini et al. ⁴
$\text{CO}(\text{g})$	$\text{C}(\text{s}; \text{graphite}); 1/2 \text{O}_2(\text{g})$	Tabulated in 100° increments by Rossini et al. ⁴
$\text{CO}_2(\text{g})$	$\text{C}(\text{s}; \text{graphite}); \text{O}_2(\text{g})$	Tabulated in 100° increments by Rossini et al. ⁴
$\text{Na}_2\text{O}(\text{s})$	$2\text{Na}(\text{s}); 1/2 \text{O}_2(\text{g})$	Free energy-temperature curves of Glassner ⁸
$\text{NaCl}(\text{s})$	$\text{Na}(\text{s}); 1/2 \text{Cl}_2(\text{g})$	Free energy-temperature curves of Glassner ⁸
$\text{SiO}_2(\text{quartz})$	$\text{Si}(\text{s}); \text{O}_2(\text{g})$	Free energy-temperature curves of Glassner ⁸
$\text{Al}_2\text{O}_3(\text{s})$	$\text{Al}(\text{s}); 3/2 \text{O}_2(\text{g})$	Free energy-temperature curves of Glassner ⁸

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