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**Thermal and Chemical Degradation of
Inorganic Membrane Materials**

Topical Report

**Gopala N. Krishnan
Angel Sanjurjo
Bernard J. Wood
Kai-Hung Lau**

April 1994

Work Performed Under Contract No.: DE-AC21-92MC28053

**For
U.S. Department of Energy
Office of Fossil Energy
Morgantown Energy Technology Center
Morgantown, West Virginia**

**By
SRI International
Menlo Park, California**

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333 Ravenswood Avenue
Menlo Park, California 94025**

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SUMMARY

This report describes the results of a literature review to evaluate the long-term thermal and chemical degradation of inorganic membranes that are being developed to separate gaseous products produced by the gasification or combustion of coal in fixed-, fluidized-, and entrained-bed gasifiers, direct coal-fired turbines, and pressurized-fluidized-bed combustors. Several impurities, such as H_2S , NH_3 , SO_2 , NO_x , and trace metal compounds are generated during coal conversion, and they must be removed from the coal gas or the combustor flue gas to meet environmental standards. The use of membranes to separate these noxious gases is an attractive alternative to their removal by sorbents such as zinc titanate or calcium oxide. Inorganic membranes that have a high separation efficiency and exhibit both thermal and chemical stability would improve the economics of power generation from coal. The U.S. Department of Energy is supporting investigations to develop inorganic membranes for separating hydrogen from coal gas streams and noxious impurities from hot coal- and flue-gas streams. Membrane materials that have been investigated in the past include glass (silica), alumina, zirconia, carbon, and metals (Pd and Pt).

Many studies examined membrane performance in relatively clean gaseous environments. But coal gasification and combustion gas streams at high temperatures can be an aggressive threat to the efficient operation of inorganic membranes. These gas streams contain several components, such as H_2O , CO , H_2S , SO_2 , and alkali vapor, that could react with Al_2O_3 , ZrO_2 , SiO_2 , Pd, and other membrane materials in the temperature range of interest (500° to 1200°C). The residual particulate flyash material, if present after passage through cyclones or filters, contains several components such as alkali salts that could react with the membrane materials at high temperatures to form different phases. Thus, several thermal and chemical degradation mechanisms could unfavorably alter the properties of inorganic membranes exposed to high temperature coal gas and flue gas streams.

An evaluation of potential degradation mechanisms, using existing theories and data available in the literature, has been conducted as part of a research program at SRI International. A literature search was made using computerized data bases, and several hundred citations were obtained. Relevant technical articles were reviewed critically to ascertain the role of sintering, hydrothermal attack, reaction with ash particles, interaction with alkali impurities, and the deposition of carbon on membranes in hot coal gas and combustion gas environments.

Sintering of highly porous inorganic membranes is a degradation mechanism that limits the temperature at which the membranes can be used for gas separation. Crystallites of the materials used in these membranes are of several nanometers in size, but they are in relatively unstable thermodynamic states. At high temperatures, they tend to revert to a lower energy state by agglomeration or through phase transformations. The pore size distributions in all the oxide membranes considered change when they are exposed to temperatures above 500°C. Although membranes can be made with median pore diameter less than 5 nm, the size often increases to about 10 nm when the material is heated to about 500°C. As the temperature is increased further, enlargement of pores and decrease in surface area become more severe. At temperatures above 1000°C, the median pore size is likely to be above 50 nm. Such changes are due to phase transformation or diffusion of atoms on the surface or in the bulk.

Coal gasification and combustion gas streams contain a significant fraction of steam (10 to 25% v/v). At the high temperatures and high pressures encountered in coal gasification, steam can have a deleterious effect on the properties of the membrane materials. The hydrothermal environment generally enhances sintering of the oxide membrane materials. Similarly, phase transformations in the oxide ceramics are also accelerated in the presence of steam. These effects are attributable to the formation of mobile hydroxide species on the surfaces that interact with ion vacancies normally present in the membrane material. Among common ceramic materials, the hydrothermal effect is most severe in silica, less so in alumina and titania, and minimal in zirconia. Metal membranes such as Pd and Pt are not affected by steam, but they are prone to poisoning by H₂S, arsenic, and other trace metal vapor impurities in the hot coal gas stream.

A fraction of the mineral matter in coal escapes the gasifier or combustor in the form of flyash. The composition of flyash depends on the type of coal, the combustion or gasification conditions, and the particle size of the ash. Although most of the flyash is removed by cyclones and barrier filters, a small fraction in the form of fine particulate matter (fume) may still reach the membrane modules. The constituents of these particles are silica, silicates, aluminosilicates, ferrous oxides, alkali and alkaline earth compounds. The alkali compounds especially are likely to react with certain ceramic membrane materials, forming chemical phases that weaken the membrane or modify its permeability.

The separation of the various components of the hot coal gas streams during permeation through the membrane changes the gas phase composition and shifts the equilibria between the constituents. In such cases, solids may be deposited by reaction in the gas phase inside the membrane pores. For example, preferential removal of hydrogen from the hot coal gas changes the C/H and C/O ratios, which may lead to deposition of carbon by disproportionation of CO or by decomposition of hydrocarbons. Thermochemical calculations indicate that the gas stream

from an oxygen-blown, entrained-bed gasifier (Texaco) has the potential to deposit carbon. The composition of coal gas from fluidized-bed gasifiers is outside the carbon deposition region only above 800°C. However, preferential removal of hydrogen from the hot coal gas could endow it with enough carburizing potential to deposit carbon. Fixed-bed gasifiers operate at relatively low temperatures and the gas streams contain a significant quantity of tar components. Under hydrogen-deficient conditions, these hydrocarbon components could pyrolyze and deposit carbon in the pores of inorganic membranes.

In summary, during exposure to coal gasification and combustion gas streams, inorganic membranes could be degraded by thermal sintering, hydrothermal attack, reaction with ash components, attack by vapor- and solid-phase alkali compounds, reaction with sulfur oxides, and deposition of carbon from the gas phase. The gas stream from a fixed-bed gasifier is generally below 600°C and the quantity of fume is likely to be low. Also, because of the low temperature, most of the alkali compounds will be retained in the ash, which can be effectively removed. However, the gas stream contains significant amounts of tar components, which could lead to carbon deposition on a membrane.

Fluidized-bed gasifiers operate at higher temperature than fixed-bed units and tar is not generally present. The vapor-phase alkali level is high enough to favor attack by sodium and potassium compounds. High steam levels encountered under oxygen-blown operation could lead to hydrothermal sintering of membranes. At temperatures below 800°C, the gas composition is inside the carbon deposition regime and deposition of carbon is likely. Removal of hydrogen through the membrane could force also the gas to a different equilibrium composition that favors deposition of carbon inside the membrane pores.

The degradation mechanisms that prevail in entrained-bed gasifier streams are similar to those in fluidized-bed gasifier streams, except that alkali levels could be higher in the former. The gas from an oxygen-blown entrained-bed gasifier is sufficiently carburizing that carbon deposition is likely even without removal of H₂.

Exposure of membranes to combustor gas streams from direct coal-fueled turbines and pressurized fluidized-bed combustors may lead to degradation by hydrothermal attack, or by reaction with SO₂, alkali sulfates, and ash particles.

The results of this study reveal several thermal and chemical mechanisms that could degrade the properties of inorganic membrane materials. In coal gasification streams, the most dominant mechanisms are hydrothermal sintering, attack by fine ash particles (fume) and vapor phase alkali species, poisoning by sulfur and trace metal impurities, and deposition of carbon. In

coal combustion gas streams, membrane degradation is most likely to occur by reaction with ash particulates and sulfur oxides.

It is recommended that experiments be performed under well-defined conditions to determine the rate and extent of various degradation mechanisms. For ceramic membrane materials, the degradation by hydrothermal sintering, attack by ash particulate material, and reaction with alkali species deserve primary attention. For metal membrane material, the degradation due to sulfur species such as H_2S must be determined. Changes in the physical, chemical, and mechanical properties of the membrane materials as a function of temperature, gas composition, pressure, and exposure duration must be evaluated. Long-term permeation experiments under gas streams representative of coal gasifiers and combustors must be performed. Determination of changes in the characteristics of membranes during exposure to an actual coal gasifier or combustor gas stream is also desirable.

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I. INTRODUCTION

Advanced coal gasification systems such as integrated coal gasification combined cycle (IGCC) processes offer many advantages over conventional pulverized coal combustors. IGCC systems have a high energy conversion efficiency, reduced pollutant emissions, modular construction, and potentially low capital and operating costs. The gasification process allows the contaminants to be removed in their reduced or reactive state. The volume of a coal gas stream is less than that of a combustor flue gas stream in a plant of comparable size; hence, capital and operating costs for contaminant removal are less. Hot gas cleanup minimizes the quantity of waste water requiring treatment and disposal, because the quench/scrubbing operation is eliminated. Fixed-, fluidized-, and entrained-bed reactors have been developed and tested for coal gasification.

Pressurized fluidized-bed coal combustors (PFBC) also have several advantages over atmospheric pressure units, including higher thermal efficiency, smaller plant size, and lower capital and operating costs. These advanced combustors are being tested at near-commercial scale levels. Another advanced concept being developed for electric power generation is the direct coal-fired gas turbine (DCFT) in which slurry coal is burnt in a compact combustor adjacent to a gas turbine.

Coal is a complex and heterogeneous substance that contains several impurities including sulfur, chlorine, nitrogen, and metal compounds. During gasification or combustion, many of these impurities are converted to gaseous species such as H_2S , HCl , NH_3 , SO_2 , NO_x , NaCl , and AsH_3 . Effective removal of impurities is necessary to protect electric power generating equipment such as gas turbines and fuel cells or to meet environmental standards. Coal gas streams exiting a gasifier are at a high temperature (500° to 1200°C). To preserve the enthalpy represented by this hot gas and thereby improve the thermal efficiency of processes using coal gas, there is a strong incentive to remove impurities at temperatures equal to or above the use temperatures. Indeed, the primary recommendation of DOE Coal Gasification Research Needs (COGRAN) Panel was the development of hot gas cleanup techniques [COGRAN, 1987]. The use of membranes to separate these noxious gases is an attractive alternative to their removal by sorbents such as zinc ferrite, zinc titanate or calcium oxide. Inorganic membranes that have a high separation efficiency and exhibit both thermal and chemical stability would improve the economics of power generation from coal. Furthermore, coal gas contains a significant fraction of hydrogen, a commercially valuable chemical feedstock. Membranes can separate the

hydrogen from the rest of coal gas mixture effectively and thus improve the economics of hydrogen production from coal.

II. PROJECT DESCRIPTION

The overall objective of this program is to evaluate the long-term thermal and chemical degradation of inorganic membranes that are being developed to separate gaseous products produced by the gasification or combustion of coal in fixed-, fluidized-, and entrained-bed gasifiers, direct coal-fired turbines, and pressurized-fluidized-bed combustors.

The specific objectives of this program are to (1) identify and evaluate long-term degradation mechanisms for inorganic membranes exposed to hot coal gasification and combustion gas streams using data from the existing literature, (2) quantify the extent of the degradation process for the three most serious mechanisms by performing experiments under laboratory-scale conditions, and (3) develop a predictive model that allows estimation of membrane degradation under operating conditions. To achieve the above objectives, the program is divided into the following tasks:

- Task 1. Development of evaluation methodology
- Task 2. Evaluation of potential long-term degradation mechanism
- Task 3. Submission of a topical report and a plan for experimental testing
- Task 4. Experimental testing
- Task 5. Model development.

This report is submitted in partial fulfillment of Task 3 objectives. Tasks 4 and 5 are separate options that may be exercised by the U.S. Department of Energy at the conclusion of Task 3.

III. INORGANIC MEMBRANES FOR GAS SEPARATION

Inorganic membranes have been an item of commerce for more than 30 years. Many inorganic membrane products available today perform the task of microfiltration and ultrafiltration, and some can be used for gas separation applications (Table III-1). Glass membranes are made by Corning Glass, Asahi Glass, Fuji Filters, and Schott Glass. An alumina membrane (Membralox) was manufactured by Alcoa, Pittsburgh, PA, about 3 years ago. These Vycor-like and alumina products could be made in tubular form (6- to 7-mm I.D.). They have gas-selective pores of approximately 4 to 10 nm diameter in the walls of the membrane tubes. Pores of this size are much smaller than the mean free path of gaseous molecules under a wide range of pressure and temperature conditions. Consequently, gases are separated according to the well-known Knudsen mechanism which states that the selectivity for two gases is inversely proportional to the ratio of the square root of the molecular weights of the gases.

Because the selectivity imparted by Knudsen diffusion is too low to be commercially important for most gas separation applications (a notable exception is the uranium enrichment process at the Oak Ridge Gaseous Diffusion plant), a variety of research and development efforts have ensued in recent years aimed at obtaining industrially important separation factors with industrially acceptable gas fluxes. These materials are glasses, metals, carbon, and metal oxides. The metal membranes are designed specifically for H_2 separation (via dissolution/diffusion of H_2), whereas the nonmetals are multipurpose membranes with pore sizes as large as the gas molecules themselves (molecular sieve mechanism) [Way and Roberts, 1989].

GAS SEPARATION BY INORGANIC MEMBRANES

The U.S. Department of Energy is supporting investigations to develop inorganic membranes for separating hydrogen from coal gas streams and noxious impurities from hot coal- and flue gas streams. SRI International investigated the use of hollow fiber glass membranes to separate H_2/CO , CO_2/N_2 , and NH_3/N_2 mixtures at temperatures below $400^\circ C$ [Roberts et al., 1992]. High selectivities for one of the components were obtained, but lack of a suitable sealant between the fibers prevented assembly of these fibers into modules. Porous alumina membrane tubes that are being developed by Oak Ridge National Laboratory have exhibited high permeability and moderate selectivity [Egan et al., 1990]. Ceramem Corporation is developing

Table III-1
POTENTIAL POROUS INORGANIC GAS SEPARATION MEMBRANES

Manufacturer*	Trade Name	Membrane Material	Support Material	Membrane Pore Diameter	Geometry of Membrane Element	Tube or Channel Inside Diameter (mm)
Alcoa/SCT	Membralox®	ZrO ₂ Al ₂ O ₃	Al ₂ O ₃ Al ₂ O ₃	20-100 nm 0.2-5 μm	Monolith, tube	4 and 6
Norton	Ceraflo®	Al ₂ O ₃	Al ₂ O ₃	0.2-1.0 μm 6 μm (symmetric)	Monolith, tube	3
NGK		Al ₂ O ₃	Al ₂ O ₃	0.2-5 μm	Tube	7 and 22
Du Pont	PRD-86	Al ₂ O ₃ , Mullite, Cordierite	None	0.06-1 μm	Tube	0.5-2.0
Alcan/Anotec	Anopore®	Al ₂ O ₃ Al ₂ O ₃	Al ₂ O ₃ Al ₂ O ₃	20 nm 0.1 μm 0.2 μm	Plate	
Gaston County Filtration Systems	Ucarsep®	ZrO ₂	C	4 nm	Tube	6
Rhone- Poulenc/ SFEC	Carbosep®	ZrO ₂ ZrO ₂	C C	~4 nm 0.08- 0.14 μm	Tube	6
Du Pont/ CARRE		Zr(OH) ₄	SS	0.2-0.5 μm	Tube	~2
TDK	Dynaceram®	ZrO ₂	Al ₂ O ₃	~10 nm	Tube	~5
Asahi Glass		Glass	None	8 nm-10 μm	Tube/plate	3 and 10
Schott Glass		Glass	None	10 nm and 0.1 μm	Tube	5-15
Fuji Filters		Glass Glass	None None	4-90 nm 0.25-1.2 μm	Tube	
Ceram-Filtre	FITAMM	SiC	None	0.1-8 μm	Monolith	25
Fairey	Strata-Pore®	Ceramics	Ceramics	1-10 μm	Tube/plate	
	Microfiltrex®	SS	SS	0.2-1 mm	Tube/plate	10
Mott		SS, Ni, Au, Ag, Pt, etc.	None	≥0.5 μm	Tube	3.2-19
Pall		SS, Ni, etc.	None	≥0.5 μm	Tube	60 and 64
Osmonics	Hytrex®	Ag	None	0.2-5 μm	Tube/plate	
	Ceratrex®	Ceramics	Ceramics	0.1 μm		
Ceramem		Ceramics oxides	Cordierite	0.05-0.5 μm	Honeycomb monolith	1.8

* Some of these manufacturers are not currently producing the identified products.

asymmetric porous silica/alumina membranes and membrane modules made of cordierite for gas separation [Goldsmith et al., 1992]. The Media and Process Technology Group of Aluminum Company of America is developing alumina and zeolitic membranes [Liu et al., 1992]. Hydrogen permselective membranes formed by depositing SiO_2 and other oxides by chemical vapor deposition within the pores of a porous silica tube are being investigated at California Institute of Technology [Gavalas, 1992]. McMahon, Galvin, and Hsu [1990] studied the use of both Vycor glass and alumina membranes to separate H_2 from a simulated coal gas stream.

Several research programs have focused on separating H_2S and NH_3 from hot coal gas streams using membrane reactors. SRI International investigated the use of a catalyst packed inside a tubular alumina membrane to decompose H_2S in He and NH_3 in H_2 and found that removal of hydrogen through the membrane enhanced the decomposition of these compounds well above equilibrium levels [Roberts et al., 1993]. Bend Research Corporation used a composite metal membrane to decompose H_2S and found that >99% conversion of H_2S can be attained at 700°C [Edlund and Pledger, 1993a]. Molten carbonate salts supported on a porous ceramic substrate are being explored by Air Products and Chemicals to separate sulfur-bearing gases from simulated coal gas streams [Minford et al., 1992].

Many of the above studies are being conducted in a relatively clean environment. But coal gasification and combustion product gas streams at high temperatures can be an aggressive threat to the efficient operation of inorganic membranes. These gas streams contain several components, such as H_2O , CO , H_2S , SO_2 , and alkali vapor, that could react with Al_2O_3 , ZrO_2 , SiO_2 , and other membrane materials in the temperature range of interest (500° to 1200°C). High levels of steam can accelerate the sintering of nanopores at high temperatures by forming mobile hydroxide species. In asymmetric membranes in which a selective microporous membrane layer is bonded to a coarse-pore substrate, the composition of gas to which the support layer is exposed is different from the composition of gas to which the selective layer is exposed. In addition, under permeation conditions, the total pressure on the feed side of the membrane greatly exceeds that on the permeate side of the membrane. Consequently, the selective layer and support layer are exposed to very different partial pressures of aggressive gaseous components. For example, the high CO/H_2 ratio that would result from the preferential removal of H_2 by the membrane could lead to deposition of carbon inside the pores of the membrane. Also, residual particulate material, if present after passage through cyclones or filters, contains several components such as alkali salts that could react with the membrane materials at high temperatures to form different phases. Thus, several thermal and chemical degradation mechanisms can alter the properties of inorganic membranes exposed to high temperature coal gas and flue gas streams.

Another factor in gas/gas separation membranes used in high temperature applications is the membrane module itself. A membrane must be placed in module form (hollow fiber, spiral, plate/frame) to function commercially, and this module necessarily has seals, gaskets, and other materials that are not only exposed to the same corrosive gases as the membrane but must also be leak free and hold a high pressure differential (up to 500 psi) at the operating temperature. The ideal sealing material perfectly matches the thermal expansion characteristics of the membrane and module materials. In practice, perfect matching is not possible, and the long-term performance of a practical module will be adversely affected as the seal itself undergoes corrosive attack.

THERMAL PROPERTIES OF DENSE AND POROUS CERAMICS

The oxide ceramic materials used in fabricating membranes have high melting points and have high-temperature mechanical strength and creep resistance significantly greater than most metals. However, ceramic materials have some limitations, particularly poor thermal shock resistance, low ductility, impact strength, and thermal conductivity. These properties of the oxide ceramics preclude their use in systems subject to rapid temperature fluctuations. Although the membranes that would be used in advanced coal conversion systems normally would operate under nearly isothermal conditions, temperature fluctuations could still occur because of changes in the operating conditions of the gasifier as the electrical load requirement changes. The integrity of many ceramic membrane materials would be at risk if such changes occurred too rapidly. To assess the thermal shock resistance of inorganic membrane materials, we must consider the changes with temperature that occur in a number of thermomechanical properties, including coefficient of thermal expansion (CTE), thermal conductivity (K), modulus of elasticity, and heat capacity.

The heat capacity (C_p) for most ceramics at temperatures above 400°C is typically 6 cal/g-atom °C. Changes in C_p with temperatures parallel those of CTE. Above the Debye characteristic temperature of the material, variations of C_p and CTE with temperature are small.

For any given temperature distribution within a ceramic body, thermal stresses are directly related to thermal expansion. The CTE remains nearly constant over the temperature range of interest in membrane applications. Thus, stress will vary linearly with temperature for homogeneous bodies unless polymorphic transformation occurs as happens in silica, zirconia, and some other materials. The CTE varies considerably between different materials (Table III-2) and will be the major factor affecting thermal stresses in most glasses and many refractory and whiteware compositions. Some materials, such as aluminum titanate and fused silica, have

extremely low coefficients of expansion, but they may be unsatisfactory for other reasons, such as low strength or poor creep resistance.

Table III-2
MEAN COEFFICIENT OF LINEAR EXPANSION* FOR
SOME MEMBRANE MATERIALS

Material	$\alpha \times 10^6 (^{\circ}\text{C}^{-1})$
Al ₂ O ₃	8.8
BeO	9.0
MgO	13.5
Mullite	5.3
Spinel	7.6
ThO ₂	9.2
ZrO ₂ (stabilized)	10.0
Fused quartz	0.5
Soda-lime-silica glass	9.0
Platinum	8.9
Palladium	11.8
Vanadium	8.3
Nickel	13.3

* Average over a temperature range 20 to 1000°C

The thermally induced stress in a ceramic is in general proportional to the modulus of elasticity, the coefficient of thermal expansion, and the temperature gradient. To minimize probability of failure due to thermally-induced stress, the modulus of elasticity and thermal conductivity must be high while the coefficient of thermal expansion must be low. The high thermal conductivities of metals makes them generally less susceptible to thermal shock. In membrane modules with different materials these properties must be matched by careful selection to minimize failure. Table III-3 lists the thermal conductivities for metals and common ceramic materials.

Table III-3
THERMAL CONDUCTIVITY OF MATERIALS*

Material	k (cal. sec. ⁻¹ °C. cm. ⁻² cm)		
	100°C	400°C	1000°C
Al ₂ O ₃	0.072	0.031	0.015
BeO	0.525	0.222	0.049
Graphite	0.426	0.268	0.149
MgO	0.086	0.039	0.017
Mullite	0.015	0.011	0.010
Spinel	0.036	0.024	0.014
ThO ₂	0.025	0.014	0.008
ZrO ₂ (stabilized)	0.0047	0.0049	0.0055
Fused quartz	0.0038	0.0045	
Soda-lime-silica glass	0.0040	0.0046	
Platinum	0.188	0.172	0.179
Palladium	0.168	-	-
Vanadium	0.074	-	-
Nickel	0.20	0.14	-

*Data for crystalline materials are for theoretical density. Values in parenthesis are estimated.

For porous materials, the total thermal conductivity of solids and void space can be approximated by the following equation:

$$K_{\text{total}} = K_{\text{ceramic}} \frac{1 - V_{\text{pore}}}{1 + V_{\text{pore}}}$$

where V_{pore} is the fractional porosity. Because the conductivity of air is much lower than that of the solid, for materials with porosity greater than 50%, the thermal conductivity is approximately equal to one-third of the conductivity of the solid:

$$K_{\text{total}} = \frac{1}{3} K_{\text{ceramic}}$$

The resistance of materials to thermal stress is difficult to quantify, but it depends on the interplay between certain mechanical and thermal properties including strength (modulus of rupture, s), thermal expansion coefficient (α), elastic modulus (E), and thermal conductivity (K). A thermal stress resistance parameter R can be defined as $[s(1 - \mu)/E\alpha]$, where μ is Poisson's ratio. The larger the value of R , the less likely that changes in temperature will cause mechanical damage such as cracking, crazing, or spalling.

The product of R and the thermal conductivity gives a transient thermal sensitivity parameter, R' . This parameter is a measure of the resistance of the material to sudden temperature changes. The values of R and R' have little absolute significance, but when they are calculated for different materials using consistent conventions for units at specific temperatures, they can be used as predictors of relative behavior when thermally shocked and stressed. Values of these parameters for a number of ceramics at three temperatures are displayed in Table III-4. Of the materials listed in this table, other properties not considered, fused silica would be the material of choice for applications where thermal shock events are likely to occur. Among the listed crystalline ceramics, berrilia possesses strong credentials as a material of choice for thermal shock resistant applications.

Table III-4

THERMAL STRESS RESISTANCE FACTORS FOR SOME CERAMIC MATERIALS

Material	100°C		400°C		1000°C	
	R (°C)	R' (cal/(s cm))	R	R'	R	R'
Al ₂ O ₃	37	2.7	36	1.1	40	0.60
BeO	33	17.3	31	6.9	14	0.69
MgO	22	1.9	24	0.94	26	0.45
Mullite	75	1.1	68	0.75	84	0.84
Spinel	32	1.15	32	0.77	32	0.45
ThO ₂	51	1.3	47	0.66	37	0.30
ZrO ₂ (stabilized)	66	0.31	62	0.30	53	0.29
Fused silica	2500	9.5	2400	10.1		
Soda-Lime-silica glass	94	0.38	94	0.43		
TiC	42	2.5	40	1.3	(40)	0.56
Porcelain	116	0.48	103	0.43	116	0.52
Fire-clay refractory	38	0.14	41	0.14	178	0.48

MECHANICAL PROPERTIES OF POROUS CERAMICS

Membranes must be able to resist certain mechanical stresses including mechanical vibration and pressure and thermal gradients (static and transient). Resistance to abrasion/erosion is also necessary for applications with particle-laden gases and under high flow rate conditions.

The mechanical properties of a membrane depend on the porosity, density, type of material, and the size of flaws. We review first the properties of specific materials of interest for membrane fabrication and we then discuss the effects of porosity and flaws.

The mechanical properties of ceramics can vary broadly as shown in Table III-5. Conventional oxide-base ceramics have high compressive strength but relatively low tensile strength. More covalent ceramics, such as SiC and Si₃N₄, have much higher tensile strength than the oxides. The relative strengths of several materials, including ceramics, metals, and polymers, are shown in Figure III-1 by plotting their elastic moduli as a function of density.

Table III-5

MECHANICAL PROPERTIES OF OXIDE CERAMICS

Property	Alumina	Cordierite	Mullite	Zirconia*
Compressive strength (MPa)	2714.0	340.0	551.0	—
Flexural strength (MPa)	315.0	107.0	386.0	800.0
Fracture toughness (MPa·m ^{0.5})	3.0	2.5	2.2	6.2
Hardness (GPa)	15.7	7.0	12.5	11.0
Poisson's ratio	0.23	0.25	0.25	0.23
Tensile strength (MPa)	311.0	54.0	—	—
Young's modulus (GPa)	360.0	100.0	230.0	190.0

* Y₂O₃ partially stabilized.

Figure III-1. Mechanical strength as a function of density for several classes of materials.
Note: Adapted from Green (1992).

The mechanical behavior of relatively compact ceramic bodies depends not only on the intrinsic properties of the materials but also on the geometry and on the size, number and distribution of internal and external flaws. Microcracks, pores, inclusions, grain boundaries, in general all microstructural irregularities, can affect the properties of ceramics. In porous materials many of these irregularities are intrinsic and abundant. The mode of fabrication can contribute appreciably to the type and density of irregularities and therefore it will play a significant role in determining mechanical properties. In asymmetric membranes, the mechanical properties of the separation layer may be different from those of an open structure used as a backing layer.

When powders are sintered without large external pressures, a network of interconnected pores is formed that can be used for filtration and/or gas separation. The probability of a nanopore becoming completely blocked is small, even if external pressure is applied during sintering, because formation and consolidation of channel walls under pressure reduces local stress, and thus the structure resists further deformation as the pore size diminishes. Experimentally, it has been shown that pores larger than a critical size do not coalesce during sintering. Such pores are typically produced in regions where the particle shapes do not conform well, leading to low packing density.

For membrane layers formed from powders by sintering, the Young's modulus of elasticity can be approximately estimated by the following equation:

$$E_p = E_0 (1 - aV_p)^n$$

where

E_p is Young's modulus for the porous material

E_0 is Young's modulus for the material of theoretical density

a is an empirical coefficient that typically is close to unity

V_p is the total pore volume

n is an empirical exponent that depends on the pore geometry, and is a measure of the tortuosity of the paths.

Experimentally, the value for n has been found to be 2 for very pure materials and 4 for mixed ceramics [Wagh et al., 1991]. This change in the algorithm indicates that, relative to porosity, the strength of the material decreases more rapidly in mixed ceramics than in pure ceramics (Figure III-2). Even if the membranes were made of pure ceramics, interaction with the residual

Figure III-2. Variation of Mechanical strength as a function of porosity for pure and mixed ceramics.

flyash components of the coal gasification or combustion gas stream could lead to an unanticipated decrease in the designed mechanical strength.

Addition of foreign compounds may result in the formation of liquid phases during sintering. In most cases, these will weaken the structure. The formation of foreign phases in a membrane can also occur by chemical reaction when particulate or gaseous species come into contact with the membrane.

The fracture toughness (K_{Ic}) of a material, the ability to withstand mechanical shocks, can be calculated from the following equation:

$$K_{Ic} = 0.016 \sqrt{\frac{E}{H}} \cdot \frac{P}{C^{1.5}}$$

where E is Young's modulus, H is hardness, P is pressure, and C is crack length measured for a single indentation under a pressure P [Hughan and Edwards 1988].

The fracture probability, F, can be estimated by the following equation:

$$F = 1 - 1/e^{V_p/(\sigma_f/\sigma_o)^m}$$

where m is the Weibull modulus and σ_f and σ_o are the tensile strengths of the porous and dense materials, respectively. Weibull statistics define the distribution and type of flaws that may result in failure at even lower stresses than those predicted when only porosity and phase contaminants are taken into account. Hence, the flaws are critical in determining the strength of a membrane, and not only the material, but also the porosity and the type and size of microdefects must be considered when predicting the mechanical performance of a membrane structure.

Kim et al.[1992] found that granular porous Al_2O_3 sintered at 1100°C contained many crack-like voids at junctions of three grains. These voids can act as crack nucleation points; indeed, they meander in all directions through the ceramic body, forming a network that may be interconnected. Krasulin et al.[1980], working with ZrO_2 , reported that cracks propagate both through intergranular contacts and within spherical grains.

This information suggests that even relatively well-sintered dense ceramics have a population of faults that weaken them. Porous membranes sintered under lower pressures and lower temperatures may have even larger flaw densities and varieties. Hence, in the manufacture of membranes, both internal and external flaws must be minimized. Both the size and number of

flaws contribute to the loss in the strength of the material. Alternatively, approaches that fill flaws and heal cracks in commercially available porous membranes may be of interest.

The mechanical properties of porous ceramics with nanopores cannot be estimated reliably. But the mechanical strength of ceramic membranes is provided by the macroporous substrate layer rather than by the nanopore gas-separating layer. Thus the mechanical strength of a membrane can be approximated using relations indicated above.

IV. CHARACTERISTICS OF ADVANCED COAL CONVERSION SYSTEMS

To evaluate the long-term thermal and chemical degradation of inorganic membranes that are being developed to separate gaseous products produced in advanced coal conversion processes, a knowledge of the characteristics of these processes is essential. The gasification of coal is conducted in fixed-, fluidized-, and entrained-bed gasifiers. The product gases from these gasifiers can be used in gas turbines and molten carbonate fuel cells to generate electricity more efficiently than conventional pulverized coal boilers. Alternatively, carbon monoxide and the hydrogen component of the coal gas stream can be used as chemical feedstocks. Hydrogen is a major chemical commodity that is used in petroleum refining, ammonia production, methanol synthesis, hydrogenation of fats, oils, and other unsaturated hydrocarbons, and reduction of ores.

The basic configurations of an IGCC system is shown in Figure IV-1. In the advanced IGCC systems using hot gas cleanup, flyash is removed from the gas stream in cyclones and filters. H_2S and other impurities are removed by sorbents or catalysts at temperatures ranging from 550° to 725°C . The clean gas is then burned in a gas turbine to generate electricity. Finally, the residual sensible heat is recovered in steam generators and the steam is used to produce additional electricity.

In an IGCC system using inorganic membranes, the gas stream from the gasifier is first passed through cyclones to remove a major portion of the flyash (Figure IV-2). A high temperature filter of cross-flow, candle, or granular-bed type is then used to remove the remainder of the flyash particulates. Inorganic membrane modules placed downstream of the filter are used to separate H_2 from the gas stream. Removal of H_2 from the gas stream also enhances the rate of decomposition of H_2S and NH_3 . The gas may then be passed through a water gas shift membrane reactor, where the CO reacts with added steam to produce additional H_2 that is separated by the membrane. Sulfur produced during the decomposition of H_2S is condensed in a sulfur cooler. The remaining components of the coal gas stream together with the hydrogen are burnt in a gas turbine to generate electricity. The hot gases from the gas turbines are cooled in a heat recovery steam generator and vented. The steam from the steam generator is used to generate electricity in a steam turbine. Alternatively, hydrogen from the membrane reactors may be used as a chemical feedstock.

Figure IV-1. Schematic diagram of a conventional IGCC System

Figure IV-2. Schematic diagram of an IGCC system with membrane separators.

For direct coal fueled turbine and pressurized fluidized-bed applications, the principal applications of the inorganic membranes appear to be in the removal of sulfur oxides and nitrogen oxides through facilitated transport mechanism using molten salts. We assume that such a membrane module will operate downstream of the gas turbine, but upstream of the heat recovery steam generator (Figure IV-3). In a pressurized-fluidized-bed combustor, the membrane module could be best placed downstream of the the gas turbine (Figure IV-4).

The gas streams from fixed-, fluidized-, and entrained-bed gasifiers have different compositions and temperatures (Table IV-1). The gas stream from a fixed-bed gasifier such as Lurgi is at a relatively low temperature of about 550°C and contains a significant fraction of hydrocarbons (including tars) and a high ratio of H₂/CO. The gas stream from an entrained-bed gasifier such as a Texaco oxygen-blown unit is at 1300°C, contains relatively few hydrocarbons, and has a low H₂/CO ratio. The partial pressure of NH₃ is higher in the gas stream from a fixed-bed gasifier than in those from fluidized- and entrained-bed gasifiers. The level of H₂S is not influenced by the gasifier design but depends on the nature of the coal. The particulate matter is lower in the fixed-bed design than in the other two types of gasifiers.

The gas streams from the pressurized fluidized-bed combustor and direct coal-fired turbines contain mostly N₂, CO₂, H₂O, and O₂. Small amounts of sulfur and nitrogen oxides are also present.

In both coal gasification and combustion systems, the level of steam is relatively high and this could have a deleterious effect on the stability of membrane materials. Although H₂S and NH₃ present in the hot coal gas streams may be benign to ceramic membrane materials, they could poison metal membranes such as Ni, Pd, and Pt. The alkali vapor (Na and K) species, expected to be present in ppm levels, are known to affect the properties of several ceramic materials including silica and alumina. Oxide ceramics such as CeO₂ and Al₂O₃ will also interact with SO₂ and O₂ present in the combustor gas stream, forming low-melting sulfates.

The coal gas streams contain several trace metal impurities that could poison the metal catalysts or impair the performance of inorganic membranes. Brittain et al. [1989] estimated the equilibrium partial pressure of various trace metal impurities at 625°C in an air-blown coal gasifier stream. Their calculations indicate that several metal species will be present above parts-per-billion levels. The actual quantities of the trace metals would depend on temperature, pressure, the type of coal, the gasification process, and presence of ash particles.

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Figure IV-3. Schematic diagram of a direct coal-fired turbine with a membrane separator.

Figure IV-4. Schematic diagram of an PFBC system with membrane separators.

Table IV-1

TYPICAL CHARACTERISTICS OF GAS STREAMS FROM COAL GASIFIERS AND COMBUSTORS

System Characteristics	Fixed-Bed Gasification	Fluidized-Bed Gasification	Entrained-Bed Gasification	Direct coal-Fired Turbines	Pressurized-Fluidized-bed Combustor
Process	Lurgi	KRW	Texaco		
Oxidant	Oxygen	Oxygen	Oxygen	Air	Air
Exit temperature (°C)	450-600	700-1000	1100	1000-1300	800-1000
Pressure (psig)	300	300	450	180	150
Oxygen potential	Reducing	Reducing	Reducing	Oxidizing	Oxidizing
<u>Gas composition (%)</u>					
CH ₄	4.28	4.5	0.3		
C ₂ H ₄	0.13	<0.01	<0.01		
C ₂ H ₆	0.20	<0.01	<0.01		
H ₂	20.92	30.0	29.8		
CO	7.49	45.0	41.0		
CO ₂	15.28	9.0	10.2	7.57	13.63
H ₂ S	0.6-1.1	1.1	1.0		
COS	0.03-0.06	0.1	0.1		
N ₂ /Ar	0.18	0.8	0.8	70.62	75.25
NH ₃	0.4	0.2	0.2		
H ₂ O	50.5	9.5	17.1	6.65	7.33
O ₂				15.16	3.45
SO ₂				0.005	0.34
NO _x (ppm)				50-100	200
Tars and oils (g/kg DAF coal)	80	<0.1	<0.1	0	0
Particulate loading (ppm)	1000-2000	1000-10,000	4000	~1000	1000-10,000

DAF: Dry ash-free

The gases from a coal gasifier or combustor contain ash particles in the range 1000 to 10,000 ppm. Most of the ash particles are removed by cyclones and barrier filters. However, a small fraction of the ash particles could potentially reach the membrane modules. Alvin et al. [1989] estimated the equilibrium composition of the ash particles leaving the cyclones in a KRW fluidized-bed gasifier and NYU pressurized-fluidized-bed combustor, based on the analysis of the ash collected in a ceramic filter (Table V-2). The results indicate that SiO_2 , aluminosilicates, magnesium silicates, and alkali compounds would be present in both gasifier and combustor flyash under equilibrium conditions. Iron and calcium sulfides are present in the gasifier gas stream, whereas they are oxidized to sulfates under combustor flue gas stream.

In the short residence time of the gas stream through the gasifier and particulate removal devices, the fine ash particles leaving the filters may not reach equilibrium. Under practical conditions, several other reactive phases not predicted by the equilibrium calculations are likely to be present.

Thus, the inorganic membranes for coal conversion systems would be exposed to more severe conditions than in conventional applications. The gas streams contain several major, minor, and trace components that could interact with the membrane materials leading to their degradation during service.

Table IV-2

NORMALIZED ASH CONCENTRATION IN FLUIDIZED-BED GASIFIER AND COMBUSTORS

KRW Fluidized-Bed Gasifier		NYU Fluidized-Bed Combustors	
Compound	Composition (wt%)	Compound	Composition (wt%)
C	72.11	CaSO ₄	36.88
Al ₂ SiO ₅	7.10	MgSiO ₄	22.73
FeS	6.84	Al ₂ SiO ₅	19.75
CaCO ₃	6.21	SiO ₂	12.25
MgSiO ₃	3.07	Fe ₂ O ₃	3.90
SiO ₂	2.20	NaAl ₂ Si ₆ O ₁₆	2.88
CaS	1.45	K ₂ SO ₄	1.15
K ₂ CO ₃	0.80	CaAl ₂ Si ₂ O ₈	0.45
NaAlO ₂	0.22		

* Alvin et al. [1989]

Table IV-3

PARTIAL PRESSURES OF TRACE METAL VAPOR SPECIES AT 625°C*

Vapor Species	Pressure (atm)
AsH ₃	3.7×10^{-10}
AsP	2.4×10^{-9}
BIS	1.3×10^{-8}
Cd	3.4×10^{-8}
GaCl	1.2×10^{-7}
GaF	4.2×10^{-9}
GeO	1.1×10^{-10}
GeS	3.5×10^{-7}
H ₂ Se	7.5×10^{-7}
H ₃ BO ₃	7.0×10^{-6}
HBO ₂	1.6×10^{-8}
HCl	1.2×10^{-5}
HF	6.0×10^{-6}
Hg	3.1×10^{-8}
KBO ₂	5.7×10^{-9}
KCl	5.6×10^{-6}
K ₂ Cl ₂	7.3×10^{-7}
KF	2.5×10^{-10}
KOH	2.9×10^{-10}
NaBO ₂	2.3×10^{-9}
NaCl	8.1×10^{-7}
Na ₂ Cl ₂	1.2×10^{-7}
Pb	1.8×10^{-7}
PbCl	2.7×10^{-8}
PbS	7.6×10^{-7}
SbCl	3.0×10^{-8}
SbS	1.2×10^{-9}
SnS	3.2×10^{-8}
Zn	7.2×10^{-8}

* Brittain et al. [1989]

V. DEGRADATION MECHANISMS OF INORGANIC MEMBRANE MATERIALS

Inorganic membranes that are relevant to the present application can be made of either nonporous metals such as Pt and Pd or microporous ceramics such as SiO_2 , Al_2O_3 , ZrO_2 , and TiO_2 . Generally, the dense membranes have very high selectivities with low permeabilities whereas microporous membranes have the opposite properties. Microporous ceramic membranes that are suitable for gas separation may have uniform pores (e.g. hollow fiber membranes) or asymmetric pore size distribution. The asymmetric membranes consist of sequential layers of progressively larger pores (Figure V-1). Generally, the gas separation layer must have pores less than 10 nm for effective separation of gaseous components by Knudsen diffusion. Gas separation by molecular sieving requires pore sizes in the range of 0.5 to 1 nm.

For separation of gases, the membranes must possess high selectivity and permeability for the gas component that needs to be separated from a gas mixture. For coal gasification and combustion gas stream applications, the membrane materials must possess these characteristics at elevated temperatures and pressures. Furthermore, they must withstand chemical attack by any fine particulate matter (fume) that may escape barrier filters and be inert to gas components such as H_2S , HCl , SO_2 , and alkali vapor present in the gas stream. Thus, inorganic membranes may degrade by several mechanisms including:

- Phase changes and pore size distribution changes caused by temperature or catalyzed by steam
- Reaction of inorganic membranes with the trace level and coal ash constituents
- Deposition of carbon inside the membrane pores because of the preferential removal of hydrogen.

THERMAL SINTERING AND PHASE CHANGES

Sintering of porous inorganic membranes is a degradation mechanism that limits the temperature at which they can be used for gas separation. Crystallites of the materials used in these membranes are of several nanometers in size and they are in relatively unstable thermodynamic states. At high temperatures, they tend to revert to low energy state by agglomeration or through phase transformations. In this respect, the membranes are similar to high surface area catalyst supports, which have been studied extensively. Siegel (1990) estimates that about 30 to 60% of the atoms reside in or very near the interfaces between grains if the mean grain diameter is 5 nm.

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Figure V-1. A typical structure of ceramic membranes.

This is in contrast to a population of 1 to 3% if the atoms on the surface for particles with a mean grain diameter of 100 nm.

In general, the observed sequence of events during sintering is (1) surface diffusion that leads to surface smoothness (more prevalent at temperatures above one-third of the melting point), (2) concave link and neck formation between next-neighbor particles, (3) aggregate consolidation by grain boundary and volume diffusion at temperatures above one-half of the melting point, (4) particle or pore equilibration toward a spherical shape, and (5) vaporization or melting near the melting point [Trimm, 1991].

The pore size distribution of an inorganic membrane depends on the starting materials and pretreatment conditions. For example, alumina membranes can be produced from hydroxides and oxyhydroxides of aluminum. Depending on the precipitation conditions, the precipitate may be gibbsite [α $\text{Al}(\text{OH})_3$], or bayerite [β $\text{Al}(\text{OH})_3$], boehmite [$\text{AlO}(\text{OH})$], or pseudo-boehmite [Lippens and Steggarda, 1970]. Dehydration of crystalline boehmite produces a small increase in surface area by generation of pores from interparticle spaces. Calcination leads to the development of cylindrical pores, and a good correlation was observed between the crystallite size of the boehmite and the pore size/pore volume of the alumina produced (Figure V-2). The pore size distribution of alumina prepared by precipitation techniques would depend on the hydroxide/oxy-hydroxide intermediate, the conditions of drying, and the conditions of calcining. Trihydroxides produce aluminas containing pores with radii in the range 0.9-2 nm. In contrast, pseudo-boehmite, precipitated at room temperature, has a crystallite size of ~ 3.5 nm and produces pores of radii 2 to 3.5 nm in the calcined alumina. Mixtures of the two produce aluminas with a mean pore radius increasing from ~ 1.2 to ~ 2.0 nm as the percentage of boehmite in the sample increases.

Pores produced by dehydration of the hydroxides are well known to change size on calcination, a process that depends on the conditions of calcination and, in particular, on the predominant phase produced by calcination. γ -alumina can be converted to other forms of alumina and eventually to α -alumina by heating, a process that is accelerated by the presence of steam and of some foreign ions. This conversion results in loss of surface area and in changes in pore radii. In pure alumina exposed to inert gas, the gamma phase is converted to delta phase at $\sim 800^\circ\text{C}$, to theta phase at $\sim 900^\circ\text{C}$, and finally to alpha phase at about 1000°C (Figure V-3), resulting in a decrease in surface area and increase in pore size. Calcination at temperatures higher than 500°C also results in increase in the mean pore radius (Figure V-4). Leenaars et al. [1984] found that the change from gamma to delta phase increases the pore size from ~ 3.2 nm to 4.3 nm, and the change to theta phase increases the pore size further to 5.4 nm. When alpha phase is formed, the pore size can be higher than 80 nm.

Figure V-2. Correlation between crystallite size and pore radius Trimm (1986).

Note: Path A is preferred when large crystals ($>100\mu\text{m}$) are calcined in wet air.

Path B is preferred when small crystals ($<10\mu\text{m}$) are calcined in dry air

Figure V-3. Phase transformations in alumina as a function of temperature.

Figure V-4. Pore size characteristics of alumina calcined at different temperatures.

The pore size also increases when the oxide ceramics are heated in air. Alumina zirconia, titania, and ceria porous materials may retain a median pore size of less than 10 nm at temperatures below 600°C (Table V-1). But as the temperature is increased, the average size of the micropores also increases, and at temperatures above 1000°C, they may become unsuitable for gas separation applications.

Table V-1
AVERAGE PORE DIAMETER OF OXIDE MATERIALS AS A FUNCTION OF TEMPERATURE

Material	Pore Diameter (nm)	Treatment	
		Temperature (°C)	Time (h)
Fumed SiO ₂	15.0		
SiO ₂ aerogel	11.0	300	
Al ₂ O ₃	2.0	500	5
Al ₂ O ₃	1.8	550	5
Al ₂ O ₃	7.8	500	24
Al ₂ O ₃	13.0	900	24
Al ₂ O ₃	14.4	1000	24
ZrO ₂	1.6	300	48
ZrO ₂	3.8	275	12
ZrO ₂	5.0	500	12
ZrO ₂	5.1	600	12
ZrO ₂	7.0	700	12
ZrO ₂	10.8	800	12
ZrO ₂	13.6	900	12
TiO ₂	4.6	400	3
TiO ₂	3.8	450	3
TiO ₂	20.0	600	3
CeO ₂	2.0	300	3
CeO ₂	2.0	400	3
CeO ₂	>100.0	600	3

The presence of small amounts of impurities can either accelerate or impede phase transformations. As shown in Figure V-5, addition of Mg, Fe, Zn, Mo, Co, Mn, and V to alumina enhanced the rate of transformation from gamma to alpha phase whereas the presence of Zr, Ca, Th, Ce, and La decreased it [Burtin et al., 1987]. During heating, H₂O is evolved from gamma alumina by dehydroxylation, leading to the formation of oxygen (anionic) vacancies. Before transformation to the α phase, the transition aluminas follow the sequence $\gamma \rightarrow \delta \rightarrow \theta$ until the solid is nearly dehydroxylated. Near the transition temperature, diffusion of intrinsic cation vacancies toward the crystallite surface occurs. The mutual annihilation of cation and anion vacancies leads to a structural rearrangement and the formation of the α phase.

Microporous glass membranes exhibit gradual shrinkage and loss in surface area as the temperature approaches 800°C. Removal of hydroxyl groups causes shrinkage and results in loss of surface area and increase in pore size. At temperatures above 900°C the shrinkage is greatly accelerated, resulting in rapid pore closure. A glass with a surface area of 200 m²/g sinters to a material with less than 1 m²/g when heated to 1000°C for one hour [Elmer 1983]. Silica membranes produced by sol-gel process also sinter heavily leading to closed pores at 900°C [Larbot et al., 1989].

Although zirconia has been used as a membrane material for low temperature applications, its use may be limited for high temperature applications. Zirconia undergoes a phase transformation from a monoclinic to a tetragonal phase at temperatures above 1000°C. However, starting from an amorphous state obtained during sol-gel processing, the high temperature tetragonal metastable phase is developed at about 360°C. On increasing the temperature, the transition to monoclinic phase occurs in the temperature range 550° to 600°C, nearly doubling the crystallite size from 6 to 12 nm [Julbe et al., 1993]. At temperatures above 1000°C, the crystal structure is changed to tetragonal phase. Unless the high temperature phase is stabilized by addition of another cation, the monoclinic phase is formed on cooling.

Titania membranes also undergo phase transitions. The anatase phase is usually found at temperatures below ~500°C, and at higher temperatures the rutile phase is formed. A gradual growth of pore diameter from 6 nm at 500°C to 180 nm at 1100°C occurs when heating titania membranes.

Figure V-5. Influence of foreign ions in the conversion of boehmite to alpha-alumina at 1100°C
Burtin et al. (1987).

The increases in pore size and size of the grains are due to the thermodynamic driving force to decrease in the energy of the system. Thermodynamic equilibrium in which the energy of the system is at a minimum is achieved at higher temperatures and long durations. These conditions are conducive to grain growth. The driving force to reduce surface area for grain boundaries (and pores) is the need for the system to minimize surface energy, ΔG , in accordance with the following equation:

$$\Delta G = \tau \Delta A_s$$

where τ is the surface tension and ΔA_s is the decrease in surface area. Surface energies for oxide ceramics such MgO and Al_2O_3 are about 1000 ergs/cm^2 (Table V-2). The values of surface energies for covalent ceramics such as TiC are higher than for oxides. Metals also have surface energies in the range 1000 to 1800 ergs/cm^2 . For a material containing nanopores and with surface areas of over $100 \text{ m}^2/\text{g}$, the reduction in surface energy is about 10 - 50 cal/g when the pore size is increased to 100 nm and surface area is decreased to below $10 \text{ m}^2/\text{g}$. In contrast, for materials with coarse pores and small surface area, the change in the surface energy is only 0.1 to 0.5 cal/g when the grains grow from about 100 nm to 1 cm . Therefore, the driving force for reducing pores in a separation membrane is significantly higher than for normal ceramic sintering.

Table V-2
SURFACE ENERGY IN VACUUM OR INERT GAS

Material	Temperature (°C)	Surface Energy (ergs/cm²)
Al_2O_3 solid	1850	905
Al_2O_3 liquid	2080	700
MgO solid	25	1000
TiC solid	1100	1190
Na_2SiO_3 liquid	1000	250
Na_2CO_3 crystal	25	230

The tendency for grain growth or sintering at a given temperature will be highest in the metals, followed closely by the ceramics. Grain growth can occur by several mechanisms:

- Evaporation and condensation
- Surface diffusion
- Diffusion in grain boundaries
- Bulk diffusion.

At high temperatures and in materials with a large defect concentration, movement of atoms is rapid. When the mean grain diameter is about 5 nm, about 30% to 60% of the atoms are on the surface or at grain boundaries. As the mean diameter increases to 10 nm, only 15% to 30% of the atoms are in the grain boundaries. At a grain size of 100 nm, only 1% to 3% of the atoms remain in the interface between different grains [Siegel, 1990]. Hence, for microporous materials, surface and grain boundary diffusion are more important than bulk diffusion.

Although the boiling point of ceramics that are being considered for gas separation membranes is very high, movement of atoms may occur because the vapor pressure on a curved surface is different from that of a flat surface. The vapor pressure over curved surfaces is given by the Thomson-Freundlich equation.

$$\ln \frac{P}{P_{\text{flat}}} = \frac{M\gamma}{\rho RT} \frac{1}{r}$$

where

P = pressure (Pa) at tip (or in pore) of radius r

P_{flat} = thermodynamic reference value (Pa)

M = molecular weight of vaporizing species (g/mol)

γ = surface energy (ergs/cm²)

ρ = density (g/cm³)

R = gas constant (erg/mol·K)

T = temperature (K).

For a ceramic with γ in the range of 10^3 erg/cm² ($\text{Al}_2\text{O}_3 = 900$ erg/cm) at temperatures of 1000K, the values are given in Table V-3 for sharp convex protuberances. The vapor pressure on concave surfaces will be lower than that over flat surfaces. Thus, when pores are interconnected, the necks (convex) between pores at nm level will be blunted rapidly by movement of atoms to concave surfaces. Such surfaces with 0.5 nm radius will generate a tremendous attractive force for vapor from nearby sharp convex areas between pores. Mass will be transferred from the neck to the cavity. Even for low vapor pressures expected for materials such as alumina, the pressure at the sharp peaks (0.5 nm) will be greater by a factor of 10^5 while the pressure at the nearby small pores of similar radius will be lower by a similar magnitude. The pressure gradient is thus very large in pores of nanometer size with sharp concave and convex surfaces. This gradient allows the atoms on the surface to move toward a minimum energy surface, resulting in loss of surface area and enlargement of the pores.

Table V-3
ESTIMATED VAPOR PRESSURES OF CONVEX SURFACES IN
A POROUS ALUMINA AT 725°C

<u>Surface Radius (nm)</u>	<u>P_r/P_{flat}</u>
10,000.0	1.0004
1000.0	1.004
100.0	1.04
10.0	1.36
1.0	400
0.5	$>10^5$

Although a gas phase mechanism is implicit in this argument, the actual equilibration can also be obtained by surface diffusion and/or bulk diffusion. Surface diffusion becomes important at temperatures above $0.3 T_m$ (T_m = melting point) while bulk diffusion becomes important only at $T > 0.5 T_m$.

Near contact points between particles the number of oxygen ion vacancies is the highest in oxide ceramics such as alumina. As the temperature increases, these vacancies effectively become mobile because ions in the lattice create new vacancies as they move to fill existing vacancies. The result is transport of matter from convex to concave surfaces (always from the point of view of the gas).

HYDROTHERMAL EFFECTS

Coal gasification and combustion gas streams contain a significant fraction of steam (10 to 25% v/v). At the high temperatures and high pressures encountered in coal gasification streams, steam can have a deleterious effect on the properties of the membrane materials. The hydrothermal environment generally enhances the sintering of the oxide membrane materials, primarily because of the formation of mobile hydroxide species. Thermodynamic calculations performed at SRI indicated that hydroxides of Si and Mg are more volatile than those of aluminum (Table V-4). The vapor pressures of titanium and zirconium hydroxides are much lower than those of aluminum hydroxide. Formation of a MgAl_2O_4 phase causes lowering of the vapor pressure of the more volatile $\text{Mg}(\text{OH})_2$ species. The complete vapor pressure calculations for various oxides, silicates, and aluminates are listed in Appendix A.

Table V-4

CALCULATED EQUILIBRIUM VAPOR PRESSURES OF MAJOR HYDROXIDE SPECIES AT VARIOUS TEMPERATURES

Species	Partial Pressure (atm)		
	727°C	927°C	1127°C
$\text{Al}(\text{OH})_3$	5.6×10^{-16}	1.3×10^{-13}	6.5×10^{-12}
$\text{Mg}(\text{OH})_2$	2.2×10^{-13}	8.2×10^{-11}	5.7×10^{-9}
$\text{Mg}(\text{OH})_2$ in MgAl_2O_4	1.1×10^{-14}	5.9×10^{-12}	5.7×10^{-10}
$\text{Si}(\text{OH})_4$	5.3×10^{-15}	1.2×10^{-13}	1.2×10^{-12}
$\text{SiO}(\text{OH})_2$	9.1×10^{-12}	1.6×10^{-9}	6.0×10^{-8}
$\text{Si}_2\text{O}(\text{OH})_6$	2.2×10^{-12}	1.0×10^{-12}	6.3×10^{-13}
$\text{Ti}(\text{OH})_4$	3.0×10^{-20}	2.8×10^{-17}	3.9×10^{-15}
$\text{Zr}(\text{OH})_4$	2.3×10^{-22}	5.6×10^{-19}	1.6×10^{-16}

Alumina or silica catalysts heated in the presence of steam even at a low level of 5% v/v yielded larger pores than materials heated in dry air. The diffusion of oxygen in fused silica requires a higher activation energy than diffusion of H₂O [Moulson and Roberts, 1963]. These authors found that when SiO₂ fibers are exposed to high pressure steam containing a different isotope, the oxygen atom in the SiO₂ film is replaced by the oxygen atom in the steam. Thus, the diffusing oxygen species in the film originated in the H₂O, which formed a Si-O-H species.

Enhanced diffusion in the presence of steam is used commercially to planarize the silicon wafers in the semiconductor industry. The softening and flow of the SiO₂ lattice are so dramatic at a pressure of 300 psi and a temperature of 500°C that square-shaped, μm -high steps in the oxide surface can become spherical in minutes [Norton, 1961; Spitzer and Ligenza, 1961].

In a hydrothermal environment, loss of surface area in silica catalysts occurs by the movement of surface atoms that causes collapse of micropores, thus increasing the average pore size [Iler, 1979]. The surface area of a silica gel diminished from 732 m²/g to 359 and 193 m²/g when heated in steam at 575° and 680°C, respectively. The average pore diameter increased from an original value of 3.6 nm to 7.7 and 14.1 nm at these temperatures [Schlauffer et al., 1965]. The presence of even small amount of alkali impurities (>0.05%) drastically reduced the surface areas of silica catalysts (Figure V-6) [Axelsson et al., 1988].

Based on this evidence, steam accelerates sintering, grain growth, and transition to α alumina and results in a near elimination of micropores. Similarly, phase transformations in the oxide ceramics are also accelerated in the presence of steam. These effects are attributed to the formation of hydroxide species on the surfaces, which have low melting points and high vapor pressures in comparison with the oxides. Thus, the hydroxide species are highly mobile. The presence of steam helps to maintain the surface concentration of hydroxyl species, which in turn results in the continuous production of anion vacancies in the bulk. As noted above, the rate of phase transition in alumina is governed by the interaction of anion and cation vacancies. As the partial pressure of steam increases, the surface concentration of anion vacancies increases, leading to increased mobility and rate of sintering.

The rate of surface area loss in microporous alumina depends on the temperature (activation energy = ~40 kcal/mole), steam partial pressure, and the original surface area [Johnson 1990]. When boehmite (gamma-alumina) was heated in steam at various temperatures, the median pore size increased with temperature more than when similar treatment was performed in dry air (Figure V-7). For example, treatment in steam at 814°C resulted in a pore size of about 11.0 nm, whereas treatment in air produced a pore size of 8.5 nm [Lowendahl and Otterstedt, 1990]. The increase in median pore size was accompanied by reduction in surface

Figure V-6. Influence of sodium on the reduction in surface area of silica at 750°C in 60% steam-air mixture.

Figure V-7. Pore area distribution of dry-calcined and hydrothermally treated alumina at different temperatures for 2 h (Lowendahl and Otterstedt, 1990).

area. Furthermore, the hydrothermal treatment resulted in a sharper X-ray patterns, indicating better crystallinity. The transition to γ - Al_2O_3 and finally to θ - Al_2O_3 was accelerated in the presence of H_2O .

The surface area of titania powders also decreased more severely in the presence of water vapor. For example, the surface area decreased from $34 \text{ m}^2/\text{g}$ to 19 and $10 \text{ m}^2/\text{g}$ when heated in air and steam respectively at 575°C [Hébrard et al., 1990]. The rate of decrease in the area was found to be proportional to the square root of partial pressure of steam (Figure V-8). The role of steam in this process is the production of relatively mobile hydroxyl ions on the surface. The initial sintering of rate of TiO_2 appeared to be limited by the diffusion of hydroxyl species.

The coal gasifier and combustion gas streams also contain HCl vapor resulting from the presence of chlorides in the coal. At high temperature and pressure inorganic membrane operating conditions, the possibility of HCl reacting with the membrane material exists. Many chloride species are volatile. We calculated the vapor pressures of several chloride species that will be in equilibrium with HCl and inorganic membrane materials. The significant species and calculated vapor pressures are shown in Table V-5, and the complete results are shown in Appendix B.

Table V-5

CALCULATED EQUILIBRIUM VAPOR PRESSURES OF CHLORIDE
VAPOR SPECIES AT VARIOUS TEMPERATURES

Species	Partial Pressure (atm)		
	727°C	927°C	1127°C
AlOCl_2	4.4×10^{-11}	8.8×10^{-10}	1.4×10^{-8}
MgCl_2	1.4×10^{-11}	1.8×10^{-10}	1.8×10^{-9}
SiHCl_3	1.7×10^{-23}	4.7×10^{-22}	5.2×10^{-21}
ZrCl_4	5.5×10^{-18}	2.8×10^{-17}	9.1×10^{-17}
TiOCl_2	6.9×10^{-17}	6.8×10^{-15}	1.8×10^{-13}

Figure V-8. Reduction in surface area of titanium powder at 550°C in 0.13 atm of oxygen.

EFFECT OF SUBMICRON FUME PARTICULATES

A fraction of the mineral matter in coal escapes the gasifier or combustor in the form of flyash. The composition of flyash depends on the type of coal, combustion or gasification conditions, and the particle size of the ash. Although most of the flyash is removed by cyclones and barrier filters, a small fraction in the form of fine particulate matter (fume) could still reach the membrane modules. A subpilot scale test conducted by Westinghouse Science and Technology Center with cross-flow filters at the Texaco pilot-scale gasifier facility at Montebello showed that the outlet loading varied from 5 to 20 ppm while inlet particulate loading to the filter varied from 250 to 2000 ppm [Lippert et al., 1991]. A similar test at the PFBC facility of New York University indicated that the cross-flow filter was able to reduce ash dust loading from an inlet level of 250 to 1050 ppm to about 3-30 ppm [Lippert et al., 1989]. A test at the same facility conducted by The Combustion Power Company showed that a granular-bed filter was capable of decreasing the coal flyash level from about 3000 ppm to 3-16 ppm [Wilson et al., 1989]. Thus, although the high temperature barrier filters are able to remove nearly 99% of the flyash, a small amount escapes the filters and these particles (likely to be submicron fume) could be detrimental to the operation of a membrane module.

The composition of the submicron fume that is most likely to escape the barrier filters differs significantly from that of the coarser particles retained by cyclones and barrier filters [Quann et al., 1990]. Oxides of Si, Al, Mg, Fe, and Ca are generally the major constituents of the fume (Table V-6). Several other compounds of Na, P, Mn, V, Cr, As, Sb, Zn, Co, and Ba can also be present (Table V-7). The compounds of Na, P, As, and Co are significantly enriched in the fume fraction in comparison to the coarser particles (Table V-8). The major oxides and alkali compounds pose a significant threat to the stability of the inorganic membrane materials.

Oxides of Si are acidic whereas ferrous, calcium, and magnesium are basic. Oxides of Al, Zr, and Ti are amphoteric. Acidic oxides react strongly with basic oxides at elevated temperatures, forming mixed oxides. For example, SiO_2 reacts readily with MgO , forming MgSiO_3 . Although the ash particles are generally complex oxides (silicates, aluminates, and aluminosilicates), free silica and iron oxide have been detected in pressurized fluidized-bed combustors [Alvin et al., 1989]. The particulate matter in the gas stream, if deposited on the surfaces of the membrane, could react with the membrane material. The large surface area of the fine particle ash fume and the highly porous nanostructure of the membranes would favor rapid reaction between the phases.

Table V-6
MAJOR ELEMENT ENRICHMENT FACTORS FOR SUBMICRON FUME

<u>Coal (Rank)</u>	<u>Si</u>	<u>Mg</u>	<u>Ca</u>	<u>Fe</u>	<u>Al</u>
MS(L) ¹	0.16	4.0	0.29	3.3	0.030
ND(L) ²	0.094	2.0	0.18	1.8	0.024
TX(L) ³	0.55	—	0.21	7.2	0.12
MR(S) ⁴	0.55	12.0	0.44	17.0	0.040
WY(S) ⁵	0.12	4.0	0.28	6.3	0.040
IL(B) ⁶	1.13	0.87	0.20	1.8	0.074
WK(B) ⁷	0.87	0.55	0.02	1.5	0.080
UT(B) ⁸	0.55	0.96	0.12	4.7	0.12
AL(B) ⁹	0.48	—	—	8.8	0.085
PT(B) ¹⁰	0.97	1.82	0.13	1.3	0.062
WV(B) ¹¹	0.85	1.31	0.22	1.7	0.033

1. Montana Savage	7. Western Kentucky
2. North Dakota	8. Utah
3. Texas	9. Alabama Rose
4. Montana Rosebud	10. Pittsburgh No. 8
5. Wyoming	11. West Virginia
6. Illinois	

Table V-7
MINOR AND TRACE ELEMENT ENRICHMENT FACTORS FOR SUBMICRON FUME

<u>Coal (Rank)</u>	<u>Na</u>	<u>P</u>	<u>Mn</u>	<u>V</u>	<u>Cr</u>	<u>As</u>	<u>Sb</u>	<u>Zn</u>	<u>Co</u>	<u>Ba</u>
MS(L) ¹	12	6.7	9.6	0.79	3.4	6.5	7.6	7.2	11	2.5
ND(L) ²	4.2	1.7	2.2	0.37	0.65	4.1	3.4	0.71	3.4	1.9
TX(L) ³	39	19	0.33	3.1	7.2	14	20	14.0	18.0	6.2
MR(S) ⁴	13	2	4.5	6.5	7.3	10	2.1	2.2	2.7	0.33
WY(S) ⁵	6.5	4.5	7.0	0.45	3.4	1.0	0.27	1.3	8.2	2.5
IL(B) ⁶	20	35	1.1	11	21	34	4.1	19	5.8	—
WK(B) ⁷	17	27	5.1	11	1.5	29	6.0	14	7.5	—
UT(B) ⁸	32	31	8.5	15	39	68	20.7	>50	32	—
AL(B) ⁹	17	12	13	8.8	7.1	22	18.0	>30	17	—
PT(B) ¹⁰	16	17	5.6	8.1	—	—	—	—	—	—
WV(B) ¹¹	21	26	3.8	9.5	—	—	—	—	—	—

1. Montana Savage	7. Western Kentucky
2. North Dakota	8. Utah
3. Texas	9. Alabama Rose
4. Montana Rosebud	10. Pittsburgh No. 8
5. Wyoming	11. West Virginia
6. Illinois	

Table V-8
HEAVY TRACE METAL ELEMENT ENRICHMENT FACTORS FOR SUBMICRON FUME

<u>Coal (Rank)</u>	<u>Lu</u>	<u>Sm</u>	<u>La</u>	<u>Th</u>	<u>Eu</u>	<u>Sc</u>	<u>Cs</u>
MS(L) ¹	—	0.076	0.079	—	—	0.07	—
ND(L) ²	—	—	0.094	—	—	0.017	—
TX(L) ³	1.9	1.7	0.84	1.5	1.5	0.26	—
MR(S) ⁴	—	0.26	0.29	—	0.47	0.12	—
WY(S) ⁵	—	0.059	0.065	—	0.28	0.036	—
IL(B) ⁶	1.1	1.4	0.68	—	—	0.086	15
WK(B) ⁷	1.3	3.0	0.59	—	—	0.10	—
UT(B) ⁸	—	—	0.79	—	—	0.12	—
AL(B) ⁹	—	1.4	0.73	1.2	1.3	1.5	—
PT(B) ¹⁰	—	—	—	—	—	—	—
WV(B) ¹¹	—	—	—	—	—	—	—

1. Montana Savage
2. North Dakota
3. Texas
4. Montana Rosebud
5. Wyoming
6. Illinois

7. Western Kentucky
8. Utah
9. Alabama Rose
10. Pittsburgh No. 8
11. West Virginia

Under gasification conditions, the presence of a basic ash with high alkali content could promote the reaction between the ash and alumina or silica membranes, leading to the formation of alkali silicates, aluminates, and aluminosilicates. These complex oxides have low melting points and could lead to loss of surface area and pore closure.

Vapor phase alkali levels during coal gasification are generally higher than under combustion conditions [Krishnan and Wood, 1991]. Sodium was present as NaCl, NaOH, and Na in a bench-scale fluidized-bed coal gasifier at about 820°C. Such alkali species have the potential to react with alumina and silica membrane materials, forming alkali aluminates and silicates.

Although the vapor phase alkali levels were extremely low under fluidized bed combustion conditions, the fine particles of the flyash were extremely rich in alkali sulfates [Krishnan and Wood, 1991]. Alkali sulfates also react with alumina, especially in the presence of sulfur oxides to form alkali aluminosulfates. Krishnan and Bartlett [1973 a, b] found that at temperatures above 500°C both K₂SO₄ and Na₂SO₄ reacted with alumina in the presence of 0.3% SO₂ and air to form K₃Al(SO₄)₃ and Na₃Al(SO₄)₃. Formation of these compounds could degenerate the structure of the membranes.

The interaction of reactive oxides in the effluent gas with the membrane material may result in (1) diffusion of small cations such as Na, K into the the lattice structure of the membrane and (2) formation of a different phase that may have poor mechanical properties or different thermal expansion characteristics leading to the development of thermal stresses.

The oxide membrane materials are mainly SiO₂, Al₂O₃, ZrO₂, and TiO₂. The coal or gasification system will contain both solid and gaseous oxides both under oxidizing and reducing conditions. We expect that most reactive species are capable of reacting individually. For example, basic hydroxides or oxides such as NaOH, Na₂O, and Al₂O₃ will react with more acidic oxides such as SiO₂, SO₃, and CO₂ to form corresponding less reactive compounds.

The comparative thermodynamic tendency to react is related to the enthalpy of mixing (ΔH_m) of the ionic components of the oxide (oxi-hydroxide). Values of ΔH for some reactions are known and for others can be estimated by the following empirical expression [Schwitzer et al., 1971]:

$$\Delta H_m = b_{ij}(K_i - Y_j)^{n_j}$$

where

b_{ij} = a coefficient of the basic oxide

K_i = parameter related to basicity of each cation (e.g., Ba^{+2} , Al^{+3})

Y_j = parameter related to acidity of each oxianion (e.g., SO_4^{2-} , SiO_3^{2-})

n_j = an empirical parameter with a value of 1.43 ± 0.05 for most binary oxide combinations.

The published values for K_i and Y_j are shown in Table V-9. The predicted values of ΔH_m are shown in Table V-10, along with with experimental values found in the literature.

Table V-9
ESTIMATED VALUES OF ACIDITY/BASICITY PARAMETERS
FOR CATIONS AND ANIONS

Cation	K_i	Anion	Y_j
H ⁺	14.0 ^a	CO ₃ ⁼	0 (Ref)
H ⁺	15.39	SO ₄ ⁼	-9.77
Na ⁺	19.97	SO ₃ ⁼	2.6
K ⁺	23.73	MoO ₄ ⁻²	-2.87
Mg ⁺²	8.68	CrO ₄ ⁻²	+0.13
Ca ⁺²	13.10	V ₂ O ₆ ⁻²	+1.55
Sr ⁺²	15.74	WO ₄ ⁻²	+0.87
Ba ⁺²	18.18	SiO ₂	+3.5 ^b
Fe ⁺²	8.25	Al ₂ O ₄ ⁻²	5.24
Fe ⁺³	4.29	ZrO ₃ ⁼	7.2
Mn ⁺³	5.47	TiO ₂ ⁼	5.13
Mn ⁺²	9.10		
Co ⁺²	8.95		
Ni ⁺²	7.46		
Cu ⁺²	4.53		
Pb ⁺²	9.34		
Sn ⁺⁴	1.41		
Al ⁺³	4.37		
Zr ⁺⁴	6.4		

^a Estimated from Al(OH)₃

^b Estimated from BaSiO₃.

Table V-10
ENTHALPY OF MIXING OF OXIDES

Ash Components	ΔH (kcal/mole)						
	SiO ₂	Al ₂ O ₃		TiO ₂		ZrO ₂	
	$\Delta H_{calc.}$	ΔH Litt.	ΔH Calc.	ΔH Litt.	ΔH Calc.	ΔH Litt.	$\Delta H_{calc.}$
Na ₂ O	55	55- 57	41	24	43	51	35
K ₂ O	65	66-70	56		56		51
MgO	10	9-11	6	10	61	3-5.5	2
CaO	21	21-24	17	3.6-9	18	19.3	12
TiO ₂	5	5	5	7-14	5	7-12	1
SiO ₂							
Al ₂ O ₃	8	6					
SO ₃ ²⁻			47				75

Note: The literature values were obtained from Babrish Kim et.al., Thermodynamics of Silicates Spring Verlag, Berlin, (1985) and Kubachewski, Alcock. Metallurgical Thermoch. 5th ed. Perg. Press. (1979).

The tendency for the reaction to occur between the membrane materials and coal ash components can be also illustrated in a three dimensional plot (Figure V-9). As shown in this plot and in Table V-10, sulfates are generally very stable phases. Reaction of alkali oxides with SiO₂ are more favored than with ZrO₂. Thus, if alkali species are not present as sulfates, as is the case in coal gasification streams, they may interact with the membrane material. Presence of oxides such as La₂O₃ (basic) and ZrO₂ on the membrane surfaces may minimize reaction with alkali species. Although the quantity of fume particles and the partial pressure of alkali vapor are low, it does not take a large amount of mass to plug pores of nanometer size.

Thermodynamic calculations were performed to determine the phases that could be formed in gasifier and combustor gas streams at 500°, 700°, and 900°C. The ash phase was assumed to contain SiO₂, Al₂O₃, CaO, MgO, Na₂O, K₂O, and Fe₂O₃. The membrane phases were SiO₂, Al₂O₃, ZrO₂, and TiO₂. The thermodynamically stable and significant phases are

shown in Table V-11. All membrane materials react with some of the ash components. ZrO_2 is probably the only material that did not react with the basic components of the ash.

The interaction of alkali components decrease the melting point of SiO_2 , Al_2O_3 , and TiO_2 . Hence, the deposition of alkali components are likely to increase the sintering rate of the membrane materials. Deposition of SiO_2 and other ash components also decrease the melting point of Al_2O_3 .

Table V-11

THERMODYNAMICALLY PROJECTED SOLID PHASES FORMED BETWEEN ASH COMPONENTS
AND CERAMIC MEMBRANE MATERIALS IN THE RANGE 500° TO 900°C

Ash Component	Membrane Material			
	SiO_2	Al_2O_3	ZrO_2	TiO_2
SiO_2	SiO_2	$\text{Al}_2\text{O}_3 \cdot \text{SiO}_2$ $3\text{Al}_2\text{O}_3 \cdot 2\text{SiO}_2$	$\text{ZrO}_2 \cdot \text{SiO}_2$	—
Al_2O_3	$\text{Al}_2\text{O}_3 \cdot \text{SiO}_2$ $\text{Al}_2\text{O}_3 \cdot 2\text{SiO}_2$	Al_2O_3	—	$\text{Al}_2\text{O}_3 \cdot \text{TiO}_2$
CaO	$\text{CaO} \cdot \text{SiO}_2$	$\text{CaO} \cdot \text{Al}_2\text{O}_3$ $\text{CaO} \cdot 2\text{Al}_2\text{O}_3$	$\text{CaO} \cdot \text{ZrO}_2$	$\text{CaO} \cdot \text{TiO}_2$ $3\text{CaO} \cdot 2\text{TiO}_2$ $4\text{CaO} \cdot 3\text{TiO}_2$
MgO	$\text{MgO} \cdot \text{SiO}_2$	$\text{MgO} \cdot \text{Al}_2\text{O}_3$	—	$\text{MgO} \cdot \text{TiO}_2$ $\text{MgO} \cdot 2\text{TiO}_2$ $\text{MgO} \cdot 3\text{TiO}_2$
Na_2O	$\text{Na}_2\text{O} \cdot \text{SiO}_2$ $\text{Na}_2\text{O} \cdot 2\text{SiO}_2$ $\text{Na}_2\text{O} \cdot 3\text{SiO}_2$	$\text{Na}_2\text{O} \cdot \text{Al}_2\text{O}_3$	—	$\text{Na}_2\text{O} \cdot \text{TiO}_2$ $\text{Na}_2\text{O} \cdot 2\text{TiO}_2$ $\text{Na}_2\text{O} \cdot 3\text{TiO}_2$
K_2O	$\text{K}_2\text{O} \cdot 4\text{SiO}_2$	$\text{K}_2\text{O} \cdot \text{Al}_2\text{O}_3$	—	—
Fe_2O_3	$\text{FeO} \cdot \text{SiO}_2$ $2\text{FeO} \cdot \text{SiO}_2$	$\text{FeO} \cdot \text{Al}_2\text{O}_3$	—	—

Figure V-9. The enthalpy of mixing of oxides in membranes and coal ash.

DEPOSITION OF CARBON

The separation of the various components of the hot coal gas streams during permeation through the membrane changes the gas phase composition and shifts the equilibria between the constituents. In such cases, solids may be deposited by reaction in the gas phase inside the membrane pores.

Preferential removal of hydrogen from the hot coal gas changes the C/H and C/O ratios and it could lead to deposition of C by disproportionation of CO or by decomposition of hydrocarbons:

Thermodynamic equilibrium calculations were performed to determine the conditions under which carbon will deposit from high temperature coal gas streams. Various compositions of coal gas streams can be represented by their atomic fractions of C, H, and O and plotted in a triangular graph. In these triangular plots, the apexes of the triangle, marked by C, H, and O represent compositions of 100 atom% of C, H, and O, respectively. Each side of the triangle is a baseline indicating zero content of the element denoted by the opposite apex. Lines parallel to the base lines denote atomic fractions of the element indicated by the corresponding apex, with the levels increasing from the baseline to the apex. Points in Figure V-10 illustrate the reading of coordinates from the triangular plots. Lines of 20 at% C, 60 at% H, and 20 at% O intersect at point A. Point B represent a composition with 40 at% C, 20 at% H, and 40 at% O.

The results of the thermodynamic calculations for conditions of carbon deposition are shown in Figures V-11 and V-12 for temperatures 500° and 1000°C and two total pressures (1 and 20 atm). Appendix C displays the ternary diagrams for other temperatures. Three coal gas composition, representing a typical fixed-bed (Lurgi), fluidized-bed (KRW), and entrained-bed (Texaco), are also indicated in the diagrams. The area above the boundary lines (toward the carbon apex) represents the gas composition that is in equilibrium with solid carbon. Under equilibrium conditions in gas streams with those compositions, carbon deposition will occur.

As seen from these figures, the carbon deposition boundary lines cover a wider area at 20 atm pressure than at 1 atm pressure. As the temperature is increased the carbon boundary lines move toward the apex representing 100% C. These observations indicate that high pressures and low temperatures are conducive to carbon deposition.

Figure V-10. A triangular plot representing a gas phase containing carbon, hydrogen, and oxygen atoms.

Figure V-11. Carbon deposition boundary line at 500°C

Figure V-12. Carbon deposition boundary line at 1000°C

At temperatures above 1000°C carbon deposition is not expected from gas streams representative of all three types of gasifiers (Table V-12). The gas stream from an air-blown Lurgi fixed-bed gasifier is not carburizing enough to deposit carbon in the temperature range 500° to 1000°C under equilibrium conditions. However, if tar components are present, carbon deposition may occur at 500°C.

Table V-12
POTENTIAL FOR CARBON DEPOSITION UNDER EQUILIBRIUM CONDITIONS

Temperature (°C)	Potential for Carbon Deposition		
	Fixed-Bed Gasifier¹	Fluidized-Bed Gasifier	Entrained-Bed Gasifier
1 atm Total pressure			
500	No	Yes	Yes
600	No	Yes	Yes
700	No	No	Yes
800	No	No	No
900	No	No	No
1000	No	No	No
20 atm Total pressure			
500	No	Yes	Yes
600	No	Yes	Yes
700	No	Yes	Yes
800	No	Yes	Yes
900	No	No	Yes
1000	No	No	No

¹ Carbon deposition may occur at low temperatures, if high molecular weight hydrocarbons (tar) are deposited on the membranes

The potential for carbon deposition in a gas stream from a fluidized-bed gasifier exists at temperatures below 700° and 900°C at 1 and 20 atm pressures, respectively. For an entrained-bed gasifier gas stream, carbon deposition may occur below 900° and 1000°C at 1 and 20 atm, respectively.

These thermodynamic calculations assumed that global equilibrium will be achieved, that is, all possible reactions will go to completion. However, in practice, this is not always the case even at the high temperatures encountered in the present application. Formation of methane is

generally an activated process and requires the presence of a catalyst such as nickel. The oxide membranes and noble metals are not active catalysts for these reactions. In the absence of such catalysts, the carbon potential may be higher than indicated by the equilibrium calculations and carbon deposition may occur.

Preferential removal of hydrogen from the hot coal gas could make the composition carburizing enough to deposit carbon. Fixed-bed gasifiers operate relatively at low temperatures and the gas streams contain a significant quantity of tar components. Under hydrogen-deficient conditions, these hydrocarbon components could pyrolyze and deposit carbon in the pores of the inorganic membranes. Silica and zeolitic membranes are generally prone to this carbon deposition because they are known to catalyze cracking of hydrocarbons. Fluidized- and entrained-bed gasifiers generally contain only trace levels of tar components.

DEGRADATION OF METAL MEMBRANES

Compact metals have been used for many years as selective membranes for separation and purification of gases. The most notable systems are oxygen-silver and hydrogen-palladium. In each of these cases, the metal membrane is highly permeable to the respective gas, yet nearly totally impermeable to all other gaseous species. The unique selective permeabilities of these metals are attributable to catalytic reactions on the metal surfaces that convert the gases to metal-bulk-transportable species. In the case of silver, oxygen forms a substoichiometric oxide phase through which oxygen ions diffuse by sequential occupation and generation of oxygen vacancies. In the case of palladium, gaseous hydrogen is dissociatively adsorbed on the metal surface and the hydrogen adatoms penetrate the metal bulk by dissolution forming a hydrogen rich phase, PdH. In both cases, diffusive transport is driven by establishing a pressure differential in the diffusing gas on opposite sides of the membrane, resulting in a concentration gradient in the diffusing species within the membrane bulk.

Significant interest in membranes has been directed to catalytic reactor applications, and several reviews examine membrane preparation, characteristics, and dynamics from this viewpoint. [Gryaznov, 1992; Armor, 1992; Hsieh, 1991; Shu, et. al., 1991]. Of course, much of the information in these papers addresses aspects of membrane technology of direct concern in purification applications, and they are considered in the following discussion.

The advantage of high selectivity in dense metal membranes is moderated by low inherent diffusivity. Hence, attainment of a high flux of diffusing gas is favored by the mutually incompatible conditions of high temperatures, thin membranes, and large pressure differentials. In the hydrogen-palladium system, the diffusivity of the membrane material can be modified by

addition of an alloying element. Silver forms homogeneous solid solution alloys with palladium [Hansen, 1958]. A binary alloy composed of 23 atom percent silver in palladium is about twice as permeable to hydrogen as pure palladium. The addition of silver further improves the characteristics of the membrane material by reducing the dimensional change accompanying the formation of the hydrogen-metal phase. Internal stresses produced during transport of hydrogen into and out of the metal, especially during changes in temperature, are thus smaller and less likely to produce cracks. Pd/Ag alloy tubing for hydrogen purification has been an item of commerce for many years. [Grashoff et. al., 1983].

The hydrogen permeability of palladium alloyed with metals other than silver has been investigated and they have been shown capable of either enhancing or diminishing the permeability relative to that of pure palladium. [Grashoff et. al., 1983] Rare earths, particularly yttrium, produce ordered alloys with very high permeability. Hughes and Harris [1978] demonstrated that a 10 at% yttrium/palladium alloy was four times more permeable to hydrogen than pure palladium. A recent review of membrane catalysts discusses the effect of alloying Pd with other metals on activity and selectivity for hydrogenation and dehydrogenation processes. [Armor, 1992].

To improve the diffusive transport rate through a Pd or Pd alloy membrane, major emphasis has been placed on reducing the thickness of the membrane wall. The inherent strength of the metal places a lower limit for wall thickness at about 0.008 cm for a 0.16-cm-diameter tube operating at 425°C with a pressure differential of 14 atm (206 psig). To use a thinner metal membrane under such conditions will require a porous supporting structure that will provide the needed mechanical strength.

Gryaznov [1992] reviewed the use of noble metal membrane systems as catalysts and classified the structures as monolithic, porous, and composite or asymmetric. The first class includes compact metal foils, either pure substances or alloys. Selectivity can be perfect for separation of hydrogen or for certain hydrogenation and dehydrogenation reactions, but permeability is low, thus limiting process rates.

The second class includes microporous metals or ceramics in which a noble metal catalyst is deposited in the inner surfaces of the channels. The metal catalyst is highly dispersed and therefore potentially highly active. Gas transport through such membranes is very fast, but separation of unreactive gaseous components depends on Knudsen diffusion and is thus rather poor. However, efficient formation and separation of a desired gaseous product from a reactive feedgas are facilitated by catalytic chemical interaction with the dispersed catalyst that lines the pores. The mode of action of such membranes is analogous to that of supported catalysts in general.

Combination of monolithic and porous catalytic membranes results in a third class that constitutes layered structures in which a mechanically strong porous support is covered by one or more layers of a highly selective membrane. Manufacture of such membranes has been the subject of many investigations. Techniques have covered a broad span of coating technologies and include wet impregnation [Komo et. al., 1988], electroplating [Uemiya et. al., 1991, 1991a], compression cladding [Edlund and Pledger, 1993], reactive precipitation, chemical vapor deposition, sputtering, and spray pyrolysis [Li, et. al., 1993]. Examined substrates have included metals, ceramics, and polymers, but the membrane layer is always a hydrogen-permeable metal such as palladium or a palladium alloy. Shu, et. al., [1991] discuss these various techniques for preparation of Pd-based composite membranes in their recent review of Pd membrane reactors.

For recovery of the substantial quantity of hydrogen in coal gas, palladium-based composite membranes are very attractive. They are 100% selective and can be engineered to provide reasonable permeability rates. The actual amount of metal is small, mitigating the relatively high cost of metallic palladium. They are capable of operating in the temperature range typical of hot coal gas streams. But there is one serious flaw: the affinity of palladium for hydrogen is impaired by a variety of surface modifications, the most serious of which is caused by exposure to sulfur-bearing compounds such as hydrogen sulfide. Temperature-programmed desorption of hydrogen from a Pd surface indicated that the activation energy for desorption increased in connection with the surface sulfur concentration. [Lalauze, et al, 1988]. It is likely that the hydrogen sulfide indigenous to coal gas (typically >1000 ppm) would quickly poison the membrane surface and seriously impair the permeability of the membrane.

Methods to remove, reduce, or make irrelevant the sulfur sensitivity of the metal layers in composite membranes are now eliciting interest. Edlund and Pledger [1993] have described a vanadium-based membrane coated with platinum that is reported to be capable of thermally dissociating hydrogen sulfide at 700°C and recovering the hydrogen that diffuses through the sandwich. The hydrogen permeability of the membrane was reported to remain constant during an 8 hour exposure to hydrogen sulfide at 115 psia. The possibility of applying such a device to hot coal gas purification is very attractive.

The role of H₂S in the degradation mechanism for noble metal membranes can be estimated from thermochemical calculations. The partial pressure of gaseous S₂, p(S₂), is related to the partial pressures of H₂S, p(H₂S), and H₂, p(H₂), through the equilibrium constant (K) for the H₂ + S₂ reaction:

$$K = p(\text{H}_2\text{S})/[p(\text{H}_2) \cdot p(\text{S}_2)^{0.5}]$$

$$p(\text{S}_2) = \{[p(\text{H}_2\text{S})/p(\text{H}_2)] \cdot 1/K\}^2$$

The partial pressure of O_2 in coal gas streams is typically less than 10^{-20} atm, a condition in which the oxides of Pt and Pd are unstable. The concentration of H_2S varies from 0.05 to 0.5% v/v and that of hydrogen is typically in the range 20 to 30% v/v. Thus, the ratio $\text{H}_2\text{S}/\text{H}_2$ would be in the range 0.002 to 0.025 (logs of the ratios vary from -2.7 to -1.6).

Thermochemical calculations of the partial pressures of oxygen and sulfur required to form stable sulfides and oxides of Pd and Pt show that the free metals are the stable bulk phases at equilibrium under these conditions (Figures V-13 through V-16).

Even under conditions in which bulk sulfides are unstable, H_2S (or S atoms) can chemisorb on the membrane surfaces, thereby poisoning it for H_2 transport. For the case of Pt, experimental measurements of the stability of S adsorbates on metal surfaces have been reported. In studies of the thermodynamics of H_2S chemisorption on Pt surfaces, McCarty (1983) showed that the heat of chemisorption varies from -50 to -42 kcal/mole as coverage increases from 0.1 to 0.5 fraction of a monolayer. He also determined equilibrium sulfur coverage as a function of $\text{H}_2\text{S}/\text{H}_2$ ratio and temperature. Based on the isosteres shown in Figure V-17 (McCarty, 1983), exposure of a Pt surface to hydrogen containing 1 ppm of H_2S [$(\text{H}_2\text{S})/(\text{H}_2) = 1 \times 10^{-6}$] will produce fractional monolayer sulfur coverages of 0.25 and 0.3, respectively, at 550° and 725°C. Thus, H_2S could adsorb on Pt membrane surfaces and inactivate them even at H_2S levels too low to form stable bulk sulfides.

Edlund and Pledger [1993a, 1993b] suggest that hydrogen produced by thermal dissociation of pure H_2S on a Pt surface diffuses through the metal to the opposite side of a membrane where it can be removed by pumping or by reaction with an oxidant. Their measurements were made in batch experiments with a gas mixture of 1.5% H_2S and balance N_2 at 8 atm (abs). At a residence time of 12 min, complete conversion of H_2S was observed. They did not demonstrate sustained steady state membrane separation of hydrogen produced by thermolysis of H_2S containing gas stream. It would seem prudent at this time to withhold judgment on the hydrogen permeability of Pt membranes in sulfur-contaminated gas streams.

Figure V-13. Stability Diagram for Pd-S-O system at 500°C.

Figure V-14. Stability diagram for Pd-S-O system at 700°C

Figure V-15. Stability diagram for Pt-S-O system at 500°C.

Figure V-16. Stability diagrams for Pt-S-O system at 700°C.

Figure V-17. Variation of surface coverage of sulfur atoms as a function of temperature.

It has long been recognized that the hydrogen permeability of Pd depends not only on the high capacity of the metal to dissolve hydrogen, but also on its affinity for dissociative adsorption of H_2 . Therefore, it is not surprising that the presence of an adlayer of a strongly bound substance will seriously impair hydrogen permeation through a Pd membrane. Quantitative thermochemical measurements relating sulfur coverage on Pd to the sulfur activity of the gas in contact with the metal have not been reported. However, the power of sulfur as an irreversible deactivating agent in heterogeneous catalytic processes has been well documented [Barbier, 1985] for many metals including Pd. Apesteguia et al. [1981] found that only a fraction of the sulfur adsorbed on an alumina-supported Pt catalyst could be rapidly desorbed at 500°C in a hydrogen atmosphere. Indeed, after 30 hours of exposure in such an atmosphere, the catalyst retained a coverage equivalent to 0.4 atom of sulfur for each atom of Pt. However, more recently, Hoyos et al. [1992] used the dehydrogenation of cyclohexane as a calibration reaction to measure the effect of adsorbed sulfur on the catalytic activity of alumina- and silica-alumina-supported Pd. In the absence of sulfur, catalytic activity initially decayed rapidly upon exposure to the feedstock, particularly in the case of the highly acidic silica-alumina supported catalyst, because of carbon deposition. Exposure of the catalysts to H_2S drastically reduced activity, but heating in hydrogen restored the activity in approximate proportion to the temperature. Regeneration at 673 K (400°C) almost completely restored the activity, even though infrared spectral measurements of adsorbed CO indicated that the characteristics of CO adspecies on the metal crystallites on the catalyst were modified, probably by the presence of irreversibly adsorbed sulfur atoms. This reported behavior is in conflict with the warning that exposure to sulfur compounds will irreversibly incapacitate Pd membranes designed and marketed for the production of ultrapure hydrogen [Grashoff et al, 1983]. The contradiction cannot be reconciled from currently available information, but there appears to be sufficient evidence to justify continued studies of methods and strategies for using Pd-based membranes to separate hydrogen from coal gas streams.

VI. DOMINANT DEGRADATION MECHANISMS UNDER DIFFERENT PROCESS CONDITIONS

An analysis of the available literature indicates that in coal gasification and combustion gas streams, the inorganic membranes could be degraded by thermal sintering, hydrothermal attack, reaction with ash components, attack by vapor- and solid-phase alkali compounds, reaction with sulfur oxides, and deposition of carbon from the gas phase (Table VI-1 to V-4). The gas stream from a fixed-bed gasifier is generally at temperatures below 600°C and the level of fume could be low. Similarly, because of the low temperature, most of the alkali compounds will be in the solid-state. However, this gas stream contains significant amount of tar components which could lead to carbon deposition.

Fluidized-bed gasifiers operate at higher temperatures than fixed-bed gasifiers and tar is not generally present. The vapor-phase alkali level is sufficiently high that attack by sodium and potassium compounds is likely. High steam levels encountered under oxygen-blown mode operation could lead to hydrothermal sintering of the membranes. Although the gas composition is generally outside the carbon deposition boundary, removal of hydrogen through the membrane could lead to deposition of carbon inside the membrane pores.

The degradation mechanisms that would be prevalent in entrained-bed gasifiers are similar to those for fluidized-bed gasifier except that alkali levels could be higher under entrained bed gasifier conditions. The gas from an oxygen-blown entrained-bed gasifier is sufficiently carburizing that carbon deposition is likely even with out the removal of H₂.

Hydrothermal attack and reaction with SO₂, alkali sulfates, and ash particles could degrade the membranes when exposed to combustor gas streams from direct coal-fueled turbines and pressurized fluidized-bed combustors.

The results of this study reveal several thermal and chemical mechanisms that could degrade the properties of inorganic membrane materials. In coal gasification streams, the most dominant mechanisms are hydrothermal sintering, attack by fine ash particles (fume) and vapor phase alkali species, poisoning by sulfur and trace metal impurities, and deposition of carbon. In coal combustion gas streams, membrane degradation is most likely to occur by reaction with ash particulates and sulfur oxides.

Table VI-1
LONG-TERM DEGRADATION MECHANISMS FOR INORGANIC MEMBRANES AT 550°C
UNDER GASIFICATION CONDITIONS

Characteristic	Membrane Material				
	SiO ₂	Al ₂ O ₃	TiO ₂	ZrO ₂	Metals ¹
Phase change	None	None	Yes	Yes	None
Thermal sintering	Small	Small	Significant	Significant	N.A.
Hydrothermal sintering	Significant	Small	Significant	Not Available	N.A.
Vaporization of matrix	Not significant	Not significant	Not significant	Not significant	None
Reaction with H ₂ S	None	None	None	None	Yes
Reaction with HCl	None	Not significant	Not significant	Not significant	None
Reaction with alkali species	Na ₂ SiO ₂ K ₂ O·4SiO ₂	Na ₂ O·Al ₂ O ₃ K ₂ O·Al ₂ O ₃	Na ₂ O·nTiO ₂	No data	None
Reaction with ash components	Al ₂ O ₃ ·nSiO ₂ CaO·SiO ₂ MgO·SiO ₂ FeO·nSiO ₂	Al ₂ O ₃ ·nSiO ₂ CaO·nAl ₂ O ₃ MgO·Al ₂ O ₃ FeO·Al ₂ O ₃	CaO·nTiO ₂ MgO·nTiO ₂	ZrO ₂ ·SiO ₂ CaO·ZrO ₂	None
Carbon deposition:					
Fixed-bed gasifier	No ²	No	No	No	No
Fluidized-bed gasifier	Yes	Yes	Yes	Yes	Yes
Entrained-bed gasifier	Yes	Yes	Yes	Yes	Yes
Reaction with trace metal species	None	None	None	None	Moderate

¹ Alloys of platinum and palladium.

² Carbon deposition is possible if tar components are deposited on the membrane.

Table VI-2

**LONG-TERM DEGRADATION MECHANISMS FOR INORGANIC MEMBRANES AT 700°C
UNDER GASIFICATION CONDITIONS**

Characteristic	Membrane Material				
	SiO ₂	Al ₂ O ₃	TiO ₂	ZrO ₂	Metals ¹
Phase change	None	Yes	Yes	Yes	None
Thermal sintering	Significant	Moderate	Significant	Significant	N.A.
Hydrothermal sintering	Significant	Small	Significant	No data	N.A.
Vaporization of matrix	Not significant	Not significant	Not significant	Not significant	None
Reaction with H ₂ S	None	None	None	None	Moderate
Reaction with HCl	None	Not significant	Not significant	Not significant	None
Reaction with alkali species	Na ₂ SiO ₂ K ₂ O·4SiO ₂	Na ₂ O·Al ₂ O ₃ K ₂ O·Al ₂ O ₃	Na ₂ O·nTiO ₂	No data	None
Reaction with ash components	Al ₂ O ₃ ·nSiO ₂ CaO·SiO ₂ MgO·SiO ₂ FeO·nSiO ₂	Al ₂ O ₃ ·nSiO ₂ CaO·nAl ₂ O ₃ MgO·Al ₂ O ₃ FeO·Al ₂ O ₃	CaO·nTiO ₂ MgO·nTiO ₂	ZrO ₂ ·SiO ₂ CaO·ZrO ₂	None
Carbon deposition:					
Fixed-bed gasifier	No	No	No	No	No
Fluidized-bed gasifier	Yes	Yes	Yes	Yes	Yes
Entrained-bed gasifier	Yes	Yes	Yes	Yes	Yes
Reaction with trace metal species	None	None	None	None	Moderate

¹ Alloys of platinum and palladium.

Table VI-3

LONG-TERM DEGRADATION MECHANISMS FOR INORGANIC MEMBRANES AT 900°C
UNDER GASIFICATION CONDITIONS

Characteristic	Membrane Material				
	SiO ₂	Al ₂ O ₃	TiO ₂	ZrO ₂	Metals ¹
Phase change	None	Yes	Yes	Yes	None
Thermal sintering	Yes	Significant	Significant	Significant	N.A.
Hydrothermal sintering	Significant	Significant	Significant	No data	N.A.
Vaporization of matrix	Not significant	Not significant	Not significant	Not significant	None
Reaction with H ₂ S	None	None	None	None	May be
Reaction with HCl	None	Not significant	Not significant	Not significant	None
Reaction with alkali species	Na ₂ SiO ₂ K ₂ O·4SiO ₂	Na ₂ O·Al ₂ O ₃ K ₂ O·Al ₂ O ₃	Na ₂ O·nTiO ₂	No data	None
Reaction with ash components	Al ₂ O ₃ ·nSiO ₂ CaO·SiO ₂ MgO·SiO ₂ FeO·nSiO ₂	Al ₂ O ₃ ·nSiO ₂ CaO·nAl ₂ O ₃ MgO·Al ₂ O ₃ FeO·Al ₂ O ₃	CaO·nTiO ₂ MgO·nTiO ₂	ZrO ₂ ·SiO ₂ CaO·ZrO ₂	None
Carbon deposition:					
Fixed-bed gasifier	No	No	No	No	No
Fluidized-bed gasifier	No	No	No	No	No
Entrained-bed gasifier	Yes	Yes	Yes	Yes	Yes
Reaction with trace metal species	None	None	None	None	Moderate

¹ Alloys of platinum and palladium.

Table VI-4

**LONG-TERM DEGRADATION MECHANISMS FOR INORGANIC MEMBRANES AT 700°C
UNDER PRESSURIZED-FLUIDIZED-BED COMBUSTOR CONDITIONS**

Characteristic	Membrane Material			
	SiO ₂	Al ₂ O ₃	TiO ₂	ZrO ₂
Phase change	None	Yes	Yes	Yes
Thermal sintering	Yes	Moderate	Significant	Significant
Hydrothermal sintering	Significant	Moderate	Significant	Not Available
Vaporization of matrix	Not significant	Not significant	Not significant	Not significant
Reaction with SO ₂	None	Al ₂ (SO ₄) ₃	Not significant	Not significant
Reaction with HCl	None	Not significant	Not significant	Not significant
Reaction with alkali species	Na ₂ SiO ₂ K ₂ O·4SiO ₂	Na ₂ O·Al ₂ O ₃ K ₂ O·Al ₂ O ₃ Na ₂ Al ₂ (SO ₄) ₄	Na ₂ O·nTiO ₂	No data
Reaction with ash components	Al ₂ O ₃ ·nSiO ₂ CaO·SiO ₂ MgO·SiO ₂ FeO·nSiO ₂	Al ₂ O ₃ ·nSiO ₂ CaO·nAl ₂ O ₃ MgO·Al ₂ O ₃ FeO·Al ₂ O ₃	CaO·nTiO ₂ MgO·nTiO ₂	ZrO ₂ ·SiO ₂ CaO·ZrO ₂
Reaction with trace metal species	None	None	None	None

VII. CONCLUSIONS AND RECOMMENDATIONS

From our analysis of the data available in the literature, we conclude the following:

- Inorganic membranes made of oxide ceramics and noble metals are subjected to several thermal and chemical degradation mechanisms that could affect the efficiency of the membranes during service.
- Many oxide membranes including those made of alumina, zirconia, and titania undergo phase transitions in the temperature of interest. Such phase transitions could lead to loss of surface area and coarsening of pores.
- Hydrothermal sintering and the coarsening of pores occur with porous oxides on exposure to steam at high temperature and high pressures. Because coal gasifier and combustor gas streams contain a significant fraction of steam, this mode of degradation could be dominant in membrane materials during service in such systems.
- Although cyclones and barrier filters remove nearly 99% of the flyash from the gas stream, the remaining particles can still pose a problem for the inorganic membranes. These particles, which are in submicron in size are rich in alkali species that are detrimental to the integrity of the membrane materials.
- The coal gas stream from fluidized- and fixed-bed gasifiers are carburizing enough to deposit carbon below a temperature of 900°C. Although the gas composition of a fixed-bed gasifier gas stream is outside the carbon boundary region, tar components could still pyrolyze on the membrane surfaces.
- Chemisorption of sulfur atoms on the surface of noble metal membranes could lead to deactivation of the surface and loss of hydrogen permeation rate.

Based on the above conclusions, we recommend the following:

- Perform bench-scale experiments under well-defined conditions to determine the rate and extent of various degradation mechanisms. For ceramic membrane materials, the degradation by hydrothermal sintering, attack by ash particulate material, and reaction with alkali species deserve primary attention. For metal membrane material, the degradation due to sulfur species such as H₂S must be determined.
- Perform exposure tests with coupons of inorganic membrane materials under simulated conditions associated with coal gasifiers and combustors in the temperature range 550° to 900°C and at pressures up to 225 psig. Characterize the changes in membrane properties as a function of temperature, pressure and experimental parameters.
- Evaluate changes in the permeation properties of the membranes at high temperatures and pressures using simulated gas streams representative of a selected gasifier and a pressurized-fluidized-bed combustor.

- To determine changes that will be induced under real process conditions, perform exposure tests with an actual hot coal gas stream at a pressurized fixed-bed gasifier facility. Evaluate the changes in the physical, chemical, and mechanical properties of the membrane materials.
- Using theoretical and empirical approaches, results from the experimental program, and other data available in the literature develop a predictive model that can be used to estimate the long-term degradation of inorganic membrane materials under process conditions.

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APPENDIX A

CALCULATED PARTIAL PRESSURES OF OXIDES AND HYDROXIDES UNDER COAL COMBUSTION GAS STREAM CONDITIONS

**CALCULATED PARTIAL PRESSURES OF SPECIES OVER METAL OXIDES IN
THE PRESENCE OF Ar/O₂/H₂O MIXTURE AT 1 ATM PRESSURE**

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
Al₂O₃-α(c,l)						
Ar	0.70000	0.70000	0.70000	0.70000	0.69999	0.69998
O ₂	0.05000	0.05000	0.05000	0.05000	0.04999	0.04998
H ₂ O	0.25000	0.25000	0.25000	0.24999	0.24998	0.24995
Al	1.23 x 10 ⁻⁴⁵	4.20 x 10 ⁻⁴⁰	1.61 x 10 ⁻³⁵	1.19 x 10 ⁻³¹	2.46 x 10 ⁻²⁸	1.81 x 10 ⁻²⁵
AlO	3.44 x 10 ⁻³⁵	6.50 x 10 ⁻³¹	2.23 x 10 ⁻²⁷	2.16 x 10 ⁻²⁴	7.74 x 10 ⁻²²	1.25 x 10 ⁻¹⁹
AlO ₂	2.74 x 10 ⁻³¹	1.02 x 10 ⁻²⁷	9.10 x 10 ⁻²⁵	2.83 x 10 ⁻²²	3.83 x 10 ⁻²⁰	2.68 x 10 ⁻¹⁸
Al ₂ O	1.44 x 10 ⁻⁵⁸	2.52 x 10 ⁻⁵¹	2.42 x 10 ⁻⁴⁵	2.71 x 10 ⁻⁴⁰	5.67 x 10 ⁻³⁶	3.08 x 10 ⁻³²
Al ₂ O ₂	5.68 x 10 ⁻⁵⁰	6.69 x 10 ⁻⁴⁴	6.78 x 10 ⁻³⁹	1.14 x 10 ⁻³⁴	4.68 x 10 ⁻³¹	6.23 x 10 ⁻²⁸
AlOH	1.12 x 10 ⁻³⁰	6.17 x 10 ⁻²⁷	7.60 x 10 ⁻²⁴	3.10 x 10 ⁻²¹	5.31 x 10 ⁻¹⁹	4.54 x 10 ⁻¹⁷
Al(OH) ₂	1.54 x 10 ⁻²⁴	7.93 x 10 ⁻²²	1.37 x 10 ⁻¹⁹	1.06 x 10 ⁻¹⁷	4.40 x 10 ⁻¹⁶	1.11 x 10 ⁻¹⁴
Al(OH) ₃	5.62 x 10 ⁻¹⁶	1.14 x 10 ⁻¹⁴	1.34 x 10 ⁻¹³	1.08 x 10 ⁻¹²	6.51 x 10 ⁻¹²	3.08 x 10 ⁻¹¹
AlO(OH)	9.71 x 10 ⁻²⁶	6.98 x 10 ⁻²³	1.58 x 10 ⁻²⁰	1.54 x 10 ⁻¹⁸	7.70 x 10 ⁻¹⁷	2.27 x 10 ⁻¹⁵
AlHO	6.11 x 10 ⁻⁴¹	2.62 x 10 ⁻³⁶	1.79 x 10 ⁻³²	3.13 x 10 ⁻²⁹	1.87 x 10 ⁻²⁶	4.72 x 10 ⁻²⁴
O	3.48 x 10 ⁻¹¹	5.53 x 10 ⁻¹⁰	5.56 x 10 ⁻⁹	3.92 x 10 ⁻⁸	2.10 x 10 ⁻⁷	8.99 x 10 ⁻⁷
O ₃	9.73 x 10 ⁻¹⁴	4.49 x 10 ⁻¹³	1.67 x 10 ⁻¹²	5.09 x 10 ⁻¹²	1.33 x 10 ⁻¹¹	3.04 x 10 ⁻¹¹
OH	1.25 x 10 ⁻⁷	7.39 x 10 ⁻⁷	3.26 x 10 ⁻⁶	1.14 x 10 ⁻⁵	3.36 x 10 ⁻⁵	8.53 x 10 ⁻⁵
H	2.22 x 10 ⁻¹⁴	9.84 x 10 ⁻¹³	2.33 x 10 ⁻¹¹	3.42 x 10 ⁻¹⁰	3.43 x 10 ⁻⁹	2.54 x 10 ⁻⁸
H ₂	9.69 x 10 ⁻¹¹	1.46 x 10 ⁻⁹	1.41 x 10 ⁻⁸	9.64 x 10 ⁻⁸	5.02 x 10 ⁻⁷	2.10 x 10 ⁻⁶
H ₂ O ₂	1.53 x 10 ⁻¹⁰	4.95 x 10 ⁻¹⁰	1.32 x 10 ⁻⁹	3.05 x 10 ⁻⁹	6.27 x 10 ⁻⁹	1.17 x 10 ⁻⁸
Σ P(Al) (atm)	5.62 x 10 ⁻¹⁶	1.14 x 10 ⁻¹⁴	1.34 x 10 ⁻¹³	1.08 x 10 ⁻¹²	6.51 x 10 ⁻¹²	3.08 x 10 ⁻¹¹
Σ P(Al-O) (atm)	2.74 x 10 ⁻³¹	1.02 x 10 ⁻²⁷	9.12 x 10 ⁻²⁵	2.85 x 10 ⁻²²	3.91 x 10 ⁻²⁰	2.81 x 10 ⁻¹⁸
Al ₂ O ₃ -α(2327 ^a)	1 ^b	1	1	1	1	1
Al(934)	0	0	0	0	0	0
Al(OH) ₃ (c)	0	0	0	0	0	0

Notes: ΣP(Al) = Sum of vapor pressures of species containing Al, O, and H
 ΣP(Al-O) = Sum of vapor pressures of species containing Al and O only
 a = Melting point in degrees Kelvin
 b = One (1) and zero (0) represent the presence and absence of the solid phase respectively.

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
K₂O(c,l)						
Ar	0.77707	0.77373	0.76082	0.72209	0.64640	0.64096
O ₂	0.05551	0.05526	0.05433	0.05154	0.04609	0.04572
H ₂ O	0.16652	0.16580	0.16304	0.15476	0.13862	0.13756
K	5.51 x 10 ⁻¹⁰	2.62 x 10 ⁻⁸	6.44 x 10 ⁻⁷	9.70 x 10 ⁻⁶	8.96 x 10 ⁻⁵	2.95 x 10 ⁻⁴
KO	1.42 x 10 ⁻¹⁰	5.24 x 10 ⁻⁹	1.03 x 10 ⁻⁷	1.26 x 10 ⁻⁶	9.42 x 10 ⁻⁶	2.69 x 10 ⁻⁵
KO ₂	3.46 x 10 ⁻⁷	2.51 x 10 ⁻⁶	1.27 x 10 ⁻⁵	4.82 x 10 ⁻⁵	1.28 x 10 ⁻⁴	1.56 x 10 ⁻⁴
K ₂	2.46 x 10 ⁻²⁰	3.10 x 10 ⁻¹⁷	1.14 x 10 ⁻¹⁴	1.69 x 10 ⁻¹²	9.96 x 10 ⁻¹¹	7.78 x 10 ⁻¹⁰
K ₂ O	7.28 x 10 ⁻¹⁴	1.04 x 10 ⁻¹¹	6.20 x 10 ⁻¹⁰	1.95 x 10 ⁻⁸	2.95 x 10 ⁻⁷	7.44 x 10 ⁻⁷
K ₂ O ₂	1.50 x 10 ⁻¹²	6.21 x 10 ⁻¹¹	1.31 x 10 ⁻⁹	1.69 x 10 ⁻⁸	1.16 x 10 ⁻⁷	1.54 x 10 ⁻⁷
KOH	7.78 x 10 ⁻⁴	4.52 x 10 ⁻³	1.91 x 10 ⁻²	6.34 x 10 ⁻²	1.53 x 10 ⁻¹	1.68 x 10 ⁻¹
K ₂ (OH) ₂	1.27 x 10 ⁻⁴	6.84 x 10 ⁻⁴	2.66 x 10 ⁻³	8.12 x 10 ⁻³	1.58 x 10 ⁻²	7.42 x 10 ⁻³
O	3.67 x 10 ⁻¹¹	5.82 x 10 ⁻¹⁰	5.79 x 10 ⁻⁹	3.98 x 10 ⁻⁸	2.02 x 10 ⁻⁷	8.60 x 10 ⁻⁷
O ₃	1.14 x 10 ⁻¹³	5.22 x 10 ⁻¹³	1.89 x 10 ⁻¹²	5.33 x 10 ⁻¹²	1.17 x 10 ⁻¹¹	2.66 x 10 ⁻¹¹
OH	1.04 x 10 ⁻⁷	6.17 x 10 ⁻⁷	2.68 x 10 ⁻⁶	9.06 x 10 ⁻⁶	2.45 x 10 ⁻⁵	6.19 x 10 ⁻⁵
H	1.77 x 10 ⁻¹⁴	7.81 x 10 ⁻¹³	1.84 x 10 ⁻¹¹	2.67 x 10 ⁻¹⁰	2.61 x 10 ⁻⁹	1.93 x 10 ⁻⁸
H ₂	6.13 x 10 ⁻¹¹	9.22 x 10 ⁻¹⁰	8.83 x 10 ⁻⁹	5.88 x 10 ⁻⁸	2.90 x 10 ⁻⁷	1.21 x 10 ⁻⁶
H ₂ O ₂	1.07 x 10 ⁻¹⁰	3.45 x 10 ⁻¹⁰	9.00 x 10 ⁻¹⁰	1.92 x 10 ⁻⁹	3.34 x 10 ⁻⁹	6.16 x 10 ⁻⁹
Σ P(K) (atm)	9.05 x 10 ⁻⁴	5.21 x 10 ⁻³	2.18 x 10 ⁻²	7.16 x 10 ⁻²	1.69 x 10 ⁻¹	1.76 x 10 ⁻¹
Σ P(K-O) (atm)	3.47 x 10 ⁻⁷	2.52 x 10 ⁻⁶	1.28 x 10 ⁻⁵	4.95 x 10 ⁻⁵	1.38 x 10 ⁻⁴	1.84 x 10 ⁻⁴
K ₂ O(590) ^a	0 ^b	0	0	0	0	0
K ₂ O ₂ (818)	0	0	0	0	0	0
KOH(679)	1	1	1	1	0	0
KO ₂ (808)	0	0	0	0	0	0
K(336)	0	0	0	0	0	0

Notes: ΣP(K) = Sum of vapor pressures of species containing K, O, and H

ΣP(K-O) = Sum of vapor pressures of species containing K and O only

a = Melting point in degrees Kelvin

b = One (1) and zero (0) represent the presence and absence of the solid phase respectively.

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
	MgO(c.l)					
Ar	0.70000	0.70000	0.70000	0.70000	0.69999	0.69998
O ₂	0.05000	0.05000	0.05000	0.05000	0.04999	0.04998
H ₂ O	0.25000	0.25000	0.25000	0.24999	0.24998	0.24995
Mg	1.09 x 10 ⁻²⁷	3.61 x 10 ⁻²⁴	3.06 x 10 ⁻²¹	9.07 x 10 ⁻¹⁹	1.18 x 10 ⁻¹⁶	8.00 x 10 ⁻¹⁵
MgO	3.15 x 10 ⁻²⁴	3.16 x 10 ⁻²¹	1.00 x 10 ⁻¹⁸	1.32 x 10 ⁻¹⁶	8.60 x 10 ⁻¹⁵	3.21 x 10 ⁻¹³
MgOH	2.45 x 10 ⁻²²	1.25 x 10 ⁻¹⁹	2.24 x 10 ⁻¹⁷	1.79 x 10 ⁻¹⁵	7.60 x 10 ⁻¹⁴	1.94 x 10 ⁻¹²
Mg(OH) ₂	2.17 x 10 ⁻¹³	5.52 x 10 ⁻¹²	8.21 x 10 ⁻¹¹	8.07 x 10 ⁻¹⁰	5.74 x 10 ⁻⁹	3.14 x 10 ⁻⁸
O	3.48 x 10 ⁻¹¹	5.53 x 10 ⁻¹⁰	5.56 x 10 ⁻⁹	3.92 x 10 ⁻⁸	2.10 x 10 ⁻⁷	8.99 x 10 ⁻⁷
O ₃	9.73 x 10 ⁻¹⁴	4.49 x 10 ⁻¹³	1.67 x 10 ⁻¹²	5.09 x 10 ⁻¹²	1.33 x 10 ⁻¹¹	3.04 x 10 ⁻¹¹
OH	1.25 x 10 ⁻⁷	7.39 x 10 ⁻⁷	3.26 x 10 ⁻⁶	1.14 x 10 ⁻⁵	3.36 x 10 ⁻⁵	8.53 x 10 ⁻⁵
H	2.22 x 10 ⁻¹⁴	9.84 x 10 ⁻¹³	2.33 x 10 ⁻¹¹	3.42 x 10 ⁻¹⁰	3.43 x 10 ⁻⁹	2.54 x 10 ⁻⁸
H ₂	9.69 x 10 ⁻¹¹	1.46 x 10 ⁻⁹	1.41 x 10 ⁻⁸	9.64 x 10 ⁻⁸	5.02 x 10 ⁻⁷	2.10 x 10 ⁻⁶
H ₂ O ₂	1.53 x 10 ⁻¹⁰	4.95 x 10 ⁻¹⁰	1.32 x 10 ⁻⁹	3.05 x 10 ⁻⁹	6.27 x 10 ⁻⁹	1.17 x 10 ⁻⁸
Σ P(Mg) (atm)	2.17 x 10 ⁻¹³	5.52 x 10 ⁻¹²	8.21 x 10 ⁻¹¹	8.07 x 10 ⁻¹⁰	5.74 x 10 ⁻⁹	3.14 x 10 ⁻⁸
Σ P(Mg-O) (atm)	3.15 x 10 ⁻²⁴	3.16 x 10 ⁻²¹	1.00 x 10 ⁻¹⁸	1.32 x 10 ⁻¹⁶	8.60 x 10 ⁻¹⁵	3.21 x 10 ⁻¹³
MgO(3105)	1	1	1	1	1	1
Mg(OH) ₂ (c)	0	0	0	0	0	0
Mg(923)	0	0	0	0	0	0

Notes: ΣP(Mg) = Sum of vapor pressures of species containing Mg, O, and H

ΣP(Mg-O) = Sum of vapor pressures of species containing Mg and O only

a = Melting point in degrees Kelvin

b = One (1) and zero (0) represent the presence and absence of the solid phase respectively.

Species	Partial Pressure (atm)						
	T(K) =	1000	1100	1200	1300	1400	1500
MgAl ₂ O ₄ (c,l)							
Ar		0.70000	0.70000	0.70000	0.70000	0.69999	0.69998
O ₂		0.05000	0.05000	0.05000	0.05000	0.04999	0.04998
H ₂ O		0.25000	0.25000	0.25000	0.24999	0.24998	0.24995
Mg		5.56 x 10 ⁻²⁹	2.10 x 10 ⁻²⁵	2.19 x 10 ⁻²²	7.73 x 10 ⁻²⁰	1.17 x 10 ⁻¹⁷	8.93 x 10 ⁻¹⁶
MgO		1.60 x 10 ⁻²⁵	1.84 x 10 ⁻²²	7.19 x 10 ⁻²⁰	1.12 x 10 ⁻¹⁷	8.48 x 10 ⁻¹⁶	3.59 x 10 ⁻¹⁴
MgOH		1.25 x 10 ⁻²³	7.27 x 10 ⁻²¹	1.60 x 10 ⁻¹⁸	1.52 x 10 ⁻¹⁶	7.49 x 10 ⁻¹⁵	2.17 x 10 ⁻¹³
Mg(OH) ₂		1.10 x 10 ⁻¹⁴	3.21 x 10 ⁻¹³	5.87 x 10 ⁻¹²	6.88 x 10 ⁻¹¹	5.66 x 10 ⁻¹⁰	3.51 x 10 ⁻⁹
Al		1.23 x 10 ⁻⁴⁵	4.20 x 10 ⁻⁴⁰	1.61 x 10 ⁻³⁵	1.19 x 10 ⁻³¹	2.46 x 10 ⁻²⁸	1.81 x 10 ⁻²⁵
AlO		3.44 x 10 ⁻³⁵	6.50 x 10 ⁻³¹	2.23 x 10 ⁻²⁷	2.16 x 10 ⁻²⁴	7.74 x 10 ⁻²²	1.25 x 10 ⁻¹⁹
AlO ₂		2.74 x 10 ⁻³¹	1.02 x 10 ⁻²⁷	9.10 x 10 ⁻²⁵	2.83 x 10 ⁻²²	3.83 x 10 ⁻²⁰	2.68 x 10 ⁻¹⁸
Al ₂ O		1.44 x 10 ⁻⁵⁸	2.52 x 10 ⁻⁵¹	2.42 x 10 ⁻⁴⁵	2.71 x 10 ⁻⁴⁰	5.67 x 10 ⁻³⁶	3.08 x 10 ⁻³²
Al ₂ O ₂		5.68 x 10 ⁻⁵⁰	6.69 x 10 ⁻⁴⁴	6.78 x 10 ⁻³⁹	1.14 x 10 ⁻³⁴	4.68 x 10 ⁻³¹	6.23 x 10 ⁻²⁸
AlOH		1.12 x 10 ⁻³⁰	6.17 x 10 ⁻²⁷	7.60 x 10 ⁻²⁴	3.10 x 10 ⁻²¹	5.31 x 10 ⁻¹⁹	4.54 x 10 ⁻¹⁷
Al(OH) ₂		1.54 x 10 ⁻²⁴	7.93 x 10 ⁻²²	1.37 x 10 ⁻¹⁹	1.06 x 10 ⁻¹⁷	4.40 x 10 ⁻¹⁶	1.11 x 10 ⁻¹⁴
Al(OH) ₃		5.62 x 10 ⁻¹⁶	1.14 x 10 ⁻¹⁴	1.34 x 10 ⁻¹³	1.08 x 10 ⁻¹²	6.51 x 10 ⁻¹²	3.08 x 10 ⁻¹¹
AlO(OH)		9.71 x 10 ⁻²⁶	6.98 x 10 ⁻²³	1.58 x 10 ⁻²⁰	1.54 x 10 ⁻¹⁸	7.70 x 10 ⁻¹⁷	2.27 x 10 ⁻¹⁵
AlHO		6.11 x 10 ⁻⁴¹	2.62 x 10 ⁻³⁶	1.79 x 10 ⁻³²	3.13 x 10 ⁻²⁹	1.87 x 10 ⁻²⁶	4.72 x 10 ⁻²⁴
O		3.48 x 10 ⁻¹¹	5.53 x 10 ⁻¹⁰	5.56 x 10 ⁻⁹	3.92 x 10 ⁻⁸	2.10 x 10 ⁻⁷	8.99 x 10 ⁻⁷
O ₃		9.73 x 10 ⁻¹⁴	4.49 x 10 ⁻¹³	1.67 x 10 ⁻¹²	5.09 x 10 ⁻¹²	1.33 x 10 ⁻¹¹	3.04 x 10 ⁻¹¹
OH		1.25 x 10 ⁻⁷	7.39 x 10 ⁻⁷	3.26 x 10 ⁻⁶	1.14 x 10 ⁻⁵	3.36 x 10 ⁻⁵	8.53 x 10 ⁻⁵
H		2.22 x 10 ⁻¹⁴	9.84 x 10 ⁻¹³	2.33 x 10 ⁻¹¹	3.42 x 10 ⁻¹⁰	3.43 x 10 ⁻⁹	2.54 x 10 ⁻⁸
H ₂		9.69 x 10 ⁻¹¹	1.46 x 10 ⁻⁹	1.41 x 10 ⁻⁸	9.64 x 10 ⁻⁸	5.02 x 10 ⁻⁷	2.10 x 10 ⁻⁶
H ₂ O ₂		1.53 x 10 ⁻¹⁰	4.95 x 10 ⁻¹⁰	1.32 x 10 ⁻⁹	3.05 x 10 ⁻⁹	6.27 x 10 ⁻⁹	1.17 x 10 ⁻⁸
Σ P(Mg) (atm)		1.10 x 10 ⁻¹⁴	3.21 x 10 ⁻¹³	5.87 x 10 ⁻¹²	6.88 x 10 ⁻¹¹	5.66 x 10 ⁻¹⁰	3.51 x 10 ⁻⁹
Σ P(Mg-O) (atm)		1.60 x 10 ⁻²⁵	1.84 x 10 ⁻²²	7.19 x 10 ⁻²⁰	1.12 x 10 ⁻¹⁷	8.48 x 10 ⁻¹⁶	3.59 x 10 ⁻¹⁴
Σ P(Al) (atm)		5.62 x 10 ⁻¹⁶	1.14 x 10 ⁻¹⁴	1.34 x 10 ⁻¹³	1.08 x 10 ⁻¹²	6.51 x 10 ⁻¹²	3.08 x 10 ⁻¹¹
Σ P(Al-O) (atm)		2.74 x 10 ⁻³¹	1.02 x 10 ⁻²⁷	9.12 x 10 ⁻²⁵	2.85 x 10 ⁻²²	3.91 x 10 ⁻²⁰	2.81 x 10 ⁻¹⁸
MgAl ₂ O ₄ (2408)		1	1	1	1	1	1
MgO(3105)		0	0	0	0	0	0
Mg(OH) ₂ (c)		0	0	0	0	0	0
Mg(923)		0	0	0	0	0	0
Al ₂ O ₃ -α(2327)		1	1	1	1	1	1
Al(OH) ₃ (c)		0	0	0	0	0	0
Al(934)		0	0	0	0	0	0

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
Na₂O(c,l)						
Ar	0.77775	0.77753	0.77635	0.77166	0.75683	0.71751
O ₂	0.05555	0.05554	0.05545	0.05511	0.05405	0.05130
H ₂ O	0.16666	0.16661	0.16636	0.16536	0.16220	0.15399
Na	1.59 x 10 ⁻¹⁰	9.62 x 10 ⁻⁹	2.85 x 10 ⁻⁷	4.93 x 10 ⁻⁶	5.61 x 10 ⁻⁵	4.66 x 10 ⁻⁴
NaO	1.61 x 10 ⁻¹²	9.64 x 10 ⁻¹¹	2.83 x 10 ⁻⁹	4.83 x 10 ⁻⁸	5.41 x 10 ⁻⁷	4.36 x 10 ⁻⁶
NaO ₂	1.48 x 10 ⁻⁸	1.58 x 10 ⁻⁷	1.11 x 10 ⁻⁶	5.60 x 10 ⁻⁶	2.19 x 10 ⁻⁵	6.99 x 10 ⁻⁵
Na ₂	1.31 x 10 ⁻²⁰	2.09 x 10 ⁻¹⁷	9.20 x 10 ⁻¹⁵	1.52 x 10 ⁻¹²	1.19 x 10 ⁻¹⁰	5.29 x 10 ⁻⁹
Na ₂ O	5.41 x 10 ⁻¹⁶	1.59 x 10 ⁻¹³	1.72 x 10 ⁻¹¹	8.70 x 10 ⁻¹⁰	2.45 x 10 ⁻⁸	4.43 x 10 ⁻⁷
Na ₂ O ₂	2.03 x 10 ⁻¹⁵	1.87 x 10 ⁻¹³	7.68 x 10 ⁻¹²	1.71 x 10 ⁻¹⁰	2.37 x 10 ⁻⁹	2.28 x 10 ⁻⁸
NaOH	3.75 x 10 ⁻⁵	3.14 x 10 ⁻⁴	1.80 x 10 ⁻³	7.71 x 10 ⁻³	2.64 x 10 ⁻²	7.57 x 10 ⁻²
Na ₂ (OH) ₂	1.30 x 10 ⁻⁶	8.51 x 10 ⁻⁶	3.89 x 10 ⁻⁵	1.35 x 10 ⁻⁴	3.81 x 10 ⁻⁴	9.11 x 10 ⁻⁴
O	3.67 x 10 ⁻¹¹	5.83 x 10 ⁻¹⁰	5.85 x 10 ⁻⁹	4.12 x 10 ⁻⁸	2.18 x 10 ⁻⁷	9.11 x 10 ⁻⁷
O ₃	1.14 x 10 ⁻¹³	5.25 x 10 ⁻¹³	1.95 x 10 ⁻¹²	5.89 x 10 ⁻¹²	1.49 x 10 ⁻¹¹	3.16 x 10 ⁻¹¹
OH	1.04 x 10 ⁻⁷	6.19 x 10 ⁻⁷	2.73 x 10 ⁻⁶	9.52 x 10 ⁻⁶	2.76 x 10 ⁻⁵	6.74 x 10 ⁻⁵
H	1.77 x 10 ⁻¹⁴	7.82 x 10 ⁻¹³	1.85 x 10 ⁻¹¹	2.71 x 10 ⁻¹⁰	2.71 x 10 ⁻⁹	1.98 x 10 ⁻⁸
H ₂	6.13 x 10 ⁻¹¹	9.25 x 10 ⁻¹⁰	8.91 x 10 ⁻⁹	6.07 x 10 ⁻⁸	3.13 x 10 ⁻⁷	1.28 x 10 ⁻⁶
H ₂ O ₂	1.07 x 10 ⁻¹⁰	3.48 x 10 ⁻¹⁰	9.28 x 10 ⁻¹⁰	2.12 x 10 ⁻⁹	4.23 x 10 ⁻⁹	7.30 x 10 ⁻⁹
Σ P(Na) (atm)	3.88 x 10 ⁻⁵	3.22 x 10 ⁻⁴	1.84 x 10 ⁻³	7.86 x 10 ⁻³	2.69 x 10 ⁻²	7.71 x 10 ⁻²
Σ P(Na-O) (atm)	1.48 x 10 ⁻⁸	1.58 x 10 ⁻⁷	1.11 x 10 ⁻⁶	5.64 x 10 ⁻⁶	2.25 x 10 ⁻⁵	7.47 x 10 ⁻⁵
Na ₂ O(1405) ^a	0 ^b	0	0	0	0	0
Na ₂ O ₂ (948)	0	0	0	0	0	0
NaOH(596)	1	1	1	1	1	1
NaO ₂ (800)	0	0	0	0	0	0
Na(371)	0	0	0	0	0	0

Notes: ΣP(Na) = Sum of vapor pressures of species containing Na, O, and H

ΣP(Na-O) = Sum of vapor pressures of species containing Na and O only

a = Melting point in degrees Kelvin

b = One (1) and zero (0) represent the presence and absence of the solid phase respectively.

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Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
	SiO ₂ (c,l) (Q)					
Ar	0.70000	0.70000	0.70000	0.70000	0.69999	0.69998
O ₂	0.05000	0.05000	0.05000	0.05000	0.04999	0.04998
H ₂ O	0.25000	0.25000	0.25000	0.24999	0.24998	0.24995
Si	2.36 x 10 ⁻⁵³	6.27 x 10 ⁻⁴⁷	1.40 x 10 ⁻⁴¹	4.56 x 10 ⁻³⁷	3.33 x 10 ⁻³³	7.38 x 10 ⁻³⁰
SiO	1.95 x 10 ⁻²⁸	1.21 x 10 ⁻²⁴	1.73 x 10 ⁻²¹	7.83 x 10 ⁻¹⁹	1.46 x 10 ⁻¹⁶	1.35 x 10 ⁻¹⁴
SiO ₂	4.28 x 10 ⁻²⁴	3.87 x 10 ⁻²¹	1.11 x 10 ⁻¹⁸	1.31 x 10 ⁻¹⁶	7.71 x 10 ⁻¹⁵	2.62 x 10 ⁻¹³
SiOH	4.75 x 10 ⁻⁴⁵	6.86 x 10 ⁻⁴⁰	1.35 x 10 ⁻³⁵	5.64 x 10 ⁻³²	7.10 x 10 ⁻²⁹	3.42 x 10 ⁻²⁶
Si(OH) ₂	2.00 x 10 ⁻³²	6.24 x 10 ⁻²⁹	5.07 x 10 ⁻²⁶	1.44 x 10 ⁻²³	1.81 x 10 ⁻²¹	1.19 x 10 ⁻¹⁹
Si(OH) ₃	5.71 x 10 ⁻²⁹	2.58 x 10 ⁻²⁶	4.22 x 10 ⁻²⁴	3.12 x 10 ⁻²²	1.25 x 10 ⁻²⁰	3.08 x 10 ⁻¹⁹
Si(OH) ₄	5.38 x 10 ⁻¹⁵	2.95 x 10 ⁻¹⁴	1.23 x 10 ⁻¹³	4.10 x 10 ⁻¹³	1.16 x 10 ⁻¹²	2.88 x 10 ⁻¹²
SiO(OH)	4.79 x 10 ⁻¹⁹	1.55 x 10 ⁻¹⁶	1.90 x 10 ⁻¹⁴	1.08 x 10 ⁻¹²	3.42 x 10 ⁻¹¹	6.80 x 10 ⁻¹⁰
SiO(OH) ₂	9.06 x 10 ⁻¹²	1.50 x 10 ⁻¹⁰	1.56 x 10 ⁻⁹	1.11 x 10 ⁻⁸	5.95 x 10 ⁻⁸	2.55 x 10 ⁻⁷
Si ₂ O(OH) ₆	2.16 x 10 ⁻¹²	1.42 x 10 ⁻¹²	1.03 x 10 ⁻¹²	7.76 x 10 ⁻¹³	6.26 x 10 ⁻¹³	5.30 x 10 ⁻¹³
O	3.48 x 10 ⁻¹¹	5.53 x 10 ⁻¹⁰	5.56 x 10 ⁻⁹	3.92 x 10 ⁻⁸	2.10 x 10 ⁻⁷	8.99 x 10 ⁻⁷
O ₃	9.73 x 10 ⁻¹⁴	4.49 x 10 ⁻¹³	1.67 x 10 ⁻¹²	5.09 x 10 ⁻¹²	1.33 x 10 ⁻¹¹	3.04 x 10 ⁻¹¹
OH	1.25 x 10 ⁻⁷	7.39 x 10 ⁻⁷	3.26 x 10 ⁻⁶	1.14 x 10 ⁻⁵	3.36 x 10 ⁻⁵	8.53 x 10 ⁻⁵
H	2.22 x 10 ⁻¹⁴	9.84 x 10 ⁻¹³	2.33 x 10 ⁻¹¹	3.42 x 10 ⁻¹⁰	3.43 x 10 ⁻⁹	2.54 x 10 ⁻⁸
H ₂	9.69 x 10 ⁻¹¹	1.46 x 10 ⁻⁹	1.41 x 10 ⁻⁸	9.64 x 10 ⁻⁸	5.02 x 10 ⁻⁷	2.10 x 10 ⁻⁶
H ₂ O ₂	1.53 x 10 ⁻¹⁰	4.95 x 10 ⁻¹⁰	1.32 x 10 ⁻⁹	3.05 x 10 ⁻⁹	6.27 x 10 ⁻⁹	1.17 x 10 ⁻⁸
Σ P(Si) (atm)	1.12 x 10 ⁻¹¹	1.52 x 10 ⁻¹⁰	1.56 x 10 ⁻⁹	1.11 x 10 ⁻⁸	5.95 x 10 ⁻⁸	2.56 x 10 ⁻⁷
Σ P(Si-O) (atm)	4.28 x 10 ⁻²⁴	3.87 x 10 ⁻²¹	1.12 x 10 ⁻¹⁸	1.31 x 10 ⁻¹⁶	7.85 x 10 ⁻¹⁵	2.75 x 10 ⁻¹³
SiO ₂ (1996) ^a	1	1	1	1	1	1
Si(1685)	0	0	0	0	0	0

Notes: ΣP(Si) = Sum of vapor pressures of species containing Si, O, and H

ΣP(Si-O) = Sum of vapor pressures of species containing Si and O only

a = Melting point in degrees Kelvin

b = One (1) and zero (0) represent the presence and absence of the solid phase respectively.

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
	TiO ₂ (c,l)					
Ar	0.70000	0.70000	0.70000	0.70000	0.69999	0.69998
O ₂	0.05000	0.05000	0.05000	0.05000	0.04999	0.04998
H ₂ O	0.25000	0.25000	0.25000	0.24999	0.24998	0.24995
Ti	2.86 x 10 ⁻⁵⁶	1.36 x 10 ⁻⁴⁹	4.92 x 10 ⁻⁴⁴	2.44 x 10 ⁻³⁹	2.56 x 10 ⁻³⁵	7.70 x 10 ⁻³²
TiO	7.49 x 10 ⁻³⁸	3.61 x 10 ⁻³³	2.83 x 10 ⁻²⁹	5.50 x 10 ⁻²⁶	3.57 x 10 ⁻²³	9.67 x 10 ⁻²¹
TiO ₂	1.40 x 10 ⁻²³	1.32 x 10 ⁻²⁰	3.91 x 10 ⁻¹⁸	4.75 x 10 ⁻¹⁶	2.87 x 10 ⁻¹⁴	9.90 x 10 ⁻¹³
TiOH	1.77 x 10 ⁻⁴⁶	4.61 x 10 ⁻⁴¹	1.48 x 10 ⁻³⁶	9.50 x 10 ⁻³³	1.72 x 10 ⁻²⁹	1.13 x 10 ⁻²⁶
Ti(OH) ₂	1.10 x 10 ⁻³²	6.34 x 10 ⁻²⁹	8.58 x 10 ⁻²⁶	3.81 x 10 ⁻²³	7.05 x 10 ⁻²¹	6.47 x 10 ⁻¹⁹
Ti(OH) ₃	1.48 x 10 ⁻²⁴	4.78 x 10 ⁻²²	5.94 x 10 ⁻²⁰	3.53 x 10 ⁻¹⁸	1.17 x 10 ⁻¹⁶	2.45 x 10 ⁻¹⁵
Ti(OH) ₄	3.03 x 10 ⁻²⁰	1.25 x 10 ⁻¹⁸	2.82 x 10 ⁻¹⁷	3.99 x 10 ⁻¹⁶	3.91 x 10 ⁻¹⁵	2.85 x 10 ⁻¹⁴
TiO(OH)	9.40 x 10 ⁻²⁹	2.80 x 10 ⁻²⁵	2.18 x 10 ⁻²²	6.02 x 10 ⁻²⁰	7.37 x 10 ⁻¹⁸	4.72 x 10 ⁻¹⁶
TiO(OH) ₂	3.34 x 10 ⁻²⁶	1.68 x 10 ⁻²³	2.98 x 10 ⁻²¹	2.39 x 10 ⁻¹⁹	1.02 x 10 ⁻¹⁷	2.64 x 10 ⁻¹⁶
O	3.48 x 10 ⁻¹¹	5.53 x 10 ⁻¹⁰	5.56 x 10 ⁻⁹	3.92 x 10 ⁻⁸	2.10 x 10 ⁻⁷	8.99 x 10 ⁻⁷
O ₃	9.73 x 10 ⁻¹⁴	4.49 x 10 ⁻¹³	1.67 x 10 ⁻¹²	5.09 x 10 ⁻¹²	1.33 x 10 ⁻¹¹	3.04 x 10 ⁻¹¹
OH	1.25 x 10 ⁻⁷	7.39 x 10 ⁻⁷	3.26 x 10 ⁻⁶	1.14 x 10 ⁻⁵	3.36 x 10 ⁻⁵	8.53 x 10 ⁻⁵
H	2.22 x 10 ⁻¹⁴	9.84 x 10 ⁻¹³	2.33 x 10 ⁻¹¹	3.42 x 10 ⁻¹⁰	3.43 x 10 ⁻⁹	2.54 x 10 ⁻⁸
H ₂	9.69 x 10 ⁻¹¹	1.46 x 10 ⁻⁹	1.41 x 10 ⁻⁸	9.64 x 10 ⁻⁸	5.02 x 10 ⁻⁷	2.10 x 10 ⁻⁶
H ₂ O ₂	1.53 x 10 ⁻¹⁰	4.95 x 10 ⁻¹⁰	1.32 x 10 ⁻⁹	3.05 x 10 ⁻⁹	6.27 x 10 ⁻⁹	1.17 x 10 ⁻⁸
Σ P(Ti) (atm)	3.03 x 10 ⁻²⁰	1.26 x 10 ⁻¹⁸	3.22 x 10 ⁻¹⁷	8.78 x 10 ⁻¹⁶	3.27 x 10 ⁻¹⁴	1.02 x 10 ⁻¹²
Σ P(Ti-O) (atm)	1.40 x 10 ⁻²³	1.32 x 10 ⁻²⁰	3.91 x 10 ⁻¹⁸	4.75 x 10 ⁻¹⁶	2.87 x 10 ⁻¹⁴	9.90 x 10 ⁻¹³
TiO ₂ -r(2130) ^a	1 ^b	1	1	1	1	1
Ti ₄ O ₇ (1950)	0	0	0	0	0	0
Ti ₃ O ₅ (2050)	0	0	0	0	0	0
Ti ₂ O ₃ (2115)	0	0	0	0	0	0
TiO(2023)	0	0	0	0	0	0
Ti(1939)	0	0	0	0	0	0

Notes: ΣP(Ti) = Sum of vapor pressures of species containing Ti, O, and H

ΣP(Ti-O) = Sum of vapor pressures of species containing Ti and O only

a = Melting point in degrees Kelvin

b = One (1) and zero (0) represent the presence and absence of the solid phase respectively.

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
ZrO₂(c,l)						
Ar	7.00 x 10 ⁻¹	7.00 x 10 ⁻¹	7.00 x 10 ⁻¹	7.00 x 10 ⁻¹	7.00 x 10 ⁻¹	7.00 x 10 ⁻¹
O ₂	5.00 x 10 ⁻²	5.00 x 10 ⁻²	5.00 x 10 ⁻²	5.00 x 10 ⁻²	5.00 x 10 ⁻²	5.00 x 10 ⁻²
H ₂ O	2.50 x 10 ⁻¹	2.50 x 10 ⁻¹	2.50 x 10 ⁻¹	2.50 x 10 ⁻¹	2.50 x 10 ⁻¹	2.50 x 10 ⁻¹
Zr	3.10 x 10 ⁻⁷¹	3.57 x 10 ⁻⁶³	1.84 x 10 ⁻⁵⁶	8.66 x 10 ⁻⁵¹	6.26 x 10 ⁻⁴⁶	1.00 x 10 ⁻⁴¹
ZrO	1.29 x 10 ⁻⁴⁷	4.53 x 10 ⁻⁴²	1.87 x 10 ⁻³⁷	1.49 x 10 ⁻³³	3.27 x 10 ⁻³⁰	2.53 x 10 ⁻²⁷
ZrO ₂	1.48 x 10 ⁻³⁰	6.20 x 10 ⁻²⁷	6.34 x 10 ⁻²⁴	2.19 x 10 ⁻²¹	3.24 x 10 ⁻¹⁹	2.41 x 10 ⁻¹⁷
ZrOH	5.24 x 10 ⁻⁵⁷	1.25 x 10 ⁻⁵⁰	2.54 x 10 ⁻⁴⁵	7.75 x 10 ⁻⁴¹	5.34 x 10 ⁻³⁷	1.11 x 10 ⁻³³
Zr(OH) ₂	3.15 x 10 ⁻⁴³	1.64 x 10 ⁻³⁸	1.39 x 10 ⁻³⁴	2.91 x 10 ⁻³¹	2.04 x 10 ⁻²⁸	5.89 x 10 ⁻²⁶
Zr(OH) ₃	1.37 x 10 ⁻³³	2.86 x 10 ⁻³⁰	1.68 x 10 ⁻²⁷	3.72 x 10 ⁻²⁵	3.83 x 10 ⁻²³	2.11 x 10 ⁻²¹
Zr(OH) ₄	2.28 x 10 ⁻²²	1.60 x 10 ⁻²⁰	5.60 x 10 ⁻¹⁹	1.15 x 10 ⁻¹⁷	1.55 x 10 ⁻¹⁶	1.47 x 10 ⁻¹⁵
ZrO(OH)	2.08 x 10 ⁻³⁷	4.13 x 10 ⁻³³	1.56 x 10 ⁻²⁹	1.64 x 10 ⁻²⁶	6.31 x 10 ⁻²⁴	1.08 x 10 ⁻²¹
ZrO(OH) ₂	1.88 x 10 ⁻²⁸	1.52 x 10 ⁻²⁵	4.03 x 10 ⁻²³	4.51 x 10 ⁻²¹	2.57 x 10 ⁻¹⁹	8.46 x 10 ⁻¹⁸
O	3.48 x 10 ⁻¹¹	5.53 x 10 ⁻¹⁰	5.56 x 10 ⁻⁹	3.92 x 10 ⁻⁸	2.10 x 10 ⁻⁷	8.99 x 10 ⁻⁷
O ₃	9.73 x 10 ⁻¹⁴	4.49 x 10 ⁻¹³	1.67 x 10 ⁻¹²	5.09 x 10 ⁻¹²	1.33 x 10 ⁻¹¹	3.04 x 10 ⁻¹¹
OH	1.25 x 10 ⁻⁷	7.39 x 10 ⁻⁷	3.26 x 10 ⁻⁶	1.14 x 10 ⁻⁵	3.36 x 10 ⁻⁵	8.53 x 10 ⁻⁵
H	2.22 x 10 ⁻¹⁴	9.84 x 10 ⁻¹³	2.33 x 10 ⁻¹¹	3.42 x 10 ⁻¹⁰	3.43 x 10 ⁻⁹	2.54 x 10 ⁻⁸
H ₂	9.69 x 10 ⁻¹¹	1.46 x 10 ⁻⁹	1.41 x 10 ⁻⁸	9.64 x 10 ⁻⁸	5.02 x 10 ⁻⁷	2.10 x 10 ⁻⁶
H ₂ O ₂	1.53 x 10 ⁻¹⁰	4.95 x 10 ⁻¹⁰	1.32 x 10 ⁻⁹	3.05 x 10 ⁻⁹	6.27 x 10 ⁻⁹	1.17 x 10 ⁻⁸
Σ P(Zr) (atm)	2.28 x 10 ⁻²²	1.60 x 10 ⁻²⁰	5.60 x 10 ⁻¹⁹	1.15 x 10 ⁻¹⁷	1.55 x 10 ⁻¹⁶	1.51 x 10 ⁻¹⁵
Σ P(Zr-O) (atm)	1.48 x 10 ⁻³⁰	6.20 x 10 ⁻²⁷	6.34 x 10 ⁻²⁴	2.19 x 10 ⁻²¹	3.24 x 10 ⁻¹⁹	2.41 x 10 ⁻¹⁷
ZrO ₂ (2950) ^a	1 ^b	1	1	1	1	1
Zr(2125)	0	0	0	0	0	0

Notes: ΣP(Zr) = Sum of vapor pressures of species containing Zr, O, and H

ΣP(Zr-O) = Sum of vapor pressures of species containing Zr and O only

a = Melting point in degrees Kelvin

b = One (1) and zero (0) represent the presence and absence of the solid phase respectively.

Species	Partial Pressure (atm)					
T(K) =	1000	1100	1200	1300	1400	1500
Na ₂ Si ₃ O ₇ (c)						
Ar	0.70000	0.70000	0.70000	0.70000	0.69999	0.69998
O ₂	0.05000	0.05000	0.05000	0.05000	0.04999	0.04998
H ₂ O	0.25000	0.25000	0.25000	0.24999	0.24998	0.24994
Na	3.63 x 10 ⁻¹⁵	3.84 x 10 ⁻¹³	1.83 x 10 ⁻¹¹	4.77 x 10 ⁻¹⁰	7.70 x 10 ⁻⁰⁹	8.51 x 10 ⁻⁰⁸
NaO	3.49 x 10 ⁻¹⁷	3.65 x 10 ⁻¹⁵	1.73 x 10 ⁻¹³	4.45 x 10 ⁻¹²	7.15 x 10 ⁻¹¹	7.86 x 10 ⁻¹⁰
NaO ₂	3.04 x 10 ⁻¹³	5.69 x 10 ⁻¹²	6.41 x 10 ⁻¹¹	4.91 x 10 ⁻¹⁰	2.79 x 10 ⁻⁰⁹	1.24 x 10 ⁻⁰⁸
Na ₂	6.81 x 10 ⁻³⁰	3.33 x 10 ⁻²⁶	3.79 x 10 ⁻²³	1.43 x 10 ⁻²⁰	2.24 x 10 ⁻¹⁸	1.76 x 10 ⁻¹⁶
Na ₂ O	2.67 x 10 ⁻²⁵	2.41 x 10 ⁻²²	6.75 x 10 ⁻²⁰	7.76 x 10 ⁻¹⁸	4.44 x 10 ⁻¹⁶	1.46 x 10 ⁻¹⁴
Na ₂ O ₂	9.49 x 10 ⁻²⁵	2.68 x 10 ⁻²²	2.86 x 10 ⁻²⁰	1.45 x 10 ⁻¹⁸	4.13 x 10 ⁻¹⁷	7.41 x 10 ⁻¹⁶
NaOH	1.02 x 10 ⁻⁹	1.49 x 10 ⁻⁸	1.38 x 10 ⁻⁷	8.96 x 10 ⁻⁷	4.42 x 10 ⁻⁶	1.75 x 10 ⁻⁵
Na ₂ (OH) ₂	9.59 x 10 ⁻¹⁶	1.93 x 10 ⁻¹⁴	2.29 x 10 ⁻¹³	1.82 x 10 ⁻¹²	1.06 x 10 ⁻¹¹	4.86 x 10 ⁻¹¹
Si	2.32 x 10 ⁻⁵³	6.17 x 10 ⁻⁴⁷	1.38 x 10 ⁻⁴¹	4.58 x 10 ⁻³⁷	3.40 x 10 ⁻³³	7.64 x 10 ⁻³⁰
SiO	1.92 x 10 ⁻²⁸	1.19 x 10 ⁻²⁴	1.71 x 10 ⁻²¹	7.87 x 10 ⁻¹⁹	1.49 x 10 ⁻¹⁶	1.40 x 10 ⁻¹⁴
SiO ₂	6.71 x 10 ⁻²²	3.83 x 10 ⁻¹⁹	7.52 x 10 ⁻¹⁷	6.49 x 10 ⁻¹⁵	2.94 x 10 ⁻¹³	7.96 x 10 ⁻¹²
SiOH	4.67 x 10 ⁻⁴⁵	6.75 x 10 ⁻⁴⁰	1.33 x 10 ⁻³⁵	5.67 x 10 ⁻³²	7.25 x 10 ⁻²⁹	3.54 x 10 ⁻²⁶
Si(OH) ₂	1.97 x 10 ⁻³²	6.15 x 10 ⁻²⁹	5.00 x 10 ⁻²⁶	1.45 x 10 ⁻²³	1.85 x 10 ⁻²¹	1.24 x 10 ⁻¹⁹
Si(OH) ₃	5.62 x 10 ⁻²⁹	2.54 x 10 ⁻²⁶	4.17 x 10 ⁻²⁴	3.13 x 10 ⁻²²	1.28 x 10 ⁻²⁰	3.19 x 10 ⁻¹⁹
Si(OH) ₄	5.30 x 10 ⁻¹⁵	2.90 x 10 ⁻¹⁴	1.21 x 10 ⁻¹³	4.11 x 10 ⁻¹³	1.18 x 10 ⁻¹²	2.98 x 10 ⁻¹²
SiO(OH)	3.20 x 10 ⁻²⁶	4.64 x 10 ⁻²³	1.99 x 10 ⁻²⁰	3.32 x 10 ⁻¹⁸	2.65 x 10 ⁻¹⁶	1.17 x 10 ⁻¹⁴
SiO(OH) ₂	8.91 x 10 ⁻¹²	1.48 x 10 ⁻¹⁰	1.54 x 10 ⁻⁹	1.11 x 10 ⁻⁸	6.07 x 10 ⁻⁸	2.64 x 10 ⁻⁷
O	3.48 x 10 ⁻¹¹	5.53 x 10 ⁻¹⁰	5.56 x 10 ⁻⁹	3.92 x 10 ⁻⁸	2.10 x 10 ⁻⁷	8.99 x 10 ⁻⁷
O ₃	9.73 x 10 ⁻¹⁴	4.49 x 10 ⁻¹³	1.67 x 10 ⁻¹²	5.09 x 10 ⁻¹²	1.33 x 10 ⁻¹¹	3.04 x 10 ⁻¹¹
OH	1.25 x 10 ⁻⁷	7.39 x 10 ⁻⁷	3.26 x 10 ⁻⁶	1.14 x 10 ⁻⁵	3.36 x 10 ⁻⁵	8.53 x 10 ⁻⁵
H	2.22 x 10 ⁻¹⁴	9.84 x 10 ⁻¹³	2.33 x 10 ⁻¹¹	3.42 x 10 ⁻¹⁰	3.43 x 10 ⁻⁹	2.54 x 10 ⁻⁸
H ₂	9.69 x 10 ⁻¹¹	1.46 x 10 ⁻⁹	1.41 x 10 ⁻⁸	9.64 x 10 ⁻⁸	5.02 x 10 ⁻⁷	2.10 x 10 ⁻⁶
H ₂ O ₂	1.53 x 10 ⁻¹⁰	4.95 x 10 ⁻¹⁰	1.32 x 10 ⁻⁹	3.05 x 10 ⁻⁹	6.27 x 10 ⁻⁹	1.17 x 10 ⁻⁸
Σ P(Na) (atm)	1.02 x 10 ⁻⁹	1.50 x 10 ⁻⁸	1.38 x 10 ⁻⁷	8.97 x 10 ⁻⁷	4.43 x 10 ⁻⁶	1.76 x 10 ⁻⁵
Σ P(Na-O) (atm)	3.08 x 10 ⁻¹³	6.07 x 10 ⁻¹²	8.26 x 10 ⁻¹¹	9.73 x 10 ⁻¹⁰	1.06 x 10 ⁻⁸	9.83 x 10 ⁻⁸
Σ P(Si) (atm)	8.92 x 10 ⁻¹²	1.48 x 10 ⁻¹⁰	1.54 x 10 ⁻⁹	1.11 x 10 ⁻⁸	6.07 x 10 ⁻⁸	2.64 x 10 ⁻⁷
Σ P(Si-O) (atm)	6.71 x 10 ⁻²²	3.83 x 10 ⁻¹⁹	7.52 x 10 ⁻¹⁷	6.49 x 10 ⁻¹⁵	2.95 x 10 ⁻¹³	7.98 x 10 ⁻¹²

Species	Partial Pressure (atm)					
T(K) =	1000	1100	1200	1300	1400	1500
	Na ₂ Si ₃ O ₇ (c)					
Na ₂ O(1405) ^a	0 ^b	0	0	0	0	0
Na ₂ O ₂ (948)	0	0	0	0	0	0
NaOH(596)	0	0	0	0	0	0
NaO ₂ (800)	0	0	0	0	0	0
Na(370.98)	0	0	0	0	0	0
Na ₂ SiO ₃ (1362)	0	0	0	0	0	0
Na ₂ Si ₂ O ₅ (1147)	0	0	0	0	0	0
Na ₂ Si ₃ O ₇ (c)	1	1	1	1	1	1
Na ₄ SiO ₄ (1393)	0	0	0	0	0	0
Na ₆ Si ₂ O ₇ (c)	0	0	0	0	0	0
SiO ₂ (1696)	1	1	1	1	1	1
Si(1685)	0	0	0	0	0	0

Notes: $\Sigma P(\text{Na})$ = Sum of vapor pressures of species containing Na, O, and H

$\Sigma P(\text{Na-O})$ = Sum of vapor pressures of species containing Na and O only

$\Sigma P(\text{Si})$ = Sum of vapor pressures of species containing Si, O, and H

$\Sigma P(\text{Si-O})$ = Sum of vapor pressures of species containing Si and O only

a = Melting point in degrees Kelvin

b = One (1) and zero (0) represent the presence and absence of the solid phase respectively.

Species	Partial Pressure (atm)						
	T(K) =	1000	1100	1200	1300	1400	1500
K ₂ Si ₂ O ₅ (c,l)							
Ar		0.70000	0.70000	0.70000	0.70000	0.69999	0.69997
O ₂		0.05000	0.05000	0.05000	0.05000	0.04999	0.04998
H ₂ O		0.25000	0.25000	0.25000	0.24999	0.24997	0.24993
K		5.12 x 10 ⁻¹⁵	4.86 x 10 ⁻¹³	2.08 x 10 ⁻¹¹	3.91 x 10 ⁻¹⁰	4.59 x 10 ⁻⁹	3.82 x 10 ⁻⁸
KO		1.25 x 10 ⁻¹⁵	9.23 x 10 ⁻¹⁴	3.20 x 10 ⁻¹²	5.00 x 10 ⁻¹¹	5.03 x 10 ⁻¹⁰	3.65 x 10 ⁻⁹
KO ₂		2.90 x 10 ⁻¹²	4.21 x 10 ⁻¹¹	3.78 x 10 ⁻¹⁰	1.88 x 10 ⁻⁹	7.11 x 10 ⁻⁹	2.21 x 10 ⁻⁸
K ₂		2.13 x 10 ⁻³⁰	1.06 x 10 ⁻²⁶	1.19 x 10 ⁻²³	2.74 x 10 ⁻²¹	2.61 x 10 ⁻¹⁹	1.31 x 10 ⁻¹⁷
K ₂ O		5.98 x 10 ⁻²⁴	3.40 x 10 ⁻²¹	6.23 x 10 ⁻¹⁹	3.11 x 10 ⁻¹⁷	8.06 x 10 ⁻¹⁶	1.31 x 10 ⁻¹⁴
K ₂ O ₂		1.17 x 10 ⁻²²	1.93 x 10 ⁻²⁰	1.27 x 10 ⁻¹⁸	2.66 x 10 ⁻¹⁷	3.30 x 10 ⁻¹⁶	2.84 x 10 ⁻¹⁵
KOH		8.63 x 10 ⁻⁹	1.00 x 10 ⁻⁷	7.51 x 10 ⁻⁷	3.22 x 10 ⁻⁶	1.07 x 10 ⁻⁵	3.00 x 10 ⁻⁵
K ₂ (OH) ₂		1.56 x 10 ⁻¹⁴	3.37 x 10 ⁻¹³	4.10 x 10 ⁻¹²	2.10 x 10 ⁻¹¹	7.79 x 10 ⁻¹¹	2.37 x 10 ⁻¹⁰
Si		2.32 x 10 ⁻⁵³	6.17 x 10 ⁻⁴⁷	1.38 x 10 ⁻⁴¹	4.58 x 10 ⁻³⁷	3.40 x 10 ⁻³³	7.64 x 10 ⁻³⁰
SiO		1.92 x 10 ⁻²⁸	1.19 x 10 ⁻²⁴	1.71 x 10 ⁻²¹	7.87 x 10 ⁻¹⁹	1.49 x 10 ⁻¹⁶	1.40 x 10 ⁻¹⁴
SiO ₂		6.71 x 10 ⁻²²	3.83 x 10 ⁻¹⁹	7.52 x 10 ⁻¹⁷	6.49 x 10 ⁻¹⁵	2.94 x 10 ⁻¹³	7.96 x 10 ⁻¹²
SiOH		4.67 x 10 ⁻⁴⁵	6.75 x 10 ⁻⁴⁰	1.33 x 10 ⁻³⁵	5.67 x 10 ⁻³²	7.25 x 10 ⁻²⁹	3.54 x 10 ⁻²⁶
Si(OH) ₂		1.97 x 10 ⁻³²	6.15 x 10 ⁻²⁹	5.00 x 10 ⁻²⁶	1.45 x 10 ⁻²³	1.85 x 10 ⁻²¹	1.23 x 10 ⁻¹⁹
Si(OH) ₃		5.62 x 10 ⁻²⁹	2.54 x 10 ⁻²⁶	4.17 x 10 ⁻²⁴	3.13 x 10 ⁻²²	1.28 x 10 ⁻²⁰	3.19 x 10 ⁻¹⁹
Si(OH) ₄		5.30 x 10 ⁻¹⁵	2.90 x 10 ⁻¹⁴	1.21 x 10 ⁻¹³	4.11 x 10 ⁻¹³	1.18 x 10 ⁻¹²	2.98 x 10 ⁻¹²
SiO(OH)		3.20 x 10 ⁻²⁶	4.64 x 10 ⁻²³	1.99 x 10 ⁻²⁰	3.32 x 10 ⁻¹⁸	2.65 x 10 ⁻¹⁶	1.17 x 10 ⁻¹⁴
SiO(OH) ₂		8.91 x 10 ⁻¹²	1.48 x 10 ⁻¹⁰	1.54 x 10 ⁻⁹	1.11 x 10 ⁻⁸	6.07 x 10 ⁻⁸	2.64 x 10 ⁻⁷
O		3.48 x 10 ⁻¹¹	5.53 x 10 ⁻¹⁰	5.56 x 10 ⁻⁹	3.92 x 10 ⁻⁸	2.10 x 10 ⁻⁷	8.99 x 10 ⁻⁷
O ₃		9.73 x 10 ⁻¹⁴	4.49 x 10 ⁻¹³	1.67 x 10 ⁻¹²	5.09 x 10 ⁻¹²	1.33 x 10 ⁻¹¹	3.04 x 10 ⁻¹¹
OH		1.25 x 10 ⁻⁷	7.39 x 10 ⁻⁷	3.26 x 10 ⁻⁶	1.14 x 10 ⁻⁵	3.36 x 10 ⁻⁵	8.53 x 10 ⁻⁵
H		2.22 x 10 ⁻¹⁴	9.84 x 10 ⁻¹³	2.33 x 10 ⁻¹¹	3.42 x 10 ⁻¹⁰	3.43 x 10 ⁻⁹	2.54 x 10 ⁻⁸
H ₂		9.69 x 10 ⁻¹¹	1.46 x 10 ⁻⁹	1.41 x 10 ⁻⁸	9.64 x 10 ⁻⁸	5.02 x 10 ⁻⁷	2.10 x 10 ⁻⁶
H ₂ O ₂		1.53 x 10 ⁻¹⁰	4.95 x 10 ⁻¹⁰	1.32 x 10 ⁻⁹	3.05 x 10 ⁻⁹	6.27 x 10 ⁻⁹	1.17 x 10 ⁻⁸
Σ P(K) (atm)		8.64 x 10 ⁻⁹	1.00 x 10 ⁻⁷	7.51 x 10 ⁻⁷	3.22 x 10 ⁻⁶	1.07 x 10 ⁻⁵	3.00 x 10 ⁻⁵
Σ P(K-O) (atm)		2.91 x 10 ⁻¹²	4.27 x 10 ⁻¹¹	4.02 x 10 ⁻¹⁰	2.32 x 10 ⁻⁹	1.22 x 10 ⁻⁸	6.40 x 10 ⁻⁸
Σ P(Si) (atm)		8.92 x 10 ⁻¹²	1.48 x 10 ⁻¹⁰	1.54 x 10 ⁻⁹	1.11 x 10 ⁻⁸	6.07 x 10 ⁻⁸	2.64 x 10 ⁻⁷
Σ P(Si-O) (atm)		6.71 x 10 ⁻²²	3.83 x 10 ⁻¹⁹	7.52 x 10 ⁻¹⁷	6.49 x 10 ⁻¹⁵	2.95 x 10 ⁻¹³	7.98 x 10 ⁻¹²

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
K₂Si₂O₅(c,l)						
K ₂ O(590) ^a	0 ^b	0	0	0	0	0
K ₂ O ₂ (818)	0	0	0	0	0	0
KOH(679)	0	0	0	0	0	0
KO ₂ (808)	0	0	0	0	0	0
K(336)	0	0	0	0	0	0
K ₂ SiO ₃ (1249)	0	0	0	0	0	0
K ₂ Si ₂ O ₅ (1318)	1	1	1	0	0	0
K ₂ Si ₄ O ₉ (1043)	0	0	0	1	1	1
SiO ₂ (1696)	1	1	1	1	1	1
Si(1685)	0	0	0	0	0	0

Notes: $\Sigma P(K)$ = Sum of vapor pressures of species containing K, O, and H
 $\Sigma P(K-O)$ = Sum of vapor pressures of species containing K and O only
 $\Sigma P(Si)$ = Sum of vapor pressures of species containing Si, O, and H
 $\Sigma P(Si-O)$ = Sum of vapor pressures of species containing Si and O only
a = Melting point in degrees Kelvin
b = One (1) and zero (0) represent the presence and absence of the solid phase respectively.

Table 1 (Continued)

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
	Na₂Al₂O₄(c)					
Ar	0.70000	0.70000	0.70000	0.69999	0.69996	0.69986
O ₂	0.05000	0.05000	0.05000	0.05000	0.04999	0.04997
H ₂ O	0.25000	0.25000	0.24999	0.24998	0.24991	0.24973
Na	2.62 x 10 ⁻¹³	1.86 x 10 ⁻¹¹	6.73 x 10 ⁻¹⁰	1.39 x 10 ⁻⁸	1.85 x 10 ⁻⁷	1.73 x 10 ⁻⁶
NaO	2.52 x 10 ⁻¹⁵	1.77 x 10 ⁻¹³	6.34 x 10 ⁻¹²	1.30 x 10 ⁻¹⁰	1.72 x 10 ⁻⁹	1.60 x 10 ⁻⁸
NaO ₂	2.19 x 10 ⁻¹¹	2.75 x 10 ⁻¹⁰	2.35 x 10 ⁻⁹	1.43 x 10 ⁻⁸	6.70 x 10 ⁻⁸	2.52 x 10 ⁻⁷
Na ₂	3.55 x 10 ⁻²⁶	7.79 x 10 ⁻²³	5.12 x 10 ⁻²⁰	1.21 x 10 ⁻¹⁷	1.29 x 10 ⁻¹⁵	7.27 x 10 ⁻¹⁴
Na ₂ O	1.39 x 10 ⁻²¹	5.63 x 10 ⁻¹⁹	9.10 x 10 ⁻¹⁷	6.62 x 10 ⁻¹⁵	2.56 x 10 ⁻¹³	6.01 x 10 ⁻¹²
Na ₂ O ₂	4.94 x 10 ⁻²¹	6.27 x 10 ⁻¹⁹	3.85 x 10 ⁻¹⁷	1.24 x 10 ⁻¹⁵	2.38 x 10 ⁻¹⁴	3.06 x 10 ⁻¹³
NaOH	7.36 x 10 ⁻⁸	7.23 x 10 ⁻⁷	5.07 x 10 ⁻⁶	2.62 x 10 ⁻⁵	1.06 x 10 ⁻⁴	3.55 x 10 ⁻⁴
Na ₂ (OH) ₂	5.00 x 10 ⁻¹²	4.51 x 10 ⁻¹¹	3.08 x 10 ⁻¹⁰	1.55 x 10 ⁻⁹	6.15 x 10 ⁻⁹	2.00 x 10 ⁻⁸
Al	1.23 x 10 ⁻⁴⁵	4.20 x 10 ⁻⁴⁰	1.61 x 10 ⁻³⁵	1.19 x 10 ⁻³¹	2.46 x 10 ⁻²⁸	1.81 x 10 ⁻²⁵
AlO	3.44 x 10 ⁻³⁵	6.50 x 10 ⁻³¹	2.23 x 10 ⁻²⁷	2.16 x 10 ⁻²⁴	7.74 x 10 ⁻²²	1.25 x 10 ⁻¹⁹
AlO ₂	2.74 x 10 ⁻³¹	1.02 x 10 ⁻²⁷	9.10 x 10 ⁻²⁵	2.83 x 10 ⁻²²	3.83 x 10 ⁻²⁰	2.68 x 10 ⁻¹⁸
Al ₂ O	1.44 x 10 ⁻⁵⁸	2.52 x 10 ⁻⁵¹	2.42 x 10 ⁻⁴⁵	2.71 x 10 ⁻⁴⁰	5.67 x 10 ⁻³⁶	3.08 x 10 ⁻³²
Al ₂ O ₂	5.68 x 10 ⁻⁵⁰	6.69 x 10 ⁻⁴⁴	6.78 x 10 ⁻³⁹	1.14 x 10 ⁻³⁴	4.68 x 10 ⁻³¹	6.23 x 10 ⁻²⁸
AlOH	1.12 x 10 ⁻³⁰	6.17 x 10 ⁻²⁷	7.60 x 10 ⁻²⁴	3.10 x 10 ⁻²¹	5.31 x 10 ⁻¹⁹	4.54 x 10 ⁻¹⁷
Al(OH) ₂	1.54 x 10 ⁻²⁴	7.93 x 10 ⁻²²	1.37 x 10 ⁻¹⁹	1.06 x 10 ⁻¹⁷	4.40 x 10 ⁻¹⁶	1.11 x 10 ⁻¹⁴
Al(OH) ₃	5.62 x 10 ⁻¹⁶	1.14 x 10 ⁻¹⁴	1.34 x 10 ⁻¹³	1.08 x 10 ⁻¹²	6.50 x 10 ⁻¹²	3.08 x 10 ⁻¹¹
AlO(OH)	9.71 x 10 ⁻²⁶	6.98 x 10 ⁻²³	1.58 x 10 ⁻²⁰	1.54 x 10 ⁻¹⁸	7.70 x 10 ⁻¹⁷	2.27 x 10 ⁻¹⁵
AlHO	6.11 x 10 ⁻⁴¹	2.62 x 10 ⁻³⁶	1.79 x 10 ⁻³²	3.13 x 10 ⁻²⁹	1.87 x 10 ⁻²⁶	4.72 x 10 ⁻²⁴
O	3.48 x 10 ⁻¹¹	5.53 x 10 ⁻¹⁰	5.56 x 10 ⁻⁹	3.92 x 10 ⁻⁸	2.10 x 10 ⁻⁷	8.99 x 10 ⁻⁷
O ₃	9.73 x 10 ⁻¹⁴	4.49 x 10 ⁻¹³	1.67 x 10 ⁻¹²	5.09 x 10 ⁻¹²	1.33 x 10 ⁻¹¹	3.04 x 10 ⁻¹¹
OH	1.25 x 10 ⁻⁷	7.39 x 10 ⁻⁷	3.26 x 10 ⁻⁶	1.14 x 10 ⁻⁵	3.36 x 10 ⁻⁵	8.53 x 10 ⁻⁵
H	2.22 x 10 ⁻¹⁴	9.84 x 10 ⁻¹³	2.33 x 10 ⁻¹¹	3.42 x 10 ⁻¹⁰	3.43 x 10 ⁻⁹	2.54 x 10 ⁻⁸
H ₂	9.69 x 10 ⁻¹¹	1.46 x 10 ⁻⁹	1.41 x 10 ⁻⁸	9.64 x 10 ⁻⁸	5.02 x 10 ⁻⁷	2.10 x 10 ⁻⁶
H ₂ O ₂	1.53 x 10 ⁻¹⁰	4.95 x 10 ⁻¹⁰	1.32 x 10 ⁻⁹	3.05 x 10 ⁻⁹	6.26 x 10 ⁻⁹	1.17 x 10 ⁻⁸
Σ P(Na) (atm)	7.36 x 10 ⁻⁸	7.23 x 10 ⁻⁷	5.07 x 10 ⁻⁶	2.62 x 10 ⁻⁵	1.06 x 10 ⁻⁴	3.57 x 10 ⁻⁴
Σ P(Na-O) (atm)	2.22 x 10 ⁻¹¹	2.94 x 10 ⁻¹⁰	3.03 x 10 ⁻⁹	2.84 x 10 ⁻⁸	2.54 x 10 ⁻⁷	2.00 x 10 ⁻⁶
Σ P(Al) (atm)	5.62 x 10 ⁻¹⁶	1.14 x 10 ⁻¹⁴	1.34 x 10 ⁻¹³	1.08 x 10 ⁻¹²	6.50 x 10 ⁻¹²	3.08 x 10 ⁻¹¹
Σ P(Al-O) (atm)	2.74 x 10 ⁻³¹	1.02 x 10 ⁻²⁷	9.12 x 10 ⁻²⁵	2.85 x 10 ⁻²²	3.91 x 10 ⁻²⁰	2.81 x 10 ⁻¹⁸

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
	Na₂Al₂O₄(c)					
Na ₂ O(1405) ^a	0 ^b	0	0	0	0	0
Na ₂ O ₂ (948)	0	0	0	0	0	0
NaOH(596)	0	0	0	0	0	0
NaO ₂ (800)	0	0	0	0	0	0
Na(370.98)	0	0	0	0	0	0
Na ₂ Al ₂ O ₄ (c)	1	1	1	1	1	1
Al ₂ O ₃ -α(2327)	1	1	1	1	1	1
Al(934)	0	0	0	0	0	0
Al(OH) ₃ (c)	0	0	0	0	0	0

Notes: $\Sigma P(\text{Na})$ = Sum of vapor pressures of species containing Na, O, and H

$\Sigma P(\text{Na-O})$ = Sum of vapor pressures of species containing Na and O only

$\Sigma P(\text{Al})$ = Sum of vapor pressures of species containing Al, O, and H

$\Sigma P(\text{Al-O})$ = Sum of vapor pressures of species containing Al and O only

a = Melting point in degrees Kelvin

b = One (1) and zero (0) represent the presence and absence of the solid phase respectively.

Species	Partial Pressure (atm)						
	T(K) =	1000	1100	1200	1300	1400	1500
Na ₂ Al ₂ Si ₂ O ₈ (c)							
Ar		0.70000	0.70000	0.70000	0.70000	0.69999	0.69998
O ₂		0.05000	0.05000	0.05000	0.05000	0.04999	0.04998
H ₂ O		0.25000	0.25000	0.25000	0.24999	0.24998	0.24995
Na		3.73 x 10 ⁻¹⁶	4.01 x 10 ⁻¹⁴	2.03 x 10 ⁻¹²	5.77 x 10 ⁻¹¹	1.03 x 10 ⁻⁹	1.25 x 10 ⁻⁸
NaO		3.59 x 10 ⁻¹⁸	3.62 x 10 ⁻¹⁶	1.91 x 10 ⁻¹⁴	5.38 x 10 ⁻¹³	9.59 x 10 ⁻¹²	1.16 x 10 ⁻¹⁰
NaO ₂		3.12 x 10 ⁻¹⁴	5.95 x 10 ⁻¹³	7.10 x 10 ⁻¹²	5.94 x 10 ⁻¹¹	3.74 x 10 ⁻¹⁰	1.83 x 10 ⁻⁹
Na ₂		7.19 x 10 ⁻³²	3.64 x 10 ⁻²⁸	4.66 x 10 ⁻²⁵	2.08 x 10 ⁻²²	4.04 x 10 ⁻²⁰	3.82 x 10 ⁻¹⁸
Na ₂ O		2.81 x 10 ⁻²⁷	2.63 x 10 ⁻²⁴	8.29 x 10 ⁻²²	1.14 x 10 ⁻¹⁹	8.00 x 10 ⁻¹⁸	3.16 x 10 ⁻¹⁶
Na ₂ O ₂		1.00 x 10 ⁻²⁶	2.93 x 10 ⁻²⁴	3.51 x 10 ⁻²²	2.12 x 10 ⁻²⁰	7.44 x 10 ⁻¹⁹	1.61 x 10 ⁻¹⁷
NaOH		1.05 x 10 ⁻¹⁰	1.56 x 10 ⁻⁹	1.53 x 10 ⁻⁸	1.08 x 10 ⁻⁷	5.93 x 10 ⁻⁷	2.57 x 10 ⁻⁶
Na ₂ (OH) ₂		1.01 x 10 ⁻¹⁷	2.11 x 10 ⁻¹⁶	2.81 x 10 ⁻¹⁵	2.67 x 10 ⁻¹⁴	1.92 x 10 ⁻¹³	1.05 x 10 ⁻¹²
Si		8.37 x 10 ⁻⁵⁴	2.60 x 10 ⁻⁴⁷	6.64 x 10 ⁻⁴²	2.47 x 10 ⁻³⁷	2.02 x 10 ⁻³³	4.91 x 10 ⁻³⁰
SiO		6.92 x 10 ⁻²⁹	5.03 x 10 ⁻²⁵	8.21 x 10 ⁻²²	4.24 x 10 ⁻¹⁹	8.86 x 10 ⁻¹⁷	8.98 x 10 ⁻¹⁵
SiO ₂		2.42 x 10 ⁻²²	1.61 x 10 ⁻¹⁹	3.62 x 10 ⁻¹⁷	3.50 x 10 ⁻¹⁵	1.74 x 10 ⁻¹³	5.12 x 10 ⁻¹²
SiOH		1.69 x 10 ⁻⁴⁵	2.85 x 10 ⁻⁴⁰	6.41 x 10 ⁻³⁶	3.05 x 10 ⁻³²	4.29 x 10 ⁻²⁹	2.28 x 10 ⁻²⁶
Si(OH) ₂		7.09 x 10 ⁻³³	2.59 x 10 ⁻²⁹	2.41 x 10 ⁻²⁶	7.79 x 10 ⁻²⁴	1.10 x 10 ⁻²¹	7.94 x 10 ⁻²⁰
Si(OH) ₃		2.03 x 10 ⁻²⁹	1.07 x 10 ⁻²⁶	2.00 x 10 ⁻²⁴	1.69 x 10 ⁻²²	7.58 x 10 ⁻²¹	2.05 x 10 ⁻¹⁹
Si(OH) ₄		1.91 x 10 ⁻¹⁵	1.22 x 10 ⁻¹⁴	5.84 x 10 ⁻¹⁴	2.22 x 10 ⁻¹³	7.02 x 10 ⁻¹³	1.92 x 10 ⁻¹²
SiO(OH)		1.15 x 10 ⁻²⁶	1.96 x 10 ⁻²³	9.56 x 10 ⁻²¹	1.79 x 10 ⁻¹⁸	1.57 x 10 ⁻¹⁶	7.53 x 10 ⁻¹⁵
SiO(OH) ₂		3.22 x 10 ⁻¹²	6.23 x 10 ⁻¹¹	7.39 x 10 ⁻¹⁰	5.99 x 10 ⁻⁹	3.60 x 10 ⁻⁸	1.70 x 10 ⁻⁷
Al		1.23 x 10 ⁻⁴⁵	4.20 x 10 ⁻⁴⁰	1.61 x 10 ⁻³⁵	1.15 x 10 ⁻³¹	2.24 x 10 ⁻²⁸	1.57 x 10 ⁻²⁵
AlO		3.44 x 10 ⁻³⁵	6.50 x 10 ⁻³¹	2.23 x 10 ⁻²⁷	2.08 x 10 ⁻²⁴	7.03 x 10 ⁻²²	1.08 x 10 ⁻¹⁹
AlO ₂		2.74 x 10 ⁻³¹	1.02 x 10 ⁻²⁷	9.10 x 10 ⁻²⁵	2.72 x 10 ⁻²²	3.49 x 10 ⁻²⁰	2.32 x 10 ⁻¹⁸
Al ₂ O		1.44 x 10 ⁻⁵⁸	2.52 x 10 ⁻⁵¹	2.42 x 10 ⁻⁴⁵	2.52 x 10 ⁻⁴⁰	4.68 x 10 ⁻³⁶	2.31 x 10 ⁻³²
Al ₂ O ₂		5.68 x 10 ⁻⁵⁰	6.69 x 10 ⁻⁴⁴	6.78 x 10 ⁻³⁹	1.06 x 10 ⁻³⁴	3.87 x 10 ⁻³¹	4.66 x 10 ⁻²⁸
AlOH		1.12 x 10 ⁻³⁰	6.17 x 10 ⁻²⁷	7.60 x 10 ⁻²⁴	2.98 x 10 ⁻²¹	4.83 x 10 ⁻¹⁹	3.93 x 10 ⁻¹⁷
Al(OH) ₂		1.54 x 10 ⁻²⁴	7.93 x 10 ⁻²²	1.37 x 10 ⁻¹⁹	1.02 x 10 ⁻¹⁷	4.00 x 10 ⁻¹⁶	9.57 x 10 ⁻¹⁵
Al(OH) ₃		5.62 x 10 ⁻¹⁶	1.14 x 10 ⁻¹⁴	1.34 x 10 ⁻¹³	1.04 x 10 ⁻¹²	5.91 x 10 ⁻¹²	2.67 x 10 ⁻¹¹
AlO(OH)		9.71 x 10 ⁻²⁶	6.98 x 10 ⁻²³	1.58 x 10 ⁻²⁰	1.48 x 10 ⁻¹⁸	7.00 x 10 ⁻¹⁷	1.97 x 10 ⁻¹⁵
AlHO		6.11 x 10 ⁻⁴¹	2.62 x 10 ⁻³⁶	1.79 x 10 ⁻³²	3.02 x 10 ⁻²⁹	1.70 x 10 ⁻²⁶	4.09 x 10 ⁻²⁴
O		3.48 x 10 ⁻¹¹	5.53 x 10 ⁻¹⁰	5.56 x 10 ⁻⁹	3.92 x 10 ⁻⁸	2.10 x 10 ⁻⁷	8.99 x 10 ⁻⁷
O ₃		9.73 x 10 ⁻¹⁴	4.49 x 10 ⁻¹³	1.67 x 10 ⁻¹²	5.09 x 10 ⁻¹²	1.33 x 10 ⁻¹¹	3.04 x 10 ⁻¹¹

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
Na₂Al₂Si₂O₈(c)						
OH	1.25 x 10 ⁻⁷	7.39 x 10 ⁻⁷	3.26 x 10 ⁻⁶	1.14 x 10 ⁻⁵	3.36 x 10 ⁻⁵	8.53 x 10 ⁻⁵
H	2.22 x 10 ⁻¹⁴	9.84 x 10 ⁻¹³	2.33 x 10 ⁻¹¹	3.42 x 10 ⁻¹⁰	3.43 x 10 ⁻⁹	2.54 x 10 ⁻⁸
H ₂	9.69 x 10 ⁻¹¹	1.46 x 10 ⁻⁹	1.41 x 10 ⁻⁸	9.64 x 10 ⁻⁸	5.02 x 10 ⁻⁷	2.10 x 10 ⁻⁶
H ₂ O ₂	1.53 x 10 ⁻¹⁰	4.95 x 10 ⁻¹⁰	1.32 x 10 ⁻⁹	3.05 x 10 ⁻⁹	6.27 x 10 ⁻⁹	1.17 x 10 ⁻⁸
Σ P(Na) (atm)	1.05 x 10 ⁻¹⁰	1.56 x 10 ⁻⁹	1.53 x 10 ⁻⁸	1.08 x 10 ⁻⁷	5.94 x 10 ⁻⁷	2.59 x 10 ⁻⁶
Σ P(Na-O) (atm)	3.16 x 10 ⁻¹⁴	6.35 x 10 ⁻¹³	9.16 x 10 ⁻¹²	1.18 x 10 ⁻¹⁰	1.42 x 10 ⁻⁹	1.45 x 10 ⁻⁸
Σ P(Si) (atm)	3.22 x 10 ⁻¹²	6.23 x 10 ⁻¹¹	7.39 x 10 ⁻¹⁰	5.99 x 10 ⁻⁹	3.60 x 10 ⁻⁸	1.70 x 10 ⁻⁷
Σ P(Si-O) (atm)	2.42 x 10 ⁻²²	1.61 x 10 ⁻¹⁹	3.62 x 10 ⁻¹⁷	3.50 x 10 ⁻¹⁵	1.74 x 10 ⁻¹³	5.13 x 10 ⁻¹²
Σ P(Al) (atm)	5.62 x 10 ⁻¹⁶	1.14 x 10 ⁻¹⁴	1.34 x 10 ⁻¹³	1.04 x 10 ⁻¹²	5.91 x 10 ⁻¹²	2.67 x 10 ⁻¹¹
Σ P(Al-O) (atm)	2.74 x 10 ⁻³¹	1.02 x 10 ⁻²⁷	9.12 x 10 ⁻²⁵	2.74 x 10 ⁻²²	3.56 x 10 ⁻²⁰	2.43 x 10 ⁻¹⁸
Na ₂ O(1405)	0	0	0	0	0	0
Na ₂ O ₂ (948)	0	0	0	0	0	0
NaOH(596)	0	0	0	0	0	0
NaO ₂ (800)	0	0	0	0	0	0
Na ₂ SiO ₃ (1362)	0	0	0	0	0	0
Na ₂ Si ₂ O ₅ (1147)	0	0	0	0	0	0
Na ₂ Si ₃ O ₇ (c)	0	0	0	0	0	0
Na ₄ SiO ₄ (1393)	0	0	0	0	0	0
Na ₆ Si ₂ O ₇ (c)	0	0	0	0	0	0
SiO ₂ (1696)	0	0	0	0	0	0
Si(1685)	0	0	0	0	0	0
Al ₂ O ₃ -α(2327)	1	1	1	0	0	0
Al(934)	0	0	0	0	0	0
Na ₂ Al ₂ O ₄ (c)	0	0	0	0	0	0
Na ₂ Al ₂ Si ₂ O ₈ (c)	1	1	1	1	1	1
Na ₂ Al ₂ Si ₄ O ₁₂ (c)	0	0	0	0	0	0
Na ₂ Al ₂ Si ₆ O ₁₆ (c)	1	1	1	1	1	1
Al ₂ SiO ₅ (c)	0	0	0	0	0	0
Al ₂ Si ₂ O ₇ (c)	0	0	0	0	0	0
Al ₆ Si ₂ O ₁₃ (c)	0	0	0	1	1	1
Al(OH) ₃ (c)	0	0	0	0	0	0

For explanation of terms see notes for the previous Table.

Species	Partial Pressure (atm)						
	T(K) =	1000	1100	1200	1300	1400	1500
Na ₂ Ti ₂ O ₅ (c,l)							
Ar		0.70000	0.70000	0.70000	0.70000	0.69999	0.69996
O ₂		0.05000	0.05000	0.05000	0.05000	0.04999	0.04998
H ₂ O		0.25000	0.25000	0.25000	0.24999	0.24996	0.24990
Na		3.94 x 10 ⁻¹⁴	4.44 x 10 ⁻¹²	2.26 x 10 ⁻¹⁰	3.84 x 10 ⁻⁹	4.37 x 10 ⁻⁸	3.67 x 10 ⁻⁷
NaO		3.79 x 10 ⁻¹⁶	4.22 x 10 ⁻¹⁴	2.12 x 10 ⁻¹²	3.58 x 10 ⁻¹¹	4.05 x 10 ⁻¹⁰	3.39 x 10 ⁻⁹
NaO ₂		3.30 x 10 ⁻¹²	6.57 x 10 ⁻¹¹	7.89 x 10 ⁻¹⁰	3.95 x 10 ⁻⁹	1.58 x 10 ⁻⁸	5.36 x 10 ⁻⁸
Na ₂		8.02 x 10 ⁻²⁸	4.45 x 10 ⁻²⁴	5.76 x 10 ⁻²¹	9.22 x 10 ⁻¹⁹	7.21 x 10 ⁻¹⁷	3.29 x 10 ⁻¹⁵
Na ₂ O		3.14 x 10 ⁻²³	3.22 x 10 ⁻²⁰	1.02 x 10 ⁻¹⁷	5.02 x 10 ⁻¹⁶	1.43 x 10 ⁻¹⁴	2.72 x 10 ⁻¹³
Na ₂ O ₂		1.12 x 10 ⁻²²	3.58 x 10 ⁻²⁰	4.33 x 10 ⁻¹⁸	9.39 x 10 ⁻¹⁷	1.33 x 10 ⁻¹⁵	1.38 x 10 ⁻¹⁴
NaOH		1.11 x 10 ⁻⁸	1.73 x 10 ⁻⁷	1.70 x 10 ⁻⁶	7.20 x 10 ⁻⁶	2.50 x 10 ⁻⁵	7.55 x 10 ⁻⁵
Na ₂ (OH) ₂		1.13 x 10 ⁻¹³	2.58 x 10 ⁻¹²	3.47 x 10 ⁻¹¹	1.18 x 10 ⁻¹⁰	3.42 x 10 ⁻¹⁰	9.06 x 10 ⁻¹⁰
Ti		2.03 x 10 ⁻⁵⁶	9.59 x 10 ⁻⁵⁰	3.45 x 10 ⁻⁴⁴	2.35 x 10 ⁻³⁹	2.56 x 10 ⁻³⁵	7.70 x 10 ⁻³²
TiO		5.32 x 10 ⁻³⁸	2.54 x 10 ⁻³³	1.99 x 10 ⁻²⁹	5.30 x 10 ⁻²⁶	3.57 x 10 ⁻²³	9.67 x 10 ⁻²¹
TiO ₂		9.97 x 10 ⁻²⁴	9.32 x 10 ⁻²¹	2.75 x 10 ⁻¹⁸	4.57 x 10 ⁻¹⁶	2.87 x 10 ⁻¹⁴	9.90 x 10 ⁻¹³
TiOH		1.26 x 10 ⁻⁴⁶	3.25 x 10 ⁻⁴¹	1.04 x 10 ⁻³⁶	9.15 x 10 ⁻³³	1.72 x 10 ⁻²⁹	1.13 x 10 ⁻²⁶
Ti(OH) ₂		7.80 x 10 ⁻³³	4.46 x 10 ⁻²⁹	6.02 x 10 ⁻²⁶	3.67 x 10 ⁻²³	7.05 x 10 ⁻²¹	6.47 x 10 ⁻¹⁹
Ti(OH) ₃		1.05 x 10 ⁻²⁴	3.37 x 10 ⁻²²	4.17 x 10 ⁻²⁰	3.40 x 10 ⁻¹⁸	1.17 x 10 ⁻¹⁶	2.45 x 10 ⁻¹⁵
Ti(OH) ₄		2.15 x 10 ⁻²⁰	8.80 x 10 ⁻¹⁹	1.98 x 10 ⁻¹⁷	3.84 x 10 ⁻¹⁶	3.91 x 10 ⁻¹⁵	2.85 x 10 ⁻¹⁴
TiO(OH)		6.68 x 10 ⁻²⁹	1.97 x 10 ⁻²⁵	1.53 x 10 ⁻²²	5.79 x 10 ⁻²⁰	7.37 x 10 ⁻¹⁸	4.72 x 10 ⁻¹⁶
TiO(OH) ₂		2.37 x 10 ⁻²⁶	1.18 x 10 ⁻²³	2.09 x 10 ⁻²¹	2.30 x 10 ⁻¹⁹	1.02 x 10 ⁻¹⁷	2.64 x 10 ⁻¹⁶
O		3.48 x 10 ⁻¹¹	5.53 x 10 ⁻¹⁰	5.56 x 10 ⁻⁹	3.92 x 10 ⁻⁸	2.10 x 10 ⁻⁷	8.99 x 10 ⁻⁷
O ₃		9.73 x 10 ⁻¹⁴	4.49 x 10 ⁻¹³	1.67 x 10 ⁻¹²	5.09 x 10 ⁻¹²	1.33 x 10 ⁻¹¹	3.04 x 10 ⁻¹¹
OH		1.25 x 10 ⁻⁷	7.39 x 10 ⁻⁷	3.26 x 10 ⁻⁶	1.14 x 10 ⁻⁵	3.36 x 10 ⁻⁵	8.53 x 10 ⁻⁵
H		2.22 x 10 ⁻¹⁴	9.84 x 10 ⁻¹³	2.33 x 10 ⁻¹¹	3.42 x 10 ⁻¹⁰	3.43 x 10 ⁻⁹	2.54 x 10 ⁻⁸
H ₂		9.69 x 10 ⁻¹¹	1.46 x 10 ⁻⁹	1.41 x 10 ⁻⁸	9.64 x 10 ⁻⁸	5.02 x 10 ⁻⁷	2.10 x 10 ⁻⁶
H ₂ O ₂		1.53 x 10 ⁻¹⁰	4.95 x 10 ⁻¹⁰	1.32 x 10 ⁻⁹	3.05 x 10 ⁻⁹	6.27 x 10 ⁻⁹	1.17 x 10 ⁻⁸
Σ P(Na) (atm)		1.11 x 10 ⁻⁸	1.73 x 10 ⁻⁷	1.70 x 10 ⁻⁶	7.21 x 10 ⁻⁶	2.51 x 10 ⁻⁵	7.59 x 10 ⁻⁵
Σ P(Na-O) (atm)		3.34 x 10 ⁻¹²	7.02 x 10 ⁻¹¹	1.02 x 10 ⁻⁹	7.82 x 10 ⁻⁹	5.99 x 10 ⁻⁸	4.24 x 10 ⁻⁷
Σ P(Ti) (atm)		2.15 x 10 ⁻²⁰	8.89 x 10 ⁻¹⁹	2.26 x 10 ⁻¹⁷	8.45 x 10 ⁻¹⁶	3.27 x 10 ⁻¹⁴	1.02 x 10 ⁻¹²
Σ P(Ti-O) (atm)		9.97 x 10 ⁻²⁴	9.32 x 10 ⁻²¹	2.75 x 10 ⁻¹⁸	4.57 x 10 ⁻¹⁶	2.87 x 10 ⁻¹⁴	9.90 x 10 ⁻¹³

Species	Partial Pressure (atm)						
	T(K) =	1000	1100	1200	1300	1400	1500
		Na ₂ Ti ₂ O ₅ (c,l)					
Na ₂ O(1405) ^a	0 ^b	0	0	0	0	0	0
Na ₂ O ₂ (948)	0	0	0	0	0	0	0
NaOH(596)	0	0	0	0	0	0	0
NaO ₂ (800)	0	0	0	0	0	0	0
Na(370.98)	0	0	0	0	0	0	0
Na ₂ TiO ₃ (c)	0	0	0	0	0	0	0
Na ₂ Ti ₂ O ₅ (1258)	1	1	1	1	1	1	1
Na ₂ Ti ₃ O ₇ (c)	1	1	1	1	0	0	0
TiO ₂ -r(2130)	0	0	0	0	1	1	1
Ti ₄ O ₇ (1950)	0	0	0	0	0	0	0
Ti ₃ O ₅ (2050)	0	0	0	0	0	0	0
Ti ₂ O ₃ (2115)	0	0	0	0	0	0	0
TiO(2023)	0	0	0	0	0	0	0
Ti(1939)	0	0	0	0	0	0	0

Notes: $\Sigma P(\text{Na})$ = Sum of vapor pressures of species containing Na, O, and H
 $\Sigma P(\text{Na-O})$ = Sum of vapor pressures of species containing Na and O only
 $\Sigma P(\text{Ti})$ = Sum of vapor pressures of species containing Ti, O, and H
 $\Sigma P(\text{Ti-O})$ = Sum of vapor pressures of species containing Ti and O only
a = Melting point in degrees Kelvin
b = One (1) and zero (0) represent the presence and absence of the solid phase respectively.

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
MgSiO₃(c,l)						
Ar	0.70000	0.70000	0.70000	0.70000	0.69999	0.69998
O ₂	0.05000	0.05000	0.05000	0.05000	0.04999	0.04998
H ₂ O	0.25000	0.25000	0.25000	0.24999	0.24998	0.24995
Mg	3.93 x 10 ⁻²⁹	1.73 x 10 ⁻²⁵	1.85 x 10 ⁻²²	6.70 x 10 ⁻²⁰	1.04 x 10 ⁻¹⁷	8.06 x 10 ⁻¹⁶
MgO	1.13 x 10 ⁻²⁵	1.51 x 10 ⁻²²	6.08 x 10 ⁻²⁰	9.72 x 10 ⁻¹⁸	7.53 x 10 ⁻¹⁶	3.24 x 10 ⁻¹⁴
MgOH	8.81 x 10 ⁻²⁴	5.99 x 10 ⁻²¹	1.36 x 10 ⁻¹⁸	1.32 x 10 ⁻¹⁶	6.64 x 10 ⁻¹⁵	1.96 x 10 ⁻¹³
Mg(OH) ₂	7.79 x 10 ⁻¹⁵	2.64 x 10 ⁻¹³	4.97 x 10 ⁻¹²	5.96 x 10 ⁻¹¹	5.02 x 10 ⁻¹⁰	3.17 x 10 ⁻⁹
Si	9.84 x 10 ⁻⁵⁴	3.01 x 10 ⁻⁴⁷	7.62 x 10 ⁻⁴²	2.80 x 10 ⁻³⁷	2.26 x 10 ⁻³³	5.49 x 10 ⁻³⁰
SiO	8.13 x 10 ⁻²⁹	5.82 x 10 ⁻²⁵	9.43 x 10 ⁻²²	4.82 x 10 ⁻¹⁹	9.93 x 10 ⁻¹⁷	1.00 x 10 ⁻¹⁴
SiO ₂	2.85 x 10 ⁻²²	1.87 x 10 ⁻¹⁹	4.16 x 10 ⁻¹⁷	3.97 x 10 ⁻¹⁵	1.96 x 10 ⁻¹³	5.73 x 10 ⁻¹²
SiOH	1.98 x 10 ⁻⁴⁵	3.30 x 10 ⁻⁴⁰	7.36 x 10 ⁻³⁶	3.47 x 10 ⁻³²	4.82 x 10 ⁻²⁹	2.55 x 10 ⁻²⁶
Si(OH) ₂	8.34 x 10 ⁻³³	3.00 x 10 ⁻²⁹	2.76 x 10 ⁻²⁶	8.84 x 10 ⁻²⁴	1.23 x 10 ⁻²¹	8.89 x 10 ⁻²⁰
Si(OH) ₃	2.39 x 10 ⁻²⁹	1.24 x 10 ⁻²⁶	2.30 x 10 ⁻²⁴	1.92 x 10 ⁻²²	8.50 x 10 ⁻²¹	2.29 x 10 ⁻¹⁹
Si(OH) ₄	2.25 x 10 ⁻¹⁵	1.42 x 10 ⁻¹⁴	6.71 x 10 ⁻¹⁴	2.52 x 10 ⁻¹³	7.87 x 10 ⁻¹³	2.14 x 10 ⁻¹²
SiO(OH)	2.81 x 10 ⁻²⁴	2.89 x 10 ⁻²¹	9.35 x 10 ⁻¹⁹	1.23 x 10 ⁻¹⁶	7.94 x 10 ⁻¹⁵	2.95 x 10 ⁻¹³
SiO(OH) ₂	2.87 x 10 ⁻¹⁰	3.69 x 10 ⁻⁹	3.13 x 10 ⁻⁸	1.90 x 10 ⁻⁷	8.88 x 10 ⁻⁷	3.40 x 10 ⁻⁶
O	3.48 x 10 ⁻¹¹	5.53 x 10 ⁻¹⁰	5.56 x 10 ⁻⁹	3.92 x 10 ⁻⁸	2.10 x 10 ⁻⁷	8.99 x 10 ⁻⁷
O ₃	9.73 x 10 ⁻¹⁴	4.49 x 10 ⁻¹³	1.67 x 10 ⁻¹²	5.09 x 10 ⁻¹²	1.33 x 10 ⁻¹¹	3.04 x 10 ⁻¹¹
OH	1.25 x 10 ⁻⁷	7.39 x 10 ⁻⁷	3.26 x 10 ⁻⁶	1.14 x 10 ⁻⁵	3.36 x 10 ⁻⁵	8.53 x 10 ⁻⁵
H	2.22 x 10 ⁻¹⁴	9.84 x 10 ⁻¹³	2.33 x 10 ⁻¹¹	3.42 x 10 ⁻¹⁰	3.43 x 10 ⁻⁹	2.54 x 10 ⁻⁸
H ₂	9.69 x 10 ⁻¹¹	1.46 x 10 ⁻⁹	1.41 x 10 ⁻⁸	9.64 x 10 ⁻⁸	5.02 x 10 ⁻⁷	2.10 x 10 ⁻⁶
H ₂ O ₂	1.53 x 10 ⁻¹⁰	4.95 x 10 ⁻¹⁰	1.32 x 10 ⁻⁹	3.05 x 10 ⁻⁹	6.27 x 10 ⁻⁹	1.17 x 10 ⁻⁸
Σ P(Mg) (atm)	7.79 x 10 ⁻¹⁵	2.64 x 10 ⁻¹³	4.97 x 10 ⁻¹²	5.96 x 10 ⁻¹¹	5.02 x 10 ⁻¹⁰	3.17 x 10 ⁻⁹
Σ P(Mg-O) (atm)	1.13 x 10 ⁻²⁵	1.52 x 10 ⁻²²	6.10 x 10 ⁻²⁰	9.78 x 10 ⁻¹⁸	7.63 x 10 ⁻¹⁶	3.32 x 10 ⁻¹⁴
Σ P(Si) (atm)	2.87 x 10 ⁻¹⁰	3.69 x 10 ⁻⁹	3.13 x 10 ⁻⁸	1.90 x 10 ⁻⁷	8.88 x 10 ⁻⁷	3.40 x 10 ⁻⁶
Σ P(Si-O) (atm)	2.85 x 10 ⁻²²	1.87 x 10 ⁻¹⁹	4.16 x 10 ⁻¹⁷	3.97 x 10 ⁻¹⁵	1.96 x 10 ⁻¹³	5.74 x 10 ⁻¹²
Mg(923)	0	0	0	0	0	0
Mg(3105)	0	0	0	0	0	0
Mg(OH) ₂ (c)	0	0	0	0	0	0
MgSiO ₃ (1850)	1	1	1	1	1	1
Mg ₂ SiO ₄ (2171)	1	1	1	1	1	1
Si(1685)	0	0	0	0	0	0
SiO ₂ (1696)	0	0	0	0	0	0

Species	Partial Pressure (atm)						
	T(K) =	1000	1100	1200	1300	1400	1500
		MgTi ₂ O ₅ (s,l)					
Ar		0.70000	0.70000	0.70000	0.70000	0.69999	0.69998
O ₂		0.05000	0.05000	0.05000	0.05000	0.04999	0.04998
H ₂ O		0.25000	0.25000	0.25000	0.24999	0.24998	0.24995
Mg		4.96 x 10 ⁻²⁹	2.01 x 10 ⁻²⁵	2.01 x 10 ⁻²²	6.81 x 10 ⁻²⁰	9.86 x 10 ⁻¹⁸	7.23 x 10 ⁻¹⁶
MgO		1.43 x 10 ⁻²⁵	1.76 x 10 ⁻²²	6.60 x 10 ⁻²⁰	9.87 x 10 ⁻¹⁸	7.16 x 10 ⁻¹⁶	2.91 x 10 ⁻¹⁴
MgOH		1.11 x 10 ⁻²³	6.97 x 10 ⁻²¹	1.47 x 10 ⁻¹⁸	1.34 x 10 ⁻¹⁶	6.32 x 10 ⁻¹⁵	1.76 x 10 ⁻¹³
Mg(OH) ₂		9.84 x 10 ⁻¹⁵	3.08 x 10 ⁻¹³	5.40 x 10 ⁻¹²	6.06 x 10 ⁻¹¹	4.78 x 10 ⁻¹⁰	2.84 x 10 ⁻⁹
Ti		2.86 x 10 ⁻⁵⁶	1.36 x 10 ⁻⁴⁹	4.92 x 10 ⁻⁴⁴	2.44 x 10 ⁻³⁹	2.56 x 10 ⁻³⁵	7.70 x 10 ⁻³²
TiO		7.49 x 10 ⁻³⁸	3.61 x 10 ⁻³³	2.83 x 10 ⁻²⁹	5.50 x 10 ⁻²⁶	3.57 x 10 ⁻²³	9.67 x 10 ⁻²¹
TiO ₂		1.40 x 10 ⁻²³	1.32 x 10 ⁻²⁰	3.91 x 10 ⁻¹⁸	4.75 x 10 ⁻¹⁶	2.87 x 10 ⁻¹⁴	9.90 x 10 ⁻¹³
TiOH		1.77 x 10 ⁻⁴⁶	4.61 x 10 ⁻⁴¹	1.48 x 10 ⁻³⁶	9.50 x 10 ⁻³³	1.72 x 10 ⁻²⁹	1.13 x 10 ⁻²⁶
Ti(OH) ₂		1.10 x 10 ⁻³²	6.34 x 10 ⁻²⁹	8.58 x 10 ⁻²⁶	3.81 x 10 ⁻²³	7.05 x 10 ⁻²¹	6.47 x 10 ⁻¹⁹
Ti(OH) ₃		1.48 x 10 ⁻²⁴	4.78 x 10 ⁻²²	5.94 x 10 ⁻²⁰	3.53 x 10 ⁻¹⁸	1.17 x 10 ⁻¹⁶	2.45 x 10 ⁻¹⁵
Ti(OH) ₄		3.03 x 10 ⁻²⁰	1.25 x 10 ⁻¹⁸	2.82 x 10 ⁻¹⁷	3.99 x 10 ⁻¹⁶	3.91 x 10 ⁻¹⁵	2.85 x 10 ⁻¹⁴
TiO(OH)		9.40 x 10 ⁻²⁹	2.80 x 10 ⁻²⁵	2.18 x 10 ⁻²²	6.02 x 10 ⁻²⁰	7.37 x 10 ⁻¹⁸	4.72 x 10 ⁻¹⁶
TiO(OH) ₂		3.34 x 10 ⁻²⁶	1.68 x 10 ⁻²³	2.98 x 10 ⁻²¹	2.39 x 10 ⁻¹⁹	1.02 x 10 ⁻¹⁷	2.64 x 10 ⁻¹⁶
O		3.48 x 10 ⁻¹¹	5.53 x 10 ⁻¹⁰	5.56 x 10 ⁻⁹	3.92 x 10 ⁻⁸	2.10 x 10 ⁻⁷	8.99 x 10 ⁻⁷
O ₃		9.73 x 10 ⁻¹⁴	4.49 x 10 ⁻¹³	1.67 x 10 ⁻¹²	5.09 x 10 ⁻¹²	1.33 x 10 ⁻¹¹	3.04 x 10 ⁻¹¹
OH		1.25 x 10 ⁻⁷	7.39 x 10 ⁻⁷	3.26 x 10 ⁻⁶	1.14 x 10 ⁻⁵	3.36 x 10 ⁻⁵	8.53 x 10 ⁻⁵
H		2.22 x 10 ⁻¹⁴	9.84 x 10 ⁻¹³	2.33 x 10 ⁻¹¹	3.42 x 10 ⁻¹⁰	3.43 x 10 ⁻⁹	2.54 x 10 ⁻⁸
H ₂		9.69 x 10 ⁻¹¹	1.46 x 10 ⁻⁹	1.41 x 10 ⁻⁸	9.64 x 10 ⁻⁸	5.02 x 10 ⁻⁷	2.10 x 10 ⁻⁶
H ₂ O ₂		1.53 x 10 ⁻¹⁰	4.95 x 10 ⁻¹⁰	1.32 x 10 ⁻⁹	3.05 x 10 ⁻⁹	6.27 x 10 ⁻⁹	1.17 x 10 ⁻⁸
Σ P(Mg) (atm)		9.84 x 10 ⁻¹⁵	3.08 x 10 ⁻¹³	5.40 x 10 ⁻¹²	6.06 x 10 ⁻¹¹	4.78 x 10 ⁻¹⁰	2.84 x 10 ⁻⁹
Σ P(Mg-O) (atm)		1.43 x 10 ⁻²⁵	1.76 x 10 ⁻²²	6.62 x 10 ⁻²⁰	9.94 x 10 ⁻¹⁸	7.26 x 10 ⁻¹⁶	2.98 x 10 ⁻¹⁴
Σ P(Ti) (atm)		3.03 x 10 ⁻²⁰	1.26 x 10 ⁻¹⁸	3.22 x 10 ⁻¹⁷	8.78 x 10 ⁻¹⁶	3.27 x 10 ⁻¹⁴	1.02 x 10 ⁻¹²
Σ P(Ti-O) (atm)		1.40 x 10 ⁻²³	1.32 x 10 ⁻²⁰	3.91 x 10 ⁻¹⁸	4.75 x 10 ⁻¹⁶	2.87 x 10 ⁻¹⁴	9.90 x 10 ⁻¹³

Species	Partial Pressure (atm)						
	T(K) =	1000	1100	1200	1300	1400	1500
		MgTi ₂ O ₅ (c,l)					
Mg(923) ^a	0 ^b	0	0	0	0	0	0
MgO(3105)	0	0	0	0	0	0	0
Mg(OH) ₂ (c)	0	0	0	0	0	0	0
MgTiO ₃ (1903)	0	0	0	0	0	0	0
MgTi ₂ O ₅ (1963)	1	1	1	1	1	1	1
Mg ₂ TiO ₄ (2005)	0	0	0	0	0	0	0
Ti(1939)	0	0	0	0	0	0	0
TiO ₂ -r(2130)	1	1	1	1	1	1	1
Ti ₄ O ₇ (1950)	0	0	0	0	0	0	0
Ti ₃ O ₅ (2050)	0	0	0	0	0	0	0
Ti ₂ O ₃ (2115)	0	0	0	0	0	0	0
TiO(2023)	0	0	0	0	0	0	0

Notes: $\Sigma P(\text{Mg})$ = Sum of vapor pressures of species containing Mg, O, and H

$\Sigma P(\text{Mg-O})$ = Sum of vapor pressures of species containing Mg and O only

$\Sigma P(\text{Ti})$ = Sum of vapor pressures of species containing Ti, O, and H

$\Sigma P(\text{Ti-O})$ = Sum of vapor pressures of species containing Ti and O only

a = Melting point in degrees Kelvin

b = One (1) and zero (0) represent the presence and absence of the solid phase respectively.

APPENDIX B

CALCULATED PARTIAL PRESSURES OF CHLORIDE SPECIES UNDER COAL GASIFICATION CONDITIONS

**CALCULATED PARTIAL PRESSURES OF SPECIES OVER METAL OXIDES IN THE
PRESENCE OF TEXACO COAL GAS MIXTURE CONTAINING 300 PPM HCl
AT 1 ATM TOTAL PRESSURE**

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
Al₂O₃-α(c,l)						
Al	6.68 x 10 ⁻³¹	2.93 x 10 ⁻²⁷	2.98 x 10 ⁻²⁴	1.03 x 10 ⁻²¹	1.55 x 10 ⁻¹⁹	1.19 x 10 ⁻¹⁷
Al(OH)Cl	8.32 x 10 ⁻¹⁷	3.12 x 10 ⁻¹⁵	6.03 x 10 ⁻¹⁴	7.32 x 10 ⁻¹³	6.19 x 10 ⁻¹²	3.90 x 10 ⁻¹¹
Al(OH) ₂	4.52 x 10 ⁻²⁰	6.25 x 10 ⁻¹⁸	3.55 x 10 ⁻¹⁶	1.07 x 10 ⁻¹⁴	1.97 x 10 ⁻¹³	2.44 x 10 ⁻¹²
Al(OH) ₂ Cl	5.27 x 10 ⁻¹⁴	4.33 x 10 ⁻¹³	2.37 x 10 ⁻¹²	9.93 x 10 ⁻¹²	3.37 x 10 ⁻¹¹	9.70 x 10 ⁻¹¹
Al(OH) ₃	1.21 x 10 ⁻¹⁶	3.02 x 10 ⁻¹⁵	4.14 x 10 ⁻¹⁴	3.74 x 10 ⁻¹³	2.45 x 10 ⁻¹²	1.25 x 10 ⁻¹¹
AlC	1.55 x 10 ⁻⁴⁷	6.80 x 10 ⁻⁴³	4.64 x 10 ⁻³⁹	8.14 x 10 ⁻³⁶	4.89 x 10 ⁻³³	1.25 x 10 ⁻³⁰
AlCl	3.31 x 10 ⁻²²	6.35 x 10 ⁻²⁰	4.77 x 10 ⁻¹⁸	1.83 x 10 ⁻¹⁶	4.16 x 10 ⁻¹⁵	6.19 x 10 ⁻¹⁴
AlCl ₂	2.58 x 10 ⁻²⁴	2.13 x 10 ⁻²²	8.00 x 10 ⁻²¹	1.71 x 10 ⁻¹⁹	2.36 x 10 ⁻¹⁸	2.28 x 10 ⁻¹⁷
AlCl ₃	1.20 x 10 ⁻¹⁸	5.89 x 10 ⁻¹⁸	2.14 x 10 ⁻¹⁷	6.38 x 10 ⁻¹⁷	1.63 x 10 ⁻¹⁶	3.68 x 10 ⁻¹⁶
AlH	6.93 x 10 ⁻³⁰	1.33 x 10 ⁻²⁶	6.77 x 10 ⁻²⁴	1.31 x 10 ⁻²¹	1.19 x 10 ⁻¹⁹	5.87 x 10 ⁻¹⁸
AlHCl	1.99 x 10 ⁻²⁷	6.72 x 10 ⁻²⁵	8.06 x 10 ⁻²³	4.60 x 10 ⁻²¹	1.47 x 10 ⁻¹⁹	2.94 x 10 ⁻¹⁸
AlHCl ₂	8.42 x 10 ⁻²⁷	5.21 x 10 ⁻²⁵	1.54 x 10 ⁻²³	2.70 x 10 ⁻²²	3.15 x 10 ⁻²¹	2.65 x 10 ⁻²⁰
AlHO	2.43 x 10 ⁻³¹	6.15 x 10 ⁻²⁸	3.94 x 10 ⁻²⁵	9.27 x 10 ⁻²³	9.93 x 10 ⁻²¹	5.67 x 10 ⁻¹⁹
AlH ₂	3.39 x 10 ⁻³²	5.94 x 10 ⁻²⁹	2.77 x 10 ⁻²⁶	5.00 x 10 ⁻²⁴	4.27 x 10 ⁻²²	2.00 x 10 ⁻²⁰
AlH ₂ Cl	3.55 x 10 ⁻²⁹	7.03 x 10 ⁻²⁷	5.40 x 10 ⁻²⁵	2.12 x 10 ⁻²³	4.95 x 10 ⁻²²	7.56 x 10 ⁻²¹
AlH ₃	1.16 x 10 ⁻³⁴	1.35 x 10 ⁻³¹	4.51 x 10 ⁻²⁹	6.15 x 10 ⁻²⁷	4.14 x 10 ⁻²⁵	1.59 x 10 ⁻²³
AlN	6.14 x 10 ⁻⁴³	2.22 x 10 ⁻³⁸	1.31 x 10 ⁻³⁴	2.01 x 10 ⁻³¹	1.08 x 10 ⁻²⁸	2.49 x 10 ⁻²⁶
AlO	2.81 x 10 ⁻³⁰	1.24 x 10 ⁻²⁶	1.27 x 10 ⁻²³	4.43 x 10 ⁻²¹	6.64 x 10 ⁻¹⁹	5.06 x 10 ⁻¹⁷
AlO(OH)	5.83 x 10 ⁻²⁶	4.48 x 10 ⁻²³	1.07 x 10 ⁻²⁰	1.08 x 10 ⁻¹⁸	5.56 x 10 ⁻¹⁷	1.68 x 10 ⁻¹⁵
AlOCl	2.40 x 10 ⁻²¹	3.40 x 10 ⁻¹⁹	2.00 x 10 ⁻¹⁷	6.23 x 10 ⁻¹⁶	1.18 x 10 ⁻¹⁴	1.51 x 10 ⁻¹³
AlOCl ₂	4.41 x 10 ⁻¹¹	2.19 x 10 ⁻¹⁰	8.00 x 10 ⁻¹⁰	2.38 x 10 ⁻⁹	6.03 x 10 ⁻⁹	1.35 x 10 ⁻⁸
AlOH	4.48 x 10 ⁻²¹	1.45 x 10 ⁻¹⁸	1.67 x 10 ⁻¹⁶	9.17 x 10 ⁻¹⁵	2.82 x 10 ⁻¹³	5.45 x 10 ⁻¹²
AlOHCl ₂	6.94 x 10 ⁻¹⁶	4.48 x 10 ⁻¹⁵	2.02 x 10 ⁻¹⁴	7.22 x 10 ⁻¹⁴	2.15 x 10 ⁻¹³	5.50 x 10 ⁻¹³
AlO ₂	3.36 x 10 ⁻³⁶	5.34 x 10 ⁻³²	1.60 x 10 ⁻²⁸	1.38 x 10 ⁻²⁵	4.47 x 10 ⁻²³	6.66 x 10 ⁻²¹
Al ₂ Cl ₆	1.80 x 10 ⁻³⁷	1.24 x 10 ⁻³⁶	5.81 x 10 ⁻³⁶	2.18 x 10 ⁻³⁵	6.88 x 10 ⁻³⁵	1.88 x 10 ⁻³⁴
Al ₂ O	6.34 x 10 ⁻³⁹	3.37 x 10 ⁻³⁴	2.55 x 10 ⁻³⁰	4.83 x 10 ⁻²⁷	3.07 x 10 ⁻²⁴	8.14 x 10 ⁻²²
Al ₂ O ₂	3.77 x 10 ⁻⁴⁰	2.44 x 10 ⁻³⁵	2.20 x 10 ⁻³¹	4.81 x 10 ⁻²⁸	3.44 x 10 ⁻²⁵	1.01 x 10 ⁻²²

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
Al₂O₃-α(c,l)						
C	1.46 x 10 ⁻³⁰	7.48 x 10 ⁻²⁸	1.35 x 10 ⁻²⁵	1.10 x 10 ⁻²³	4.78 x 10 ⁻²²	1.27 x 10 ⁻²⁰
CCl	3.19 x 10 ⁻²⁷	2.25 x 10 ⁻²⁵	7.81 x 10 ⁻²⁴	1.58 x 10 ⁻²²	2.09 x 10 ⁻²¹	1.97 x 10 ⁻²⁰
CCl ₂	1.75 x 10 ⁻²⁸	3.44 x 10 ⁻²⁷	4.16 x 10 ⁻²⁶	3.45 x 10 ⁻²⁵	2.12 x 10 ⁻²⁴	1.03 x 10 ⁻²³
CCl ₃	2.08 x 10 ⁻³³	2.45 x 10 ⁻³²	1.95 x 10 ⁻³¹	1.14 x 10 ⁻³⁰	5.23 x 10 ⁻³⁰	1.98 x 10 ⁻²⁹
CCl ₄	4.41 x 10 ⁻³⁸	2.28 x 10 ⁻³⁷	9.29 x 10 ⁻³⁷	3.10 x 10 ⁻³⁶	8.84 x 10 ⁻³⁶	2.22 x 10 ⁻³⁵
CH	7.78 x 10 ⁻²⁷	9.92 x 10 ⁻²⁵	5.56 x 10 ⁻²³	1.68 x 10 ⁻²¹	3.14 x 10 ⁻²⁰	3.98 x 10 ⁻¹⁹
CHCl	8.33 x 10 ⁻²⁴	1.30 x 10 ⁻²²	1.28 x 10 ⁻²¹	8.83 x 10 ⁻²¹	4.66 x 10 ⁻²⁰	1.97 x 10 ⁻¹⁹
CHCl ₂	1.01 x 10 ⁻²³	3.59 x 10 ⁻²³	1.04 x 10 ⁻²²	2.57 x 10 ⁻²²	5.64 x 10 ⁻²²	1.12 x 10 ⁻²¹
CHCl ₃	4.93 x 10 ⁻²⁸	7.40 x 10 ⁻²⁸	1.05 x 10 ⁻²⁷	1.44 x 10 ⁻²⁷	1.91 x 10 ⁻²⁷	2.46 x 10 ⁻²⁷
CH ₂	6.32 x 10 ⁻²⁰	7.73 x 10 ⁻¹⁹	6.12 x 10 ⁻¹⁸	3.54 x 10 ⁻¹⁷	1.60 x 10 ⁻¹⁶	5.93 x 10 ⁻¹⁶
CH ₂ Cl	3.19 x 10 ⁻¹⁷	5.85 x 10 ⁻¹⁷	9.61 x 10 ⁻¹⁷	1.47 x 10 ⁻¹⁶	2.13 x 10 ⁻¹⁶	2.94 x 10 ⁻¹⁶
CH ₂ Cl ₂	2.57 x 10 ⁻¹⁹	1.32 x 10 ⁻¹⁹	7.63 x 10 ⁻²⁰	4.82 x 10 ⁻²⁰	3.29 x 10 ⁻²⁰	2.38 x 10 ⁻²⁰
CH ₂ O	2.26 x 10 ⁻⁷	1.99 x 10 ⁻⁷	1.75 x 10 ⁻⁷	1.58 x 10 ⁻⁷	1.44 x 10 ⁻⁷	1.32 x 10 ⁻⁷
CH ₃	1.18 x 10 ⁻¹⁰	9.77 x 10 ⁻¹¹	8.17 x 10 ⁻¹¹	7.04 x 10 ⁻¹¹	6.21 x 10 ⁻¹¹	5.59 x 10 ⁻¹¹
CH ₃ Cl	2.31 x 10 ⁻¹¹	4.41 x 10 ⁻¹²	1.09 x 10 ⁻¹²	3.38 x 10 ⁻¹³	1.24 x 10 ⁻¹³	5.25 x 10 ⁻¹⁴
CH ₄	1.22 x 10 ⁻³	8.20 x 10 ⁻⁵	8.40 x 10 ⁻⁶	1.22 x 10 ⁻⁶	2.36 x 10 ⁻⁷	5.68 x 10 ⁻⁸
CN	2.78 x 10 ⁻¹⁹	6.79 x 10 ⁻¹⁸	9.64 x 10 ⁻¹⁷	9.13 x 10 ⁻¹⁶	6.29 x 10 ⁻¹⁵	3.36 x 10 ⁻¹⁴
CNO	7.02 x 10 ⁻¹⁹	1.48 x 10 ⁻¹⁷	1.86 x 10 ⁻¹⁶	1.60 x 10 ⁻¹⁵	1.01 x 10 ⁻¹⁴	4.99 x 10 ⁻¹⁴
CN ₂	1.61 x 10 ⁻³⁰	1.96 x 10 ⁻²⁸	1.07 x 10 ⁻²⁶	3.16 x 10 ⁻²⁵	5.81 x 10 ⁻²⁴	7.27 x 10 ⁻²³
CO	2.26 x 10 ⁻¹	2.41 x 10 ⁻¹	2.52 x 10 ⁻¹	2.61 x 10 ⁻¹	2.69 x 10 ⁻¹	2.75 x 10 ⁻¹
COCl	3.23 x 10 ⁻¹⁷	2.82 x 10 ⁻¹⁶	1.72 x 10 ⁻¹⁵	7.91 x 10 ⁻¹⁵	2.93 x 10 ⁻¹⁴	9.12 x 10 ⁻¹⁴
COCl ₂	4.61 x 10 ⁻²⁰	1.27 x 10 ⁻¹⁹	3.00 x 10 ⁻¹⁹	6.24 x 10 ⁻¹⁹	1.18 x 10 ⁻¹⁸	2.04 x 10 ⁻¹⁸
COHCl	9.05 x 10 ⁻¹⁴	1.46 x 10 ⁻¹³	2.17 x 10 ⁻¹³	3.03 x 10 ⁻¹³	4.05 x 10 ⁻¹³	5.22 x 10 ⁻¹³
COOH	6.08 x 10 ⁻¹³	3.67 x 10 ⁻¹²	1.63 x 10 ⁻¹¹	5.72 x 10 ⁻¹¹	1.67 x 10 ⁻¹⁰	4.23 x 10 ⁻¹⁰
CO ₂	1.27 x 10 ⁻¹	1.12 x 10 ⁻¹	1.01 x 10 ⁻¹	9.16 x 10 ⁻²	8.43 x 10 ⁻²	7.82 x 10 ⁻²
Cl	9.42 x 10 ⁻¹³	1.05 x 10 ⁻¹¹	7.97 x 10 ⁻¹¹	4.38 x 10 ⁻¹⁰	1.93 x 10 ⁻⁹	6.94 x 10 ⁻⁹
ClHO	9.69 x 10 ⁻¹⁸	1.73 x 10 ⁻¹⁶	1.93 x 10 ⁻¹⁵	1.47 x 10 ⁻¹⁴	8.34 x 10 ⁻¹⁴	3.75 x 10 ⁻¹³
ClO	1.92 x 10 ⁻²⁴	3.05 x 10 ⁻²²	2.11 x 10 ⁻²⁰	7.57 x 10 ⁻¹⁹	1.62 x 10 ⁻¹⁷	2.31 x 10 ⁻¹⁶
ClO ₂	6.84 x 10 ⁻³⁹	2.05 x 10 ⁻³⁵	1.65 x 10 ⁻³²	4.68 x 10 ⁻³⁰	5.91 x 10 ⁻²⁸	3.90 x 10 ⁻²⁶
Cl ₂	5.54 x 10 ⁻¹⁸	4.58 x 10 ⁻¹⁷	2.71 x 10 ⁻¹⁶	1.22 x 10 ⁻¹⁵	4.44 x 10 ⁻¹⁵	1.37 x 10 ⁻¹⁴

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
Al₂O₃-α(c,l)						
Cl ₂ O	5.04 x 10 ⁻³⁶	2.01 x 10 ⁻³³	3.02 x 10 ⁻³¹	2.09 x 10 ⁻²⁹	7.89 x 10 ⁻²⁸	1.84 x 10 ⁻²⁶
H	1.09 x 10 ⁻⁹	1.21 x 10 ⁻⁸	8.98 x 10 ⁻⁸	4.93 x 10 ⁻⁷	2.13 x 10 ⁻⁶	7.57 x 10 ⁻⁶
HCN	3.25 x 10 ⁻⁷	2.72 x 10 ⁻⁷	2.31 x 10 ⁻⁷	2.03 x 10 ⁻⁷	1.82 x 10 ⁻⁷	1.67 x 10 ⁻⁷
HCO	7.73 x 10 ⁻¹²	4.13 x 10 ⁻¹¹	1.65 x 10 ⁻¹⁰	5.30 x 10 ⁻¹⁰	1.44 x 10 ⁻⁹	3.42 x 10 ⁻⁹
HCl	2.09 x 10 ⁻⁴	2.08 x 10 ⁻⁴	2.08 x 10 ⁻⁴	2.08 x 10 ⁻⁴	2.08 x 10 ⁻⁴	2.08 x 10 ⁻⁴
HNCO	7.62 x 10 ⁻⁹	8.59 x 10 ⁻⁹	9.40 x 10 ⁻⁹	1.02 x 10 ⁻⁸	1.08 x 10 ⁻⁸	1.15 x 10 ⁻⁸
HNO	2.25 x 10 ⁻¹⁹	1.15 x 10 ⁻¹⁷	3.03 x 10 ⁻¹⁶	4.80 x 10 ⁻¹⁵	5.11 x 10 ⁻¹⁴	3.96 x 10 ⁻¹³
HNO ₂	2.28 x 10 ⁻²⁴	3.05 x 10 ⁻²²	1.82 x 10 ⁻²⁰	5.74 x 10 ⁻¹⁹	1.10 x 10 ⁻¹⁷	1.41 x 10 ⁻¹⁶
HNO ₃	1.82 x 10 ⁻³⁶	2.43 x 10 ⁻³³	9.90 x 10 ⁻³¹	1.58 x 10 ⁻²⁸	1.22 x 10 ⁻²⁶	5.22 x 10 ⁻²⁵
HO ₂	7.94 x 10 ⁻²⁵	2.74 x 10 ⁻²²	3.56 x 10 ⁻²⁰	2.16 x 10 ⁻¹⁸	7.24 x 10 ⁻¹⁷	1.51 x 10 ⁻¹⁵
H ₂	2.32 x 10 ⁻¹	2.20 x 10 ⁻¹	2.09 x 10 ⁻¹	2.00 x 10 ⁻¹	1.93 x 10 ⁻¹	1.87 x 10 ⁻¹
H ₂ O	9.00 x 10 ⁻²	1.03 x 10 ⁻¹	1.14 x 10 ⁻¹	1.23 x 10 ⁻¹	1.31 x 10 ⁻¹	1.37 x 10 ⁻¹
H ₂ O ₂	8.27 x 10 ⁻²¹	5.59 x 10 ⁻¹⁹	1.86 x 10 ⁻¹⁷	3.57 x 10 ⁻¹⁶	4.45 x 10 ⁻¹⁵	3.94 x 10 ⁻¹⁴
N	1.76 x 10 ⁻²²	3.20 x 10 ⁻²⁰	2.47 x 10 ⁻¹⁸	9.78 x 10 ⁻¹⁷	2.29 x 10 ⁻¹⁵	3.54 x 10 ⁻¹⁴
NH	6.55 x 10 ⁻²⁰	3.91 x 10 ⁻¹⁸	1.18 x 10 ⁻¹⁶	2.09 x 10 ⁻¹⁵	2.47 x 10 ⁻¹⁴	2.10 x 10 ⁻¹³
NH ₂	1.93 x 10 ⁻¹³	1.39 x 10 ⁻¹²	7.13 x 10 ⁻¹²	2.83 x 10 ⁻¹¹	9.23 x 10 ⁻¹¹	2.57 x 10 ⁻¹⁰
NH ₂ NO ₂	2.39 x 10 ⁻³⁵	5.42 x 10 ⁻³³	5.01 x 10 ⁻³¹	2.30 x 10 ⁻²⁹	6.12 x 10 ⁻²⁸	1.05 x 10 ⁻²⁶
NH ₂ OH	1.78 x 10 ⁻¹⁸	1.60 x 10 ⁻¹⁷	9.92 x 10 ⁻¹⁷	4.62 x 10 ⁻¹⁶	1.72 x 10 ⁻¹⁵	5.40 x 10 ⁻¹⁵
NH ₃	3.72 x 10 ⁻⁵	1.88 x 10 ⁻⁵	1.05 x 10 ⁻⁵	6.37 x 10 ⁻⁶	4.16 x 10 ⁻⁶	2.87 x 10 ⁻⁶
NO	1.47 x 10 ⁻¹⁵	7.28 x 10 ⁻¹⁴	1.88 x 10 ⁻¹²	2.94 x 10 ⁻¹¹	3.08 x 10 ⁻¹⁰	2.36 x 10 ⁻⁹
NOCl	2.81 x 10 ⁻²⁵	2.61 x 10 ⁻²³	1.16 x 10 ⁻²¹	2.85 x 10 ⁻²⁰	4.44 x 10 ⁻¹⁹	4.79 x 10 ⁻¹⁸
NO ₂	5.97 x 10 ⁻²⁷	2.85 x 10 ⁻²⁴	4.90 x 10 ⁻²²	3.78 x 10 ⁻²⁰	1.54 x 10 ⁻¹⁸	3.89 x 10 ⁻¹⁷
NO ₂ Cl	1.57 x 10 ⁻³⁸	1.74 x 10 ⁻³⁵	6.11 x 10 ⁻³³	8.66 x 10 ⁻³¹	6.03 x 10 ⁻²⁹	2.38 x 10 ⁻²⁷
NO ₃	5.06 x 10 ⁻⁴⁴	6.79 x 10 ⁻⁴⁰	1.90 x 10 ⁻³⁶	1.55 x 10 ⁻³³	4.83 x 10 ⁻³¹	6.95 x 10 ⁻²⁹
N ₂	3.24 x 10 ⁻¹	3.23 x 10 ⁻¹	3.23 x 10 ⁻¹	3.23 x 10 ⁻¹	3.23 x 10 ⁻¹	3.23 x 10 ⁻¹
N ₂ O	7.76 x 10 ⁻²⁰	3.49 x 10 ⁻¹⁸	8.42 x 10 ⁻¹⁷	1.24 x 10 ⁻¹⁵	1.24 x 10 ⁻¹⁴	9.17 x 10 ⁻¹⁴
N ₂ O ₃	2.83 x 10 ⁻⁴⁸	4.39 x 10 ⁻⁴⁴	1.38 x 10 ⁻⁴⁰	1.24 x 10 ⁻³⁷	4.19 x 10 ⁻³⁵	6.45 x 10 ⁻³³
N ₂ O ₄	3.71 x 10 ⁻⁵⁹	4.93 x 10 ⁻⁵⁴	9.42 x 10 ⁻⁵⁰	3.92 x 10 ⁻⁴⁶	4.94 x 10 ⁻⁴³	2.40 x 10 ⁻⁴⁰
N ₂ O ₅	2.16 x 10 ⁻⁷⁴	5.53 x 10 ⁻⁶⁸	1.26 x 10 ⁻⁶²	4.24 x 10 ⁻⁵⁸	3.22 x 10 ⁻⁵⁴	7.39 x 10 ⁻⁵¹
N ₃	1.22 x 10 ⁻²⁷	1.45 x 10 ⁻²⁵	7.81 x 10 ⁻²⁴	2.29 x 10 ⁻²²	4.16 x 10 ⁻²¹	5.16 x 10 ⁻²⁰
O	5.25 x 10 ⁻²¹	1.52 x 10 ⁻¹⁸	1.71 x 10 ⁻¹⁶	9.30 x 10 ⁻¹⁵	2.85 x 10 ⁻¹³	5.54 x 10 ⁻¹²
OH	9.18 x 10 ⁻¹³	2.48 x 10 ⁻¹¹	3.86 x 10 ⁻¹⁰	3.91 x 10 ⁻⁹	2.83 x 10 ⁻⁸	1.56 x 10 ⁻⁷

Species	Partial Pressure (atm)					
T(K) =	1000	1100	1200	1300	1400	1500
Al ₂ O ₃ -α(c,l)						
O ₂	1.13 x 10 ⁻²¹	3.75 x 10 ⁻¹⁹	4.74 x 10 ⁻¹⁷	2.81 x 10 ⁻¹⁵	9.24 x 10 ⁻¹⁴	1.89 x 10 ⁻¹²
O ₃	3.32 x 10 ⁻⁴³	9.21 x 10 ⁻³⁹	4.87 x 10 ⁻³⁵	6.78 x 10 ⁻³²	3.33 x 10 ⁻²⁹	7.08 x 10 ⁻²⁷
Σ P(Al) (atm)	4.41 x 10 ⁻¹¹	2.20 x 10 ⁻¹⁰	8.02 x 10 ⁻¹⁰	2.39 x 10 ⁻⁹	6.08 x 10 ⁻⁹	1.36 x 10 ⁻⁸
Σ P(Al-O) (atm)	3.47 x 10 ⁻³⁰	1.54 x 10 ⁻²⁶	1.57 x 10 ⁻²³	5.47 x 10 ⁻²¹	8.19 x 10 ⁻¹⁹	6.24 x 10 ⁻¹⁷
Σ P(Al-Cl) (atm)	5.28 x 10 ⁻¹⁴	4.36 x 10 ⁻¹³	2.43 x 10 ⁻¹²	1.07 x 10 ⁻¹¹	3.99 x 10 ⁻¹¹	1.36 x 10 ⁻¹⁰
Al(934) ^a	0 ^b	0	0	0	0	0
C(5000)	0	0	0	0	0	0
Al ₄ C ₃ (c)	0	0	0	0	0	0
AlN(c)	0	0	0	0	0	0
Al ₂ O ₃ -α(2327)	1	1	1	1	1	1
AlOCl(c)	0	0	0	0	0	0
Al(OH) ₃ (c)	0	0	0	0	0	0
AlCl ₃ (466)	0	0	0	0	0	0

Notes: ΣP(Al) = Sum of vapor pressures of species containing Al, O, and H

ΣP(Al-O) = Sum of vapor pressures of species containing Al and O only

ΣP(Al-Cl) = Sum of vapor pressures of species containing Al and Cl only

a = Melting point in degrees Kelvin

b = One (1) and zero (0) represent the presence and absence of the solid phase respectively.

Species	Partial Pressure (atm)					
T(K) =	1000	1100	1200	1300	1400	1500
	MgO(c,l)					
C	1.94 x 10 ⁻³⁰	1.01 x 10 ⁻²⁷	1.83 x 10 ⁻²⁵	1.49 x 10 ⁻²³	6.49 x 10 ⁻²²	1.72 x 10 ⁻²⁰
CCl	5.15 x 10 ⁻²⁷	3.68 x 10 ⁻²⁵	1.28 x 10 ⁻²³	2.60 x 10 ⁻²²	3.44 x 10 ⁻²¹	3.25 x 10 ⁻²⁰
CCl ₂	3.44 x 10 ⁻²⁸	6.82 x 10 ⁻²⁷	8.26 x 10 ⁻²⁶	6.86 x 10 ⁻²⁵	4.24 x 10 ⁻²⁴	2.06 x 10 ⁻²³
CCl ₃	4.99 x 10 ⁻³³	5.88 x 10 ⁻³²	4.68 x 10 ⁻³¹	2.75 x 10 ⁻³⁰	1.27 x 10 ⁻²⁹	4.79 x 10 ⁻²⁹
CCl ₄	1.28 x 10 ⁻³⁷	6.62 x 10 ⁻³⁷	2.71 x 10 ⁻³⁶	9.06 x 10 ⁻³⁶	2.59 x 10 ⁻³⁵	6.54 x 10 ⁻³⁵
CH	1.23 x 10 ⁻²⁶	1.60 x 10 ⁻²⁴	8.97 x 10 ⁻²³	2.72 x 10 ⁻²¹	5.06 x 10 ⁻²⁰	6.41 x 10 ⁻¹⁹
CHCl	1.60 x 10 ⁻²³	2.54 x 10 ⁻²²	2.49 x 10 ⁻²¹	1.73 x 10 ⁻²⁰	9.10 x 10 ⁻²⁰	3.86 x 10 ⁻¹⁹
CHCl ₂	2.36 x 10 ⁻²³	8.47 x 10 ⁻²³	2.46 x 10 ⁻²²	6.09 x 10 ⁻²²	1.34 x 10 ⁻²¹	2.66 x 10 ⁻²¹
CHCl ₃	1.40 x 10 ⁻²⁷	2.11 x 10 ⁻²⁷	3.02 x 10 ⁻²⁷	4.14 x 10 ⁻²⁷	5.49 x 10 ⁻²⁷	7.08 x 10 ⁻²⁷
CH ₂	1.19 x 10 ⁻¹⁹	1.48 x 10 ⁻¹⁸	1.18 x 10 ⁻¹⁷	6.79 x 10 ⁻¹⁷	3.07 x 10 ⁻¹⁶	1.14 x 10 ⁻¹⁵
CH ₂ Cl	7.28 x 10 ⁻¹⁷	1.36 x 10 ⁻¹⁶	2.23 x 10 ⁻¹⁶	3.42 x 10 ⁻¹⁶	4.94 x 10 ⁻¹⁶	6.84 x 10 ⁻¹⁶
CH ₂ Cl ₂	7.13 x 10 ⁻¹⁹	3.72 x 10 ⁻¹⁹	2.15 x 10 ⁻¹⁹	1.36 x 10 ⁻¹⁹	9.27 x 10 ⁻²⁰	6.70 x 10 ⁻²⁰
CH ₂ O	4.50 x 10 ⁻⁷	4.00 x 10 ⁻⁷	3.53 x 10 ⁻⁷	3.17 x 10 ⁻⁷	2.89 x 10 ⁻⁷	2.66 x 10 ⁻⁷
CH ₃	2.62 x 10 ⁻¹⁰	2.23 x 10 ⁻¹⁰	1.87 x 10 ⁻¹⁰	1.61 x 10 ⁻¹⁰	1.41 x 10 ⁻¹⁰	1.27 x 10 ⁻¹⁰
CH ₃ Cl	6.26 x 10 ⁻¹¹	1.22 x 10 ⁻¹¹	3.03 x 10 ⁻¹²	9.35 x 10 ⁻¹³	3.43 x 10 ⁻¹³	1.45 x 10 ⁻¹³
CH ₄	3.23 x 10 ⁻³	2.23 x 10 ⁻⁴	2.29 x 10 ⁻⁵	3.33 x 10 ⁻⁶	6.39 x 10 ⁻⁷	1.53 x 10 ⁻⁷
CN	1.03 x 10 ⁻¹⁹	2.55 x 10 ⁻¹⁸	3.63 x 10 ⁻¹⁷	3.44 x 10 ⁻¹⁶	2.37 x 10 ⁻¹⁵	1.27 x 10 ⁻¹⁴
CNO	2.76 x 10 ⁻¹⁹	5.82 x 10 ⁻¹⁸	7.37 x 10 ⁻¹⁷	6.32 x 10 ⁻¹⁶	3.99 x 10 ⁻¹⁵	1.98 x 10 ⁻¹⁴
CN ₂	1.66 x 10 ⁻³¹	2.05 x 10 ⁻²⁹	1.12 x 10 ⁻²⁷	3.32 x 10 ⁻²⁶	6.09 x 10 ⁻²⁵	7.63 x 10 ⁻²⁴
CO	3.19 x 10 ⁻¹	3.42 x 10 ⁻¹	3.59 x 10 ⁻¹	3.72 x 10 ⁻¹	3.83 x 10 ⁻¹	3.92 x 10 ⁻¹
COCl	5.55 x 10 ⁻¹⁷	4.84 x 10 ⁻¹⁶	2.95 x 10 ⁻¹⁵	1.36 x 10 ⁻¹⁴	5.06 x 10 ⁻¹⁴	1.58 x 10 ⁻¹³
COCl ₂	9.63 x 10 ⁻²⁰	2.64 x 10 ⁻¹⁹	6.26 x 10 ⁻¹⁹	1.30 x 10 ⁻¹⁸	2.46 x 10 ⁻¹⁸	4.28 x 10 ⁻¹⁸
COHCl	1.85 x 10 ⁻¹³	2.98 x 10 ⁻¹³	4.44 x 10 ⁻¹³	6.22 x 10 ⁻¹³	8.32 x 10 ⁻¹³	1.07 x 10 ⁻¹²
COOH	1.08 x 10 ⁻¹²	6.51 x 10 ⁻¹²	2.89 x 10 ⁻¹¹	1.01 x 10 ⁻¹⁰	2.97 x 10 ⁻¹⁰	7.52 x 10 ⁻¹⁰
CO ₂	1.90 x 10 ⁻¹	1.67 x 10 ⁻¹	1.50 x 10 ⁻¹	1.37 x 10 ⁻¹	1.26 x 10 ⁻¹	1.17 x 10 ⁻¹
Cl	1.15 x 10 ⁻¹²	1.27 x 10 ⁻¹¹	9.64 x 10 ⁻¹¹	5.30 x 10 ⁻¹⁰	2.34 x 10 ⁻⁹	8.42 x 10 ⁻⁹
ClHO	1.49 x 10 ⁻¹⁷	2.62 x 10 ⁻¹⁶	2.91 x 10 ⁻¹⁵	2.22 x 10 ⁻¹⁴	1.26 x 10 ⁻¹³	5.67 x 10 ⁻¹³
ClO	2.48 x 10 ⁻²⁴	3.87 x 10 ⁻²²	2.68 x 10 ⁻²⁰	9.61 x 10 ⁻¹⁹	2.07 x 10 ⁻¹⁷	2.94 x 10 ⁻¹⁶
ClO ₂	9.40 x 10 ⁻³⁹	2.73 x 10 ⁻³⁵	2.19 x 10 ⁻³²	6.24 x 10 ⁻³⁰	7.90 x 10 ⁻²⁸	5.22 x 10 ⁻²⁶
Cl ₂	8.20 x 10 ⁻¹⁸	6.71 x 10 ⁻¹⁷	3.97 x 10 ⁻¹⁶	1.79 x 10 ⁻¹⁵	6.53 x 10 ⁻¹⁵	2.01 x 10 ⁻¹⁴
Cl ₂ O	7.94 x 10 ⁻³⁶	3.09 x 10 ⁻³³	4.64 x 10 ⁻³¹	3.22 x 10 ⁻²⁹	1.22 x 10 ⁻²⁷	2.84 x 10 ⁻²⁶

Species	Partial Pressure (atm)					
T(K) =	1000	1100	1200	1300	1400	1500
	MgO(c,l)					
H	1.29 x 10 ⁻⁹	1.44 x 10 ⁻⁸	1.07 x 10 ⁻⁷	5.86 x 10 ⁻⁷	2.53 x 10 ⁻⁶	9.00 x 10 ⁻⁶
HCN	1.43 x 10 ⁻⁷	1.22 x 10 ⁻⁷	1.04 x 10 ⁻⁷	9.11 x 10 ⁻⁸	8.18 x 10 ⁻⁸	7.47 x 10 ⁻⁸
HCO	1.30 x 10 ⁻¹¹	6.98 x 10 ⁻¹¹	2.79 x 10 ⁻¹⁰	8.97 x 10 ⁻¹⁰	2.44 x 10 ⁻⁹	5.79 x 10 ⁻⁹
HCl	3.02 x 10 ⁻⁴	3.00 x 10 ⁻⁴	3.00 x 10 ⁻⁴	3.00 x 10 ⁻⁴	3.00 x 10 ⁻⁴	3.00 x 10 ⁻⁴
HNCO	3.56 x 10 ⁻⁹	4.04 x 10 ⁻⁹	4.42 x 10 ⁻⁹	4.78 x 10 ⁻⁹	5.11 x 10 ⁻⁹	5.41 x 10 ⁻⁹
HNO	7.93 x 10 ⁻²⁰	3.98 x 10 ⁻¹⁸	1.05 x 10 ⁻¹⁶	1.67 x 10 ⁻¹⁵	1.77 x 10 ⁻¹⁴	1.37 x 10 ⁻¹³
HNO ₂	8.51 x 10 ⁻²⁵	1.11 x 10 ⁻²²	6.62 x 10 ⁻²¹	2.09 x 10 ⁻¹⁹	4.00 x 10 ⁻¹⁸	5.15 x 10 ⁻¹⁷
HNO ₃	7.24 x 10 ⁻³⁷	9.30 x 10 ⁻³⁴	3.78 x 10 ⁻³¹	6.03 x 10 ⁻²⁹	4.65 x 10 ⁻²⁷	2.00 x 10 ⁻²⁵
HO ₂	1.07 x 10 ⁻²⁴	3.59 x 10 ⁻²²	4.66 x 10 ⁻²⁰	2.83 x 10 ⁻¹⁸	9.48 x 10 ⁻¹⁷	1.97 x 10 ⁻¹⁵
H ₂	3.27 x 10 ⁻¹	3.12 x 10 ⁻¹	2.97 x 10 ⁻¹	2.83 x 10 ⁻¹	2.73 x 10 ⁻¹	2.64 x 10 ⁻¹
H ₂ O	1.35 x 10 ⁻¹	1.53 x 10 ⁻¹	1.70 x 10 ⁻¹	1.83 x 10 ⁻¹	1.94 x 10 ⁻¹	2.03 x 10 ⁻¹
H ₂ O ₂	1.32 x 10 ⁻²⁰	8.72 x 10 ⁻¹⁹	2.90 x 10 ⁻¹⁷	5.55 x 10 ⁻¹⁶	6.92 x 10 ⁻¹⁵	6.13 x 10 ⁻¹⁴
Mg	6.83 x 10 ⁻¹⁸	1.26 x 10 ⁻¹⁵	9.47 x 10 ⁻¹⁴	3.65 x 10 ⁻¹²	8.29 x 10 ⁻¹¹	1.24 x 10 ⁻⁹
Mg(OH) ₂	1.17 x 10 ⁻¹³	3.39 x 10 ⁻¹²	5.57 x 10 ⁻¹¹	5.90 x 10 ⁻¹⁰	4.44 x 10 ⁻⁹	2.54 x 10 ⁻⁸
MgCl	2.43 x 10 ⁻¹⁷	1.37 x 10 ⁻¹⁵	3.90 x 10 ⁻¹⁴	6.58 x 10 ⁻¹³	7.38 x 10 ⁻¹²	5.96 x 10 ⁻¹¹
MgCl ₂	1.40 x 10 ⁻¹¹	5.54 x 10 ⁻¹¹	1.75 x 10 ⁻¹⁰	4.62 x 10 ⁻¹⁰	1.06 x 10 ⁻⁹	2.19 x 10 ⁻⁹
MgO	3.15 x 10 ⁻²⁴	3.16 x 10 ⁻²¹	1.00 x 10 ⁻¹⁸	1.32 x 10 ⁻¹⁶	8.60 x 10 ⁻¹⁵	3.21 x 10 ⁻¹³
MgOH	1.42 x 10 ⁻¹⁷	1.83 x 10 ⁻¹⁵	1.03 x 10 ⁻¹³	3.07 x 10 ⁻¹²	5.60 x 10 ⁻¹¹	6.88 x 10 ⁻¹⁰
N	4.89 x 10 ⁻²³	8.91 x 10 ⁻²¹	6.87 x 10 ⁻¹⁹	2.72 x 10 ⁻¹⁷	6.38 x 10 ⁻¹⁶	9.85 x 10 ⁻¹⁵
NH	2.17 x 10 ⁻²⁰	1.29 x 10 ⁻¹⁸	3.89 x 10 ⁻¹⁷	6.93 x 10 ⁻¹⁶	8.17 x 10 ⁻¹⁵	6.94 x 10 ⁻¹⁴
NH ₂	7.62 x 10 ⁻¹⁴	5.49 x 10 ⁻¹³	2.81 x 10 ⁻¹²	1.11 x 10 ⁻¹¹	3.62 x 10 ⁻¹¹	1.01 x 10 ⁻¹⁰
NH ₂ NO ₂	2.96 x 10 ⁻³⁶	6.54 x 10 ⁻³⁴	6.03 x 10 ⁻³²	2.77 x 10 ⁻³⁰	7.36 x 10 ⁻²⁹	1.26 x 10 ⁻²⁷
NH ₂ OH	8.83 x 10 ⁻¹⁹	7.89 x 10 ⁻¹⁸	4.87 x 10 ⁻¹⁷	2.27 x 10 ⁻¹⁶	8.45 x 10 ⁻¹⁶	2.64 x 10 ⁻¹⁵
NH ₃	1.74 x 10 ⁻⁵	8.82 x 10 ⁻⁶	4.91 x 10 ⁻⁶	2.98 x 10 ⁻⁶	1.94 x 10 ⁻⁶	1.34 x 10 ⁻⁶
NO	4.37 x 10 ⁻¹⁶	2.12 x 10 ⁻¹⁴	5.49 x 10 ⁻¹³	8.56 x 10 ⁻¹²	8.99 x 10 ⁻¹¹	6.88 x 10 ⁻¹⁰
NOCl	1.01 x 10 ⁻²⁵	9.23 x 10 ⁻²⁴	4.08 x 10 ⁻²²	1.01 x 10 ⁻²⁰	1.57 x 10 ⁻¹⁹	1.70 x 10 ⁻¹⁸
NO ₂	1.88 x 10 ⁻²⁷	8.71 x 10 ⁻²⁵	1.50 x 10 ⁻²²	1.16 x 10 ⁻²⁰	4.71 x 10 ⁻¹⁹	1.19 x 10 ⁻¹⁷
NO ₂ Cl	6.02 x 10 ⁻³⁹	6.45 x 10 ⁻³⁶	2.26 x 10 ⁻³³	3.21 x 10 ⁻³¹	2.24 x 10 ⁻²⁹	8.87 x 10 ⁻²⁸
NO ₃	1.69 x 10 ⁻⁴⁴	2.18 x 10 ⁻⁴⁰	6.09 x 10 ⁻³⁸	4.98 x 10 ⁻³⁴	1.55 x 10 ⁻³¹	2.24 x 10 ⁻²⁹
N ₂	2.52 x 10 ⁻²	2.50 x 10 ⁻²	2.50 x 10 ⁻²	2.50 x 10 ⁻²	2.50 x 10 ⁻²	2.50 x 10 ⁻²

Species	Partial Pressure (atm)					
T(K) =	1000	1100	1200	1300	1400	1500
	MgO(c,l)					
N ₂ O	6.40 x 10 ⁻²¹	2.83 x 10 ⁻¹⁹	6.82 x 10 ⁻¹⁸	1.01 x 10 ⁻¹⁶	1.01 x 10 ⁻¹⁵	7.45 x 10 ⁻¹⁵
N ₂ O ₃	2.64 x 10 ⁻⁴⁹	3.92 x 10 ⁻⁴⁵	1.23 x 10 ⁻⁴¹	1.11 x 10 ⁻³⁸	3.74 x 10 ⁻³⁶	5.78 x 10 ⁻³⁴
N ₂ O ₄	3.67 x 10 ⁻⁶⁰	4.61 x 10 ⁻⁵⁵	8.80 x 10 ⁻⁵¹	3.67 x 10 ⁻⁴⁷	4.64 x 10 ⁻⁴⁴	2.25 x 10 ⁻⁴¹
N ₂ O ₅	2.27 x 10 ⁻⁷⁵	5.43 x 10 ⁻⁶⁹	1.23 x 10 ⁻⁶³	4.16 x 10 ⁻⁵⁹	3.17 x 10 ⁻⁵⁵	7.31 x 10 ⁻⁵²
N ₃	2.64 x 10 ⁻²⁹	3.11 x 10 ⁻²⁷	1.68 x 10 ⁻²⁵	4.93 x 10 ⁻²⁴	8.95 x 10 ⁻²³	1.11 x 10 ⁻²¹
O	5.57 x 10 ⁻²¹	1.59 x 10 ⁻¹⁸	1.79 x 10 ⁻¹⁶	9.76 x 10 ⁻¹⁵	3.00 x 10 ⁻¹³	5.82 x 10 ⁻¹²
OH	1.16 x 10 ⁻¹²	3.10 x 10 ⁻¹¹	4.82 x 10 ⁻¹⁰	4.87 x 10 ⁻⁹	3.53 x 10 ⁻⁸	1.95 x 10 ⁻⁷
O ₂	1.28 x 10 ⁻²¹	4.12 x 10 ⁻¹⁹	5.21 x 10 ⁻¹⁷	3.09 x 10 ⁻¹⁵	1.02 x 10 ⁻¹³	2.09 x 10 ⁻¹²
O ₃	3.98 x 10 ⁻⁴³	1.06 x 10 ⁻³⁸	5.61 x 10 ⁻³⁵	7.83 x 10 ⁻³²	3.85 x 10 ⁻²⁹	8.21 x 10 ⁻²⁷
Σ P(Mg) (atm)	1.41 x 10 ⁻¹¹	5.88 x 10 ⁻¹¹	2.31 x 10 ⁻¹⁰	1.06 x 10 ⁻⁹	5.65 x 10 ⁻⁹	2.96 x 10 ⁻⁸
Σ P(Mg-O) (atm)	6.83 x 10 ⁻¹⁸	1.26 x 10 ⁻¹⁵	9.47 x 10 ⁻¹⁴	3.65 x 10 ⁻¹²	8.30 x 10 ⁻¹¹	1.24 x 10 ⁻⁹
Σ P(Mg-Cl) (atm)	1.40 x 10 ⁻¹¹	5.54 x 10 ⁻¹¹	1.75 x 10 ⁻¹⁰	4.67 x 10 ⁻¹⁰	1.15 x 10 ⁻⁹	3.48 x 10 ⁻⁹
Mg(923) ^a	0 ^b	0	0	0	0	0
C(5000)	0	0	0	0	0	0
MgC ₂ (c)	0	0	0	0	0	0
Mg ₂ C ₃ (c)	0	0	0	0	0	0
Mg ₃ N ₂ (c)	0	0	0	0	0	0
MgCO ₃ (1263)	0	0	0	0	0	0
Mg(NO ₃) ₂ (c)	0	0	0	0	0	0
Mg(OH) ₂ (c)	0	0	0	0	0	0
MgO(3105)	1	1	1	1	1	1
MgCl ₂ (987)	0	0	0	0	0	0

Notes: ΣP(Mg) = Sum of vapor pressures of species containing Mg, O, and H

ΣP(Mg-O) = Sum of vapor pressures of species containing Mg and O only

ΣP(Mg-Cl) = Sum of vapor pressures of species containing Mg and Cl only

a = Melting point in degrees Kelvin

b = One (1) and zero (0) represent the presence and absence of the solid phase respectively.

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
	TiO ₂ (c,l)					
C	2.06 x 10 ⁻³⁰	1.08 x 10 ⁻²⁷	1.94 x 10 ⁻²⁵	1.58 x 10 ⁻²³	6.89 x 10 ⁻²²	1.83 x 10 ⁻²⁰
CCl	5.45 x 10 ⁻²⁷	3.89 x 10 ⁻²⁵	1.35 x 10 ⁻²³	2.74 x 10 ⁻²²	3.62 x 10 ⁻²¹	3.41 x 10 ⁻²⁰
CCl ₂	3.62 x 10 ⁻²⁸	7.15 x 10 ⁻²⁷	8.63 x 10 ⁻²⁶	7.16 x 10 ⁻²⁵	4.41 x 10 ⁻²⁴	2.15 x 10 ⁻²³
CCl ₃	5.22 x 10 ⁻³³	6.11 x 10 ⁻³²	4.85 x 10 ⁻³¹	2.84 x 10 ⁻³⁰	1.30 x 10 ⁻²⁹	4.93 x 10 ⁻²⁹
CCl ₄	1.34 x 10 ⁻³⁷	6.84 x 10 ⁻³⁷	2.78 x 10 ⁻³⁶	9.27 x 10 ⁻³⁶	2.65 x 10 ⁻³⁵	6.66 x 10 ⁻³⁵
CH	1.31 x 10 ⁻²⁶	1.71 x 10 ⁻²⁴	9.61 x 10 ⁻²³	2.91 x 10 ⁻²¹	5.43 x 10 ⁻²⁰	6.88 x 10 ⁻¹⁹
CHCl	1.70 x 10 ⁻²³	2.70 x 10 ⁻²²	2.65 x 10 ⁻²¹	1.83 x 10 ⁻²⁰	9.67 x 10 ⁻²⁰	4.10 x 10 ⁻¹⁹
CHCl ₂	2.50 x 10 ⁻²³	8.95 x 10 ⁻²³	2.59 x 10 ⁻²²	6.41 x 10 ⁻²²	1.41 x 10 ⁻²¹	2.80 x 10 ⁻²¹
CHCl ₃	1.48 x 10 ⁻²⁷	2.21 x 10 ⁻²⁷	3.16 x 10 ⁻²⁷	4.32 x 10 ⁻²⁷	5.71 x 10 ⁻²⁷	7.37 x 10 ⁻²⁷
CH ₂	1.28 x 10 ⁻¹⁹	1.60 x 10 ⁻¹⁸	1.27 x 10 ⁻¹⁷	7.35 x 10 ⁻¹⁷	3.32 x 10 ⁻¹⁶	1.23 x 10 ⁻¹⁵
CH ₂ Cl	7.79 x 10 ⁻¹⁷	1.46 x 10 ⁻¹⁶	2.40 x 10 ⁻¹⁶	3.66 x 10 ⁻¹⁶	5.30 x 10 ⁻¹⁶	7.34 x 10 ⁻¹⁶
CH ₂ Cl ₂	7.59 x 10 ⁻¹⁹	3.96 x 10 ⁻¹⁹	2.28 x 10 ⁻¹⁹	1.44 x 10 ⁻¹⁹	9.84 x 10 ⁻²⁰	7.12 x 10 ⁻²⁰
CH ₂ O	4.63 x 10 ⁻⁷	4.12 x 10 ⁻⁷	3.64 x 10 ⁻⁷	3.27 x 10 ⁻⁷	2.98 x 10 ⁻⁷	2.75 x 10 ⁻⁷
CH ₃	2.84 x 10 ⁻¹⁰	2.43 x 10 ⁻¹⁰	2.04 x 10 ⁻¹⁰	1.76 x 10 ⁻¹⁰	1.55 x 10 ⁻¹⁰	1.39 x 10 ⁻¹⁰
CH ₃ Cl	6.74 x 10 ⁻¹¹	1.32 x 10 ⁻¹¹	3.27 x 10 ⁻¹²	1.01 x 10 ⁻¹²	3.72 x 10 ⁻¹³	1.57 x 10 ⁻¹³
CH ₄	3.52 x 10 ⁻³	2.45 x 10 ⁻⁴	2.51 x 10 ⁻⁵	3.67 x 10 ⁻⁶	7.06 x 10 ⁻⁷	1.70 x 10 ⁻⁷
CN	1.09 x 10 ⁻¹⁹	2.72 x 10 ⁻¹⁸	3.86 x 10 ⁻¹⁷	3.66 x 10 ⁻¹⁶	2.52 x 10 ⁻¹⁵	1.35 x 10 ⁻¹⁴
CNO	2.81 x 10 ⁻¹⁹	5.91 x 10 ⁻¹⁸	7.47 x 10 ⁻¹⁷	6.40 x 10 ⁻¹⁶	4.04 x 10 ⁻¹⁵	2.00 x 10 ⁻¹⁴
CN ₂	1.77 x 10 ⁻³¹	2.18 x 10 ⁻²⁹	1.19 x 10 ⁻²⁷	3.53 x 10 ⁻²⁶	6.47 x 10 ⁻²⁵	8.10 x 10 ⁻²⁴
CO	3.24 x 10 ⁻¹	3.47 x 10 ⁻¹	3.63 x 10 ⁻¹	3.77 x 10 ⁻¹	3.87 x 10 ⁻¹	3.96 x 10 ⁻¹
COCl	5.61 x 10 ⁻¹⁷	4.88 x 10 ⁻¹⁶	2.97 x 10 ⁻¹⁵	1.37 x 10 ⁻¹⁴	5.07 x 10 ⁻¹⁴	1.58 x 10 ⁻¹³
COCl ₂	9.68 x 10 ⁻²⁰	2.64 x 10 ⁻¹⁹	6.24 x 10 ⁻¹⁹	1.30 x 10 ⁻¹⁸	2.44 x 10 ⁻¹⁸	4.24 x 10 ⁻¹⁸
COHCl	1.88 x 10 ⁻¹³	3.03 x 10 ⁻¹³	4.50 x 10 ⁻¹³	6.30 x 10 ⁻¹³	8.41 x 10 ⁻¹³	1.08 x 10 ⁻¹²
COOH	1.06 x 10 ⁻¹²	6.35 x 10 ⁻¹²	2.82 x 10 ⁻¹¹	9.89 x 10 ⁻¹¹	2.89 x 10 ⁻¹⁰	7.31 x 10 ⁻¹⁰
CO ₂	1.84 x 10 ⁻¹	1.61 x 10 ⁻¹	1.45 x 10 ⁻¹	1.32 x 10 ⁻¹	1.21 x 10 ⁻¹	1.13 x 10 ⁻¹
Cl	1.14 x 10 ⁻¹²	1.27 x 10 ⁻¹¹	9.56 x 10 ⁻¹¹	5.25 x 10 ⁻¹⁰	2.32 x 10 ⁻⁹	8.34 x 10 ⁻⁹
ClHO	1.42 x 10 ⁻¹⁷	2.50 x 10 ⁻¹⁶	2.78 x 10 ⁻¹⁵	2.12 x 10 ⁻¹⁴	1.20 x 10 ⁻¹³	5.40 x 10 ⁻¹³
ClO	2.36 x 10 ⁻²⁴	3.67 x 10 ⁻²²	2.53 x 10 ⁻²⁰	9.08 x 10 ⁻¹⁹	1.95 x 10 ⁻¹⁷	2.77 x 10 ⁻¹⁶
ClO ₂	8.55 x 10 ⁻³⁹	2.47 x 10 ⁻³⁵	1.98 x 10 ⁻³²	5.62 x 10 ⁻³⁰	7.10 x 10 ⁻²⁸	4.68 x 10 ⁻²⁶
Cl ₂	8.11 x 10 ⁻¹⁸	6.61 x 10 ⁻¹⁷	3.90 x 10 ⁻¹⁶	1.76 x 10 ⁻¹⁵	6.40 x 10 ⁻¹⁵	1.97 x 10 ⁻¹⁴

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
	TiO ₂ (c,l)					
Cl ₂ O	7.51 x 10 ⁻³⁶	2.91 x 10 ⁻³³	4.35 x 10 ⁻³¹	3.01 x 10 ⁻²⁹	1.14 x 10 ⁻²⁷	2.65 x 10 ⁻²⁶
H	1.30 x 10 ⁻⁹	1.45 x 10 ⁻⁸	1.08 x 10 ⁻⁷	5.92 x 10 ⁻⁷	2.55 x 10 ⁻⁶	9.09 x 10 ⁻⁶
HCN	1.53 x 10 ⁻⁷	1.31 x 10 ⁻⁷	1.11 x 10 ⁻⁷	9.77 x 10 ⁻⁸	8.77 x 10 ⁻⁸	8.02 x 10 ⁻⁸
HCO	1.33 x 10 ⁻¹¹	7.14 x 10 ⁻¹¹	2.85 x 10 ⁻¹⁰	9.17 x 10 ⁻¹⁰	2.49 x 10 ⁻⁹	5.91 x 10 ⁻⁹
HCl	3.02 x 10 ⁻⁴	3.00 x 10 ⁻⁴	3.00 x 10 ⁻⁴	3.00 x 10 ⁻⁴	3.00 x 10 ⁻⁴	3.00 x 10 ⁻⁴
HNCO	3.64 x 10 ⁻⁹	4.13 x 10 ⁻⁹	4.52 x 10 ⁻⁹	4.88 x 10 ⁻⁹	5.22 x 10 ⁻⁹	5.53 x 10 ⁻⁹
HNO	7.63 x 10 ⁻²⁰	3.83 x 10 ⁻¹⁸	1.01 x 10 ⁻¹⁶	1.60 x 10 ⁻¹⁵	1.71 x 10 ⁻¹⁴	1.32 x 10 ⁻¹³
HNO ₂	7.83 x 10 ⁻²⁵	1.02 x 10 ⁻²²	6.08 x 10 ⁻²¹	1.92 x 10 ⁻¹⁹	3.67 x 10 ⁻¹⁸	4.72 x 10 ⁻¹⁷
HNO ₃	6.37 x 10 ⁻³⁷	8.15 x 10 ⁻³⁴	3.31 x 10 ⁻³¹	5.28 x 10 ⁻²⁹	4.06 x 10 ⁻²⁷	1.74 x 10 ⁻²⁵
HO ₂	9.81 x 10 ⁻²⁵	3.29 x 10 ⁻²²	4.27 x 10 ⁻²⁰	2.59 x 10 ⁻¹⁸	8.69 x 10 ⁻¹⁷	1.81 x 10 ⁻¹⁵
H ₂	3.31 x 10 ⁻¹	3.17 x 10 ⁻¹	3.02 x 10 ⁻¹	2.89 x 10 ⁻¹	2.78 x 10 ⁻¹	2.69 x 10 ⁻¹
H ₂ O	1.31 x 10 ⁻¹	1.49 x 10 ⁻¹	1.64 x 10 ⁻¹	1.78 x 10 ⁻¹	1.88 x 10 ⁻¹	1.97 x 10 ⁻¹
H ₂ O ₂	1.22 x 10 ⁻²⁰	8.06 x 10 ⁻¹⁹	2.68 x 10 ⁻¹⁷	5.14 x 10 ⁻¹⁶	6.41 x 10 ⁻¹⁵	5.67 x 10 ⁻¹⁴
N	4.89 x 10 ⁻²³	8.91 x 10 ⁻²¹	6.87 x 10 ⁻¹⁹	2.72 x 10 ⁻¹⁷	6.38 x 10 ⁻¹⁶	9.85 x 10 ⁻¹⁵
NH	2.18 x 10 ⁻²⁰	1.30 x 10 ⁻¹⁸	3.92 x 10 ⁻¹⁷	6.99 x 10 ⁻¹⁶	8.25 x 10 ⁻¹⁵	7.01 x 10 ⁻¹⁴
NH ₂	7.71 x 10 ⁻¹⁴	5.57 x 10 ⁻¹³	2.86 x 10 ⁻¹²	1.13 x 10 ⁻¹¹	3.70 x 10 ⁻¹¹	1.03 x 10 ⁻¹⁰
NH ₂ NO ₂	2.74 x 10 ⁻³⁶	6.05 x 10 ⁻³⁴	5.58 x 10 ⁻³²	2.56 x 10 ⁻³⁰	6.81 x 10 ⁻²⁹	1.17 x 10 ⁻²⁷
NH ₂ OH	8.60 x 10 ⁻¹⁹	7.70 x 10 ⁻¹⁸	4.77 x 10 ⁻¹⁷	2.22 x 10 ⁻¹⁶	8.30 x 10 ⁻¹⁶	2.60 x 10 ⁻¹⁵
NH ₃	1.77 x 10 ⁻⁵	9.02 x 10 ⁻⁶	5.04 x 10 ⁻⁶	3.06 x 10 ⁻⁶	2.00 x 10 ⁻⁶	1.38 x 10 ⁻⁶
NO	4.18 x 10 ⁻¹⁶	2.03 x 10 ⁻¹⁴	5.24 x 10 ⁻¹³	8.16 x 10 ⁻¹²	8.57 x 10 ⁻¹¹	6.55 x 10 ⁻¹⁰
NOCl	9.64 x 10 ⁻²⁶	8.74 x 10 ⁻²⁴	3.86 x 10 ⁻²²	9.51 x 10 ⁻²¹	1.48 x 10 ⁻¹⁹	1.60 x 10 ⁻¹⁸
NO ₂	1.72 x 10 ⁻²⁷	7.93 x 10 ⁻²⁵	1.36 x 10 ⁻²²	1.05 x 10 ⁻²⁰	4.27 x 10 ⁻¹⁹	1.08 x 10 ⁻¹⁷
NO ₂ Cl	5.48 x 10 ⁻³⁹	5.83 x 10 ⁻³⁶	2.04 x 10 ⁻³³	2.89 x 10 ⁻³¹	2.01 x 10 ⁻²⁹	7.95 x 10 ⁻²⁸
NO ₃	1.48 x 10 ⁻⁴⁴	1.89 x 10 ⁻⁴⁰	5.29 x 10 ⁻³⁷	4.31 x 10 ⁻³⁴	1.34 x 10 ⁻³¹	1.93 x 10 ⁻²⁹
N ₂	2.52 x 10 ⁻²	2.50 x 10 ⁻²	2.50 x 10 ⁻²	2.50 x 10 ⁻²	2.50 x 10 ⁻²	2.50 x 10 ⁻²
N ₂ O	6.12 x 10 ⁻²¹	2.70 x 10 ⁻¹⁹	6.51 x 10 ⁻¹⁸	9.59 x 10 ⁻¹⁷	9.62 x 10 ⁻¹⁶	7.09 x 10 ⁻¹⁵
N ₂ O ₃	2.31 x 10 ⁻⁴⁹	3.40 x 10 ⁻⁴⁵	1.07 x 10 ⁻⁴¹	9.59 x 10 ⁻³⁹	3.24 x 10 ⁻³⁶	4.99 x 10 ⁻³⁴
N ₂ O ₄	3.07 x 10 ⁻⁶⁰	3.83 x 10 ⁻⁵⁵	7.29 x 10 ⁻⁵¹	3.03 x 10 ⁻⁴⁷	3.82 x 10 ⁻⁴⁴	1.85 x 10 ⁻⁴¹
N ₂ O ₅	1.81 x 10 ⁻⁷⁵	4.30 x 10 ⁻⁶⁹	9.72 x 10 ⁻⁶⁴	3.28 x 10 ⁻⁵⁹	2.49 x 10 ⁻⁵⁵	5.71 x 10 ⁻⁵²
N ₃	2.64 x 10 ⁻²⁹	3.11 x 10 ⁻²⁷	1.68 x 10 ⁻²⁵	4.93 x 10 ⁻²⁴	8.95 x 10 ⁻²³	1.11 x 10 ⁻²¹
O	5.33 x 10 ⁻²¹	1.52 x 10 ⁻¹⁸	1.71 x 10 ⁻¹⁶	9.30 x 10 ⁻¹⁵	2.85 x 10 ⁻¹³	5.54 x 10 ⁻¹²

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
TiO₂(c,l)						
OH	1.12 x 10 ⁻¹²	2.98 x 10 ⁻¹¹	4.63 x 10 ⁻¹⁰	4.69 x 10 ⁻⁹	3.39 x 10 ⁻⁸	1.88 x 10 ⁻⁷
O ₂	1.17 x 10 ⁻²¹	3.76 x 10 ⁻¹⁹	4.74 x 10 ⁻¹⁷	2.81 x 10 ⁻¹⁵	9.24 x 10 ⁻¹⁴	1.89 x 10 ⁻¹²
O ₃	3.48 x 10 ⁻⁴³	9.24 x 10 ⁻³⁹	4.87 x 10 ⁻³⁵	6.78 x 10 ⁻³²	3.33 x 10 ⁻²⁹	7.08 x 10 ⁻²⁷
Ti	1.22 x 10 ⁻³⁶	1.81 x 10 ⁻³²	5.19 x 10 ⁻²⁹	4.34 x 10 ⁻²⁶	1.38 x 10 ⁻²³	2.03 x 10 ⁻²¹
Ti(OH) ₂	3.76 x 10 ⁻²³	1.37 x 10 ⁻²⁰	1.83 x 10 ⁻¹⁸	1.14 x 10 ⁻¹⁶	3.90 x 10 ⁻¹⁵	8.28 x 10 ⁻¹⁴
Ti(OH) ₃	4.52 x 10 ⁻²⁰	4.19 x 10 ⁻¹⁸	1.81 x 10 ⁻¹⁶	4.33 x 10 ⁻¹⁵	6.57 x 10 ⁻¹⁴	6.90 x 10 ⁻¹³
Ti(OH) ₄	8.29 x 10 ⁻²¹	4.42 x 10 ⁻¹⁹	1.22 x 10 ⁻¹⁷	2.01 x 10 ⁻¹⁶	2.22 x 10 ⁻¹⁵	1.77 x 10 ⁻¹⁴
TiCl	1.43 x 10 ⁻³¹	2.21 x 10 ⁻²⁸	9.76 x 10 ⁻²⁶	1.69 x 10 ⁻²³	1.39 x 10 ⁻²¹	6.36 x 10 ⁻²⁰
TiCl ₂	3.71 x 10 ⁻²³	2.13 x 10 ⁻²¹	6.15 x 10 ⁻²⁰	1.06 x 10 ⁻¹⁸	1.21 x 10 ⁻¹⁷	1.00 x 10 ⁻¹⁶
TiCl ₃	1.19 x 10 ⁻¹⁹	6.72 x 10 ⁻¹⁹	2.85 x 10 ⁻¹⁸	9.76 x 10 ⁻¹⁸	2.81 x 10 ⁻¹⁷	7.06 x 10 ⁻¹⁷
TiCl ₄	3.07 x 10 ⁻²⁰	4.41 x 10 ⁻²⁰	6.07 x 10 ⁻²⁰	8.02 x 10 ⁻²⁰	1.03 x 10 ⁻¹⁹	1.28 x 10 ⁻¹⁹
TiN	2.91 x 10 ⁻⁴⁰	4.13 x 10 ⁻³⁶	1.14 x 10 ⁻³²	9.28 x 10 ⁻³⁰	2.87 x 10 ⁻²⁷	4.12 x 10 ⁻²⁵
TiO	4.90 x 10 ⁻²⁸	1.32 x 10 ⁻²⁴	9.20 x 10 ⁻²²	2.32 x 10 ⁻¹⁹	2.63 x 10 ⁻¹⁷	1.57 x 10 ⁻¹⁵
TiO(OH)	5.50 x 10 ⁻²⁴	4.13 x 10 ⁻²¹	1.01 x 10 ⁻¹⁸	1.04 x 10 ⁻¹⁶	5.49 x 10 ⁻¹⁵	1.69 x 10 ⁻¹³
TiO(OH) ₂	1.75 x 10 ⁻²⁶	9.97 x 10 ⁻²⁴	1.96 x 10 ⁻²¹	1.69 x 10 ⁻¹⁹	7.68 x 10 ⁻¹⁸	2.08 x 10 ⁻¹⁶
TiOCl ₂	6.87 x 10 ⁻¹⁷	8.40 x 10 ⁻¹⁶	6.78 x 10 ⁻¹⁵	3.95 x 10 ⁻¹⁴	1.78 x 10 ⁻¹³	6.57 x 10 ⁻¹³
TiO ₂	1.40 x 10 ⁻²³	1.32 x 10 ⁻²⁰	3.91 x 10 ⁻¹⁸	4.75 x 10 ⁻¹⁶	2.87 x 10 ⁻¹⁴	9.90 x 10 ⁻¹³
Σ P(Ti) (atm)	6.89 x 10 ⁻¹⁷	8.46 x 10 ⁻¹⁶	6.98 x 10 ⁻¹⁵	4.47 x 10 ⁻¹⁴	2.84 x 10 ⁻¹³	2.61 x 10 ⁻¹²
Σ P(Ti-O) (atm)	1.40 x 10 ⁻²³	1.32 x 10 ⁻²⁰	3.91 x 10 ⁻¹⁸	4.75 x 10 ⁻¹⁶	2.87 x 10 ⁻¹⁴	9.91 x 10 ⁻¹³
Σ P(Ti-Cl) (atm)	6.88 x 10 ⁻¹⁷	8.41 x 10 ⁻¹⁶	6.78 x 10 ⁻¹⁵	3.95 x 10 ⁻¹⁴	1.78 x 10 ⁻¹³	6.57 x 10 ⁻¹³
Ti(1939) ^a	0 ^b	0	0	0	0	0
TiC(3290)	0	0	0	0	0	0
TiN(c)	0	0	0	0	0	0
TiO ₂ -r(2130)	1	1	1	1	1	1
Ti ₄ O ₇ (1950)	0	0	0	0	0	0
Ti ₃ O ₅ (2050)	0	0	0	0	0	0
Ti ₂ O ₃ (2115)	0	0	0	0	0	0
TiO(2023)	0	0	0	0	0	0
TiCl ₃ (c)	0	0	0	0	0	0
TiCl ₂ (1308)	0	0	0	0	0	0
TiCl ₄ (l)	0	0	0	0	0	0

Notes: ΣP(Ti) = Sum of vapor pressures of species containing Ti, O, and H

ΣP(Ti-O) = Sum of vapor pressures of species containing Ti and O only

ΣP(Ti-Cl) = Sum of vapor pressures of species containing Ti and Cl only

a = Melting point in degrees Kelvin

b = One (1) and zero (0) represent the presence and absence of the solid phase respectively.

Species	Partial Pressure (atm)					
T(K) =	1000	1100	1200	1300	1400	1500
SiO ₂ (c,l)						
C	2.06 x 10 ⁻³⁰	1.08 x 10 ⁻²⁷	1.94 x 10 ⁻²⁵	1.58 x 10 ⁻²³	6.89 x 10 ⁻²²	1.83 x 10 ⁻²⁰
CCl	5.45 x 10 ⁻²⁷	3.89 x 10 ⁻²⁵	1.35 x 10 ⁻²³	2.74 x 10 ⁻²²	3.62 x 10 ⁻²¹	3.41 x 10 ⁻²⁰
CCl ₂	3.62 x 10 ⁻²⁸	7.15 x 10 ⁻²⁷	8.63 x 10 ⁻²⁶	7.16 x 10 ⁻²⁵	4.41 x 10 ⁻²⁴	2.15 x 10 ⁻²³
CCl ₃	5.22 x 10 ⁻³³	6.11 x 10 ⁻³²	4.85 x 10 ⁻³¹	2.84 x 10 ⁻³⁰	1.30 x 10 ⁻²⁹	4.93 x 10 ⁻²⁹
CCl ₄	1.34 x 10 ⁻³⁷	6.84 x 10 ⁻³⁷	2.78 x 10 ⁻³⁶	9.27 x 10 ⁻³⁶	2.65 x 10 ⁻³⁵	6.66 x 10 ⁻³⁵
CH	1.31 x 10 ⁻²⁶	1.71 x 10 ⁻²⁴	9.61 x 10 ⁻²³	2.91 x 10 ⁻²¹	5.43 x 10 ⁻²⁰	6.88 x 10 ⁻¹⁹
CHCl	1.70 x 10 ⁻²³	2.70 x 10 ⁻²²	2.65 x 10 ⁻²¹	1.83 x 10 ⁻²⁰	9.67 x 10 ⁻²⁰	4.10 x 10 ⁻¹⁹
CHCl ₂	2.50 x 10 ⁻²³	8.95 x 10 ⁻²³	2.59 x 10 ⁻²²	6.41 x 10 ⁻²²	1.41 x 10 ⁻²¹	2.80 x 10 ⁻²¹
CHCl ₃	1.48 x 10 ⁻²⁷	2.21 x 10 ⁻²⁷	3.16 x 10 ⁻²⁷	4.32 x 10 ⁻²⁷	5.71 x 10 ⁻²⁷	7.37 x 10 ⁻²⁷
CH ₂	1.28 x 10 ⁻¹⁹	1.60 x 10 ⁻¹⁸	1.27 x 10 ⁻¹⁷	7.35 x 10 ⁻¹⁷	3.32 x 10 ⁻¹⁶	1.23 x 10 ⁻¹⁵
CH ₂ Cl	7.79 x 10 ⁻¹⁷	1.46 x 10 ⁻¹⁶	2.40 x 10 ⁻¹⁶	3.66 x 10 ⁻¹⁶	5.30 x 10 ⁻¹⁶	7.34 x 10 ⁻¹⁶
CH ₂ Cl ₂	7.59 x 10 ⁻¹⁹	3.96 x 10 ⁻¹⁹	2.28 x 10 ⁻¹⁹	1.44 x 10 ⁻¹⁹	9.84 x 10 ⁻²⁰	7.12 x 10 ⁻²⁰
CH ₂ O	4.63 x 10 ⁻⁷	4.12 x 10 ⁻⁷	3.64 x 10 ⁻⁷	3.27 x 10 ⁻⁷	2.98 x 10 ⁻⁷	2.75 x 10 ⁻⁷
CH ₃	2.84 x 10 ⁻¹⁰	2.43 x 10 ⁻¹⁰	2.04 x 10 ⁻¹⁰	1.76 x 10 ⁻¹⁰	1.55 x 10 ⁻¹⁰	1.39 x 10 ⁻¹⁰
CH ₃ Cl	6.74 x 10 ⁻¹¹	1.32 x 10 ⁻¹¹	3.27 x 10 ⁻¹²	1.01 x 10 ⁻¹²	3.72 x 10 ⁻¹³	1.57 x 10 ⁻¹³
CH ₄	3.52 x 10 ⁻³	2.45 x 10 ⁻⁴	2.51 x 10 ⁻⁵	3.67 x 10 ⁻⁶	7.06 x 10 ⁻⁷	1.70 x 10 ⁻⁷
CN	1.09 x 10 ⁻¹⁹	2.72 x 10 ⁻¹⁸	3.86 x 10 ⁻¹⁷	3.66 x 10 ⁻¹⁶	2.52 x 10 ⁻¹⁵	1.35 x 10 ⁻¹⁴
CNO	2.81 x 10 ⁻¹⁹	5.91 x 10 ⁻¹⁸	7.47 x 10 ⁻¹⁷	6.40 x 10 ⁻¹⁶	4.04 x 10 ⁻¹⁵	2.00 x 10 ⁻¹⁴
CN ₂	1.77 x 10 ⁻³¹	2.18 x 10 ⁻²⁹	1.19 x 10 ⁻²⁷	3.53 x 10 ⁻²⁶	6.47 x 10 ⁻²⁵	8.10 x 10 ⁻²⁴
CO	3.24 x 10 ⁻¹	3.47 x 10 ⁻¹	3.63 x 10 ⁻¹	3.77 x 10 ⁻¹	3.87 x 10 ⁻¹	3.96 x 10 ⁻¹
COCl	5.61 x 10 ⁻¹⁷	4.88 x 10 ⁻¹⁶	2.97 x 10 ⁻¹⁵	1.37 x 10 ⁻¹⁴	5.07 x 10 ⁻¹⁴	1.58 x 10 ⁻¹³
COCl ₂	9.68 x 10 ⁻²⁰	2.64 x 10 ⁻¹⁹	6.24 x 10 ⁻¹⁹	1.30 x 10 ⁻¹⁸	2.44 x 10 ⁻¹⁸	4.24 x 10 ⁻¹⁸
COHCl	1.88 x 10 ⁻¹³	3.03 x 10 ⁻¹³	4.50 x 10 ⁻¹³	6.30 x 10 ⁻¹³	8.41 x 10 ⁻¹³	1.08 x 10 ⁻¹²
COOH	1.06 x 10 ⁻¹²	6.35 x 10 ⁻¹²	2.82 x 10 ⁻¹¹	9.89 x 10 ⁻¹¹	2.89 x 10 ⁻¹⁰	7.31 x 10 ⁻¹⁰
CO ₂	1.84 x 10 ⁻¹	1.61 x 10 ⁻¹	1.45 x 10 ⁻¹	1.32 x 10 ⁻¹	1.21 x 10 ⁻¹	1.13 x 10 ⁻¹
Cl	1.14 x 10 ⁻¹²	1.27 x 10 ⁻¹¹	9.56 x 10 ⁻¹¹	5.25 x 10 ⁻¹⁰	2.32 x 10 ⁻⁹	8.34 x 10 ⁻⁹
ClHO	1.42 x 10 ⁻¹⁷	2.50 x 10 ⁻¹⁶	2.78 x 10 ⁻¹⁵	2.12 x 10 ⁻¹⁴	1.20 x 10 ⁻¹³	5.40 x 10 ⁻¹³
ClO	2.36 x 10 ⁻²⁴	3.67 x 10 ⁻²²	2.53 x 10 ⁻²⁰	9.08 x 10 ⁻¹⁹	1.95 x 10 ⁻¹⁷	2.77 x 10 ⁻¹⁶
ClO ₂	8.55 x 10 ⁻³⁹	2.47 x 10 ⁻³⁵	1.98 x 10 ⁻³²	5.62 x 10 ⁻³⁰	7.10 x 10 ⁻²⁸	4.68 x 10 ⁻²⁶
Cl ₂	8.11 x 10 ⁻¹⁸	6.61 x 10 ⁻¹⁷	3.90 x 10 ⁻¹⁶	1.76 x 10 ⁻¹⁵	6.40 x 10 ⁻¹⁵	1.97 x 10 ⁻¹⁴

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
SiO₂(c,l)						
Cl ₂ O	7.51 x 10 ⁻³⁶	2.91 x 10 ⁻³³	4.35 x 10 ⁻³¹	3.01 x 10 ⁻²⁹	1.14 x 10 ⁻²⁷	2.65 x 10 ⁻²⁶
H	1.30 x 10 ⁻⁹	1.45 x 10 ⁻⁸	1.08 x 10 ⁻⁷	5.92 x 10 ⁻⁷	2.55 x 10 ⁻⁶	9.09 x 10 ⁻⁶
HCN	1.53 x 10 ⁻⁷	1.31 x 10 ⁻⁷	1.11 x 10 ⁻⁷	9.77 x 10 ⁻⁸	8.77 x 10 ⁻⁸	8.02 x 10 ⁻⁸
HCO	1.33 x 10 ⁻¹¹	7.14 x 10 ⁻¹¹	2.85 x 10 ⁻¹⁰	9.17 x 10 ⁻¹⁰	2.49 x 10 ⁻⁹	5.91 x 10 ⁻⁹
HCl	3.02 x 10 ⁻⁴	3.00 x 10 ⁻⁴	3.00 x 10 ⁻⁴	3.00 x 10 ⁻⁴	3.00 x 10 ⁻⁴	3.00 x 10 ⁻⁴
HNCO	3.64 x 10 ⁻⁹	4.13 x 10 ⁻⁹	4.52 x 10 ⁻⁹	4.88 x 10 ⁻⁹	5.22 x 10 ⁻⁹	5.53 x 10 ⁻⁹
HNO	7.63 x 10 ⁻²⁰	3.83 x 10 ⁻¹⁸	1.01 x 10 ⁻¹⁶	1.60 x 10 ⁻¹⁵	1.71 x 10 ⁻¹⁴	1.32 x 10 ⁻¹³
HNO ₂	7.83 x 10 ⁻²⁵	1.02 x 10 ⁻²²	6.08 x 10 ⁻²¹	1.92 x 10 ⁻¹⁹	3.67 x 10 ⁻¹⁸	4.72 x 10 ⁻¹⁷
HNO ₃	6.37 x 10 ⁻³⁷	8.15 x 10 ⁻³⁴	3.31 x 10 ⁻³¹	5.28 x 10 ⁻²⁹	4.06 x 10 ⁻²⁷	1.74 x 10 ⁻²⁵
HO ₂	9.81 x 10 ⁻²⁵	3.29 x 10 ⁻²²	4.27 x 10 ⁻²⁰	2.59 x 10 ⁻¹⁸	8.69 x 10 ⁻¹⁷	1.81 x 10 ⁻¹⁵
H ₂	3.31 x 10 ⁻¹	3.17 x 10 ⁻¹	3.02 x 10 ⁻¹	2.89 x 10 ⁻¹	2.78 x 10 ⁻¹	2.69 x 10 ⁻¹
H ₂ O	1.31 x 10 ⁻¹	1.49 x 10 ⁻¹	1.64 x 10 ⁻¹	1.78 x 10 ⁻¹	1.88 x 10 ⁻¹	1.97 x 10 ⁻¹
H ₂ O ₂	1.22 x 10 ⁻²⁰	8.06 x 10 ⁻¹⁹	2.68 x 10 ⁻¹⁷	5.14 x 10 ⁻¹⁶	6.41 x 10 ⁻¹⁵	5.67 x 10 ⁻¹⁴
N	4.89 x 10 ⁻²³	8.91 x 10 ⁻²¹	6.87 x 10 ⁻¹⁹	2.72 x 10 ⁻¹⁷	6.38 x 10 ⁻¹⁶	9.85 x 10 ⁻¹⁵
NH	2.18 x 10 ⁻²⁰	1.30 x 10 ⁻¹⁸	3.92 x 10 ⁻¹⁷	6.99 x 10 ⁻¹⁶	8.25 x 10 ⁻¹⁵	7.01 x 10 ⁻¹⁴
NH ₂	7.71 x 10 ⁻¹⁴	5.57 x 10 ⁻¹³	2.86 x 10 ⁻¹²	1.13 x 10 ⁻¹¹	3.70 x 10 ⁻¹¹	1.03 x 10 ⁻¹⁰
NH ₂ NO ₂	2.74 x 10 ⁻³⁶	6.05 x 10 ⁻³⁴	5.58 x 10 ⁻³²	2.56 x 10 ⁻³⁰	6.81 x 10 ⁻²⁹	1.17 x 10 ⁻²⁷
NH ₂ OH	8.60 x 10 ⁻¹⁹	7.70 x 10 ⁻¹⁸	4.77 x 10 ⁻¹⁷	2.22 x 10 ⁻¹⁶	8.30 x 10 ⁻¹⁶	2.60 x 10 ⁻¹⁵
NH ₃	1.77 x 10 ⁻⁵	9.02 x 10 ⁻⁶	5.04 x 10 ⁻⁶	3.06 x 10 ⁻⁶	2.00 x 10 ⁻⁶	1.38 x 10 ⁻⁶
NO	4.18 x 10 ⁻¹⁶	2.03 x 10 ⁻¹⁴	5.24 x 10 ⁻¹³	8.16 x 10 ⁻¹²	8.57 x 10 ⁻¹¹	6.55 x 10 ⁻¹⁰
NOCl	9.64 x 10 ⁻²⁶	8.74 x 10 ⁻²⁴	3.86 x 10 ⁻²²	9.51 x 10 ⁻²¹	1.48 x 10 ⁻¹⁹	1.60 x 10 ⁻¹⁸
NO ₂	1.72 x 10 ⁻²⁷	7.93 x 10 ⁻²⁵	1.36 x 10 ⁻²²	1.05 x 10 ⁻²⁰	4.27 x 10 ⁻¹⁹	1.08 x 10 ⁻¹⁷
NO ₂ Cl	5.48 x 10 ⁻³⁹	5.83 x 10 ⁻³⁶	2.04 x 10 ⁻³³	2.89 x 10 ⁻³¹	2.01 x 10 ⁻²⁹	7.95 x 10 ⁻²⁸
NO ₃	1.48 x 10 ⁻⁴⁴	1.89 x 10 ⁻⁴⁰	5.29 x 10 ⁻³⁷	4.31 x 10 ⁻³⁴	1.34 x 10 ⁻³¹	1.93 x 10 ⁻²⁹
N ₂	2.52 x 10 ⁻²	2.50 x 10 ⁻²	2.50 x 10 ⁻²	2.50 x 10 ⁻²	2.50 x 10 ⁻²	2.50 x 10 ⁻²
N ₂ O	6.12 x 10 ⁻²¹	2.70 x 10 ⁻¹⁹	6.51 x 10 ⁻¹⁸	9.59 x 10 ⁻¹⁷	9.62 x 10 ⁻¹⁶	7.09 x 10 ⁻¹⁵
N ₂ O ₃	2.31 x 10 ⁻⁴⁹	3.40 x 10 ⁻⁴⁵	1.07 x 10 ⁻⁴¹	9.59 x 10 ⁻³⁹	3.24 x 10 ⁻³⁶	4.99 x 10 ⁻³⁴
N ₂ O ₄	3.07 x 10 ⁻⁶⁰	3.83 x 10 ⁻⁵⁵	7.29 x 10 ⁻⁵¹	3.03 x 10 ⁻⁴⁷	3.82 x 10 ⁻⁴⁴	1.85 x 10 ⁻⁴¹
N ₂ O ₅	1.81 x 10 ⁻⁷⁵	4.30 x 10 ⁻⁶⁹	9.72 x 10 ⁻⁶⁴	3.28 x 10 ⁻⁵⁹	2.49 x 10 ⁻⁵⁵	5.71 x 10 ⁻⁵²
N ₃	2.64 x 10 ⁻²⁹	3.11 x 10 ⁻²⁷	1.68 x 10 ⁻²⁵	4.93 x 10 ⁻²⁴	8.95 x 10 ⁻²³	1.11 x 10 ⁻²¹

Species	Partial Pressure (atm)					
T(K) =	1000	1100	1200	1300	1400	1500
	SiO ₂ (c,l)					
O	5.33 x 10 ⁻²¹	1.52 x 10 ⁻¹⁸	1.71 x 10 ⁻¹⁶	9.30 x 10 ⁻¹⁵	2.85 x 10 ⁻¹³	5.54 x 10 ⁻¹²
OH	1.12 x 10 ⁻¹²	2.98 x 10 ⁻¹¹	4.63 x 10 ⁻¹⁰	4.69 x 10 ⁻⁹	3.39 x 10 ⁻⁸	1.88 x 10 ⁻⁷
O ₂	1.17 x 10 ⁻²¹	3.76 x 10 ⁻¹⁹	4.74 x 10 ⁻¹⁷	2.81 x 10 ⁻¹⁵	9.24 x 10 ⁻¹⁴	1.89 x 10 ⁻¹²
O ₃	3.48 x 10 ⁻⁴³	9.24 x 10 ⁻³⁹	4.87 x 10 ⁻³⁵	6.78 x 10 ⁻³²	3.33 x 10 ⁻²⁹	7.08 x 10 ⁻²⁷
Si	9.91 x 10 ⁻³⁴	8.21 x 10 ⁻³⁰	1.46 x 10 ⁻²⁶	8.14 x 10 ⁻²⁴	1.84 x 10 ⁻²¹	2.02 x 10 ⁻¹⁹
Si(OH) ₂	6.72 x 10 ⁻²³	1.33 x 10 ⁻²⁰	1.07 x 10 ⁻¹⁸	4.33 x 10 ⁻¹⁷	1.02 x 10 ⁻¹⁵	1.58 x 10 ⁻¹⁴
Si(OH) ₃	1.72 x 10 ⁻²⁴	2.22 x 10 ⁻²²	1.27 x 10 ⁻²⁰	3.85 x 10 ⁻¹⁹	7.16 x 10 ⁻¹⁸	8.98 x 10 ⁻¹⁷
Si(OH) ₄	1.45 x 10 ⁻¹⁵	1.03 x 10 ⁻¹⁴	5.25 x 10 ⁻¹⁴	2.07 x 10 ⁻¹³	6.71 x 10 ⁻¹³	1.85 x 10 ⁻¹²
SiC	2.28 x 10 ⁻⁴⁶	8.39 x 10 ⁻⁴²	5.02 x 10 ⁻³⁸	7.88 x 10 ⁻³⁵	4.32 x 10 ⁻³²	1.02 x 10 ⁻²⁹
SiCl	2.09 x 10 ⁻²⁸	1.66 x 10 ⁻²⁵	4.19 x 10 ⁻²³	4.52 x 10 ⁻²¹	2.49 x 10 ⁻¹⁹	8.00 x 10 ⁻¹⁸
SiCl ₂	1.53 x 10 ⁻²⁴	1.24 x 10 ⁻²²	4.78 x 10 ⁻²¹	1.05 x 10 ⁻¹⁹	1.48 x 10 ⁻¹⁸	1.46 x 10 ⁻¹⁷
SiCl ₃	1.89 x 10 ⁻²⁸	7.63 x 10 ⁻²⁷	1.67 x 10 ⁻²⁵	2.29 x 10 ⁻²⁴	2.18 x 10 ⁻²³	1.54 x 10 ⁻²²
SiCl ₄	2.22 x 10 ⁻²⁴	6.77 x 10 ⁻²⁴	1.76 x 10 ⁻²³	3.98 x 10 ⁻²³	8.10 x 10 ⁻²³	1.51 x 10 ⁻²²
SiH	1.16 x 10 ⁻³¹	3.71 x 10 ⁻²⁸	2.94 x 10 ⁻²⁵	8.32 x 10 ⁻²³	1.05 x 10 ⁻²⁰	6.90 x 10 ⁻¹⁹
SiHCl	6.00 x 10 ⁻²⁷	1.75 x 10 ⁻²⁴	1.93 x 10 ⁻²²	1.02 x 10 ⁻²⁰	3.08 x 10 ⁻¹⁹	5.88 x 10 ⁻¹⁸
SiHCl ₃	1.71 x 10 ⁻²³	1.04 x 10 ⁻²²	4.72 x 10 ⁻²²	1.71 x 10 ⁻²¹	5.20 x 10 ⁻²¹	1.37 x 10 ⁻²⁰
SiH ₂	6.55 x 10 ⁻³⁰	7.38 x 10 ⁻²⁷	2.46 x 10 ⁻²⁴	3.35 x 10 ⁻²²	2.27 x 10 ⁻²⁰	8.75 x 10 ⁻¹⁹
SiH ₂ Cl ₂	1.43 x 10 ⁻²³	1.95 x 10 ⁻²²	1.69 x 10 ⁻²¹	1.06 x 10 ⁻²⁰	5.14 x 10 ⁻²⁰	2.03 x 10 ⁻¹⁹
SiH ₃	9.71 x 10 ⁻³⁰	4.74 x 10 ⁻²⁷	7.80 x 10 ⁻²⁵	5.84 x 10 ⁻²³	2.37 x 10 ⁻²¹	5.86 x 10 ⁻²⁰
SiH ₃ Cl	3.04 x 10 ⁻²⁴	9.69 x 10 ⁻²³	1.66 x 10 ⁻²¹	1.85 x 10 ⁻²⁰	1.47 x 10 ⁻¹⁹	8.85 x 10 ⁻¹⁹
SiH ₄	2.53 x 10 ⁻²⁵	1.84 x 10 ⁻²³	6.16 x 10 ⁻²²	1.20 x 10 ⁻²⁰	1.54 x 10 ⁻¹⁹	1.41 x 10 ⁻¹⁸
SiN	5.34 x 10 ⁻³³	1.84 x 10 ⁻²⁹	1.57 x 10 ⁻²⁶	4.71 x 10 ⁻²⁴	6.27 x 10 ⁻²²	4.33 x 10 ⁻²⁰
SiO	1.25 x 10 ⁻¹⁸	4.35 x 10 ⁻¹⁶	5.55 x 10 ⁻¹⁴	3.32 x 10 ⁻¹²	1.10 x 10 ⁻¹⁰	2.27 x 10 ⁻⁹
SiO(OH)	1.87 x 10 ⁻²¹	6.84 x 10 ⁻¹⁹	9.18 x 10 ⁻¹⁷	5.74 x 10 ⁻¹⁵	1.97 x 10 ⁻¹³	4.19 x 10 ⁻¹²
SiO(OH) ₂	4.66 x 10 ⁻¹²	8.78 x 10 ⁻¹¹	1.01 x 10 ⁻⁹	7.90 x 10 ⁻⁹	4.57 x 10 ⁻⁸	2.08 x 10 ⁻⁷
SiOH	1.79 x 10 ⁻³⁰	3.63 x 10 ⁻²⁷	2.00 x 10 ⁻²⁴	4.14 x 10 ⁻²²	3.97 x 10 ⁻²⁰	2.06 x 10 ⁻¹⁸
SiO ₂	6.71 x 10 ⁻²²	3.83 x 10 ⁻¹⁹	7.52 x 10 ⁻¹⁷	6.49 x 10 ⁻¹⁵	2.94 x 10 ⁻¹³	7.96 x 10 ⁻¹²

Species	Partial Pressure (atm)					
T(K) =	1000	1100	1200	1300	1400	1500
	SiO₂(c,l)					
$\Sigma P(\text{Si})$ (atm)	4.67×10^{-12}	8.79×10^{-11}	1.01×10^{-9}	7.90×10^{-9}	4.58×10^{-8}	2.10×10^{-7}
$\Sigma P(\text{Si-O})$ (atm)	1.25×10^{-18}	4.36×10^{-16}	5.55×10^{-14}	3.33×10^{-12}	1.10×10^{-10}	2.28×10^{-9}
$\Sigma P(\text{Si-Cl})$ (atm)	3.81×10^{-23}	5.29×10^{-22}	8.86×10^{-21}	1.50×10^{-19}	2.24×10^{-18}	2.98×10^{-17}
Si(1685) ^a	0 ^b	0	0	0	0	0
C(5000)	0	0	0	0	0	0
SiC-a(3103)	0	0	0	0	0	0
Si ₃ N ₄ - α (c)	0	0	0	0	0	0
Si ₂ ON ₂ (c)	0	0	0	0	0	0
SiO ₂ (1696)	1	1	1	1	1	1

Notes: $\Sigma P(\text{Si})$ = Sum of vapor pressures of species containing Si, O, and H
 $\Sigma P(\text{Si-O})$ = Sum of vapor pressures of species containing Si and O only
 $\Sigma P(\text{Si-Cl})$ = Sum of vapor pressures of species containing Si and Cl only
a = Melting point in degrees Kelvin
b = One (1) and zero (0) represent the presence and absence of the solid phase respectively.

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
	ZrO ₂ (c,l)					
C	2.05 x 10 ⁻³⁰	1.07 x 10 ⁻²⁷	1.93 x 10 ⁻²⁵	1.57 x 10 ⁻²³	6.86 x 10 ⁻²²	1.82 x 10 ⁻²⁰
CCl	5.43 x 10 ⁻²⁶	3.88 x 10 ⁻²⁴	1.35 x 10 ⁻²²	2.73 x 10 ⁻²¹	3.61 x 10 ⁻²⁰	3.40 x 10 ⁻¹⁹
CCl ₂	3.61 x 10 ⁻²⁶	7.14 x 10 ⁻²⁵	8.62 x 10 ⁻²⁴	7.14 x 10 ⁻²³	4.40 x 10 ⁻²²	2.14 x 10 ⁻²¹
CCl ₃	5.21 x 10 ⁻³⁰	6.11 x 10 ⁻²⁹	4.85 x 10 ⁻²⁸	2.84 x 10 ⁻²⁷	1.30 x 10 ⁻²⁶	4.93 x 10 ⁻²⁶
CCl ₄	1.34 x 10 ⁻³³	6.84 x 10 ⁻³³	2.78 x 10 ⁻³²	9.28 x 10 ⁻³²	2.65 x 10 ⁻³¹	6.66 x 10 ⁻³¹
CH	1.31 x 10 ⁻²⁶	1.70 x 10 ⁻²⁴	9.55 x 10 ⁻²³	2.89 x 10 ⁻²¹	5.39 x 10 ⁻²⁰	6.83 x 10 ⁻¹⁹
CHCl	1.69 x 10 ⁻²²	2.68 x 10 ⁻²¹	2.63 x 10 ⁻²⁰	1.82 x 10 ⁻¹⁹	9.61 x 10 ⁻¹⁹	4.07 x 10 ⁻¹⁸
CHCl ₂	2.49 x 10 ⁻²¹	8.91 x 10 ⁻²¹	2.58 x 10 ⁻²⁰	6.38 x 10 ⁻²⁰	1.40 x 10 ⁻¹⁹	2.79 x 10 ⁻¹⁹
CHCl ₃	1.47 x 10 ⁻²⁴	2.21 x 10 ⁻²⁴	3.15 x 10 ⁻²⁴	4.30 x 10 ⁻²⁴	5.69 x 10 ⁻²⁴	7.34 x 10 ⁻²⁴
CH ₂	1.27 x 10 ⁻¹⁹	1.59 x 10 ⁻¹⁸	1.26 x 10 ⁻¹⁷	7.28 x 10 ⁻¹⁷	3.29 x 10 ⁻¹⁶	1.22 x 10 ⁻¹⁵
CH ₂ Cl	7.74 x 10 ⁻¹⁶	1.45 x 10 ⁻¹⁵	2.38 x 10 ⁻¹⁵	3.63 x 10 ⁻¹⁵	5.25 x 10 ⁻¹⁵	7.27 x 10 ⁻¹⁵
CH ₂ Cl ₂	7.54 x 10 ⁻¹⁷	3.93 x 10 ⁻¹⁷	2.27 x 10 ⁻¹⁷	1.43 x 10 ⁻¹⁷	9.77 x 10 ⁻¹⁸	7.07 x 10 ⁻¹⁸
CH ₂ O	4.60 x 10 ⁻⁷	4.09 x 10 ⁻⁷	3.62 x 10 ⁻⁷	3.25 x 10 ⁻⁷	2.96 x 10 ⁻⁷	2.73 x 10 ⁻⁷
CH ₃	2.81 x 10 ⁻¹⁰	2.40 x 10 ⁻¹⁰	2.01 x 10 ⁻¹⁰	1.73 x 10 ⁻¹⁰	1.53 x 10 ⁻¹⁰	1.38 x 10 ⁻¹⁰
CH ₃ Cl	6.68 x 10 ⁻¹⁰	1.30 x 10 ⁻¹⁰	3.24 x 10 ⁻¹¹	1.00 x 10 ⁻¹¹	3.68 x 10 ⁻¹²	1.55 x 10 ⁻¹²
CH ₄	3.47 x 10 ⁻³	2.42 x 10 ⁻⁴	2.48 x 10 ⁻⁵	3.61 x 10 ⁻⁶	6.95 x 10 ⁻⁷	1.67 x 10 ⁻⁷
CN	1.09 x 10 ⁻¹⁹	2.70 x 10 ⁻¹⁸	3.84 x 10 ⁻¹⁷	3.64 x 10 ⁻¹⁶	2.51 x 10 ⁻¹⁵	1.34 x 10 ⁻¹⁴
CNO	2.80 x 10 ⁻¹⁹	5.90 x 10 ⁻¹⁸	7.45 x 10 ⁻¹⁷	6.38 x 10 ⁻¹⁶	4.03 x 10 ⁻¹⁵	2.00 x 10 ⁻¹⁴
CN ₂	1.76 x 10 ⁻³¹	2.17 x 10 ⁻²⁹	1.18 x 10 ⁻²⁷	3.51 x 10 ⁻²⁶	6.43 x 10 ⁻²⁵	8.05 x 10 ⁻²⁴
CO	3.24 x 10 ⁻¹	3.47 x 10 ⁻¹	3.63 x 10 ⁻¹	3.76 x 10 ⁻¹	3.86 x 10 ⁻¹	3.95 x 10 ⁻¹
COCl	5.60 x 10 ⁻¹⁶	4.87 x 10 ⁻¹⁵	2.97 x 10 ⁻¹⁴	1.37 x 10 ⁻¹³	5.07 x 10 ⁻¹³	1.58 x 10 ⁻¹²
COCl ₂	9.68 x 10 ⁻¹⁸	2.64 x 10 ⁻¹⁷	6.24 x 10 ⁻¹⁷	1.30 x 10 ⁻¹⁶	2.44 x 10 ⁻¹⁶	4.24 x 10 ⁻¹⁶
COHCl	1.87 x 10 ⁻¹²	3.02 x 10 ⁻¹²	4.49 x 10 ⁻¹²	6.28 x 10 ⁻¹²	8.39 x 10 ⁻¹²	1.08 x 10 ⁻¹¹
COOH	1.06 x 10 ⁻¹²	6.34 x 10 ⁻¹²	2.81 x 10 ⁻¹¹	9.87 x 10 ⁻¹¹	2.89 x 10 ⁻¹⁰	7.30 x 10 ⁻¹⁰
CO ₂	1.84 x 10 ⁻¹	1.61 x 10 ⁻¹	1.45 x 10 ⁻¹	1.32 x 10 ⁻¹	1.22 x 10 ⁻¹	1.13 x 10 ⁻¹
Cl	1.14 x 10 ⁻¹¹	1.27 x 10 ⁻¹⁰	9.57 x 10 ⁻¹⁰	5.26 x 10 ⁻⁹	2.32 x 10 ⁻⁸	8.35 x 10 ⁻⁸
ClHO	1.42 x 10 ⁻¹⁶	2.50 x 10 ⁻¹⁵	2.78 x 10 ⁻¹⁴	2.12 x 10 ⁻¹³	1.20 x 10 ⁻¹²	5.41 x 10 ⁻¹²
ClO	2.36 x 10 ⁻²³	3.68 x 10 ⁻²¹	2.54 x 10 ⁻¹⁹	9.12 x 10 ⁻¹⁸	1.96 x 10 ⁻¹⁶	2.79 x 10 ⁻¹⁵
ClO ₂	8.58 x 10 ⁻³⁸	2.48 x 10 ⁻³⁴	1.99 x 10 ⁻³¹	5.66 x 10 ⁻²⁹	7.14 x 10 ⁻²⁷	4.71 x 10 ⁻²⁵
Cl ₂	8.12 x 10 ⁻¹⁶	6.62 x 10 ⁻¹⁵	3.91 x 10 ⁻¹⁴	1.76 x 10 ⁻¹³	6.42 x 10 ⁻¹³	1.97 x 10 ⁻¹²

Species	Partial Pressure (atm)					
T(K) =	1000	1100	1200	1300	1400	1500
	ZrO ₂ (c,l)					
Cl ₂ O	7.53 x 10 ⁻³⁴	2.92 x 10 ⁻³¹	4.37 x 10 ⁻²⁹	3.02 x 10 ⁻²⁷	1.14 x 10 ⁻²⁵	2.66 x 10 ⁻²⁴
H	1.30 x 10 ⁻⁹	1.45 x 10 ⁻⁸	1.08 x 10 ⁻⁷	5.90 x 10 ⁻⁷	2.55 x 10 ⁻⁶	9.07 x 10 ⁻⁶
HCN	1.52 x 10 ⁻⁷	1.30 x 10 ⁻⁷	1.11 x 10 ⁻⁷	9.70 x 10 ⁻⁸	8.70 x 10 ⁻⁸	7.95 x 10 ⁻⁸
HCO	1.32 x 10 ⁻¹¹	7.11 x 10 ⁻¹¹	2.84 x 10 ⁻¹⁰	9.13 x 10 ⁻¹⁰	2.48 x 10 ⁻⁹	5.89 x 10 ⁻⁹
HCl	3.02 x 10 ⁻³	3.00 x 10 ⁻³	3.00 x 10 ⁻³	3.00 x 10 ⁻³	3.00 x 10 ⁻³	3.00 x 10 ⁻³
HNCO	3.63 x 10 ⁻⁹	4.11 x 10 ⁻⁹	4.50 x 10 ⁻⁹	4.86 x 10 ⁻⁹	5.19 x 10 ⁻⁹	5.50 x 10 ⁻⁹
HNO	7.62 x 10 ⁻²⁰	3.83 x 10 ⁻¹⁸	1.01 x 10 ⁻¹⁶	1.60 x 10 ⁻¹⁵	1.70 x 10 ⁻¹⁴	1.32 x 10 ⁻¹³
HNO ₂	7.83 x 10 ⁻²⁵	1.02 x 10 ⁻²²	6.09 x 10 ⁻²¹	1.92 x 10 ⁻¹⁹	3.68 x 10 ⁻¹⁸	4.73 x 10 ⁻¹⁷
HNO ₃	6.38 x 10 ⁻³⁷	8.17 x 10 ⁻³⁴	3.32 x 10 ⁻³¹	5.30 x 10 ⁻²⁹	4.08 x 10 ⁻²⁷	1.75 x 10 ⁻²⁵
HO ₂	9.81 x 10 ⁻²⁵	3.30 x 10 ⁻²²	4.28 x 10 ⁻²⁰	2.60 x 10 ⁻¹⁸	8.71 x 10 ⁻¹⁷	1.81 x 10 ⁻¹⁵
H ₂	3.30 x 10 ⁻¹	3.16 x 10 ⁻¹	3.00 x 10 ⁻¹	2.87 x 10 ⁻¹	2.77 x 10 ⁻¹	2.68 x 10 ⁻¹
H ₂ O	1.30 x 10 ⁻¹	1.48 x 10 ⁻¹	1.64 x 10 ⁻¹	1.77 x 10 ⁻¹	1.88 x 10 ⁻¹	1.96 x 10 ⁻¹
H ₂ O ₂	1.22 x 10 ⁻²⁰	8.06 x 10 ⁻¹⁹	2.68 x 10 ⁻¹⁷	5.14 x 10 ⁻¹⁶	6.41 x 10 ⁻¹⁵	5.67 x 10 ⁻¹⁴
N	4.89 x 10 ⁻²³	8.90 x 10 ⁻²¹	6.86 x 10 ⁻¹⁹	2.72 x 10 ⁻¹⁷	6.37 x 10 ⁻¹⁶	9.84 x 10 ⁻¹⁵
NH	2.17 x 10 ⁻²⁰	1.30 x 10 ⁻¹⁸	3.91 x 10 ⁻¹⁷	6.97 x 10 ⁻¹⁶	8.23 x 10 ⁻¹⁵	6.99 x 10 ⁻¹⁴
NH ₂	7.67 x 10 ⁻¹⁴	5.54 x 10 ⁻¹³	2.84 x 10 ⁻¹²	1.13 x 10 ⁻¹¹	3.68 x 10 ⁻¹¹	1.02 x 10 ⁻¹⁰
NH ₂ NO ₂	2.73 x 10 ⁻³⁶	6.03 x 10 ⁻³⁴	5.57 x 10 ⁻³²	2.56 x 10 ⁻³⁰	6.80 x 10 ⁻²⁹	1.17 x 10 ⁻²⁷
NH ₂ OH	8.55 x 10 ⁻¹⁹	7.65 x 10 ⁻¹⁸	4.74 x 10 ⁻¹⁷	2.21 x 10 ⁻¹⁶	8.25 x 10 ⁻¹⁶	2.58 x 10 ⁻¹⁵
NH ₃	1.76 x 10 ⁻⁵	8.95 x 10 ⁻⁶	4.99 x 10 ⁻⁶	3.04 x 10 ⁻⁶	1.98 x 10 ⁻⁶	1.37 x 10 ⁻⁶
NO	4.18 x 10 ⁻¹⁶	2.03 x 10 ⁻¹⁴	5.25 x 10 ⁻¹³	8.18 x 10 ⁻¹²	8.59 x 10 ⁻¹¹	6.57 x 10 ⁻¹⁰
NOCl	9.65 x 10 ⁻²⁵	8.76 x 10 ⁻²³	3.87 x 10 ⁻²¹	9.54 x 10 ⁻²⁰	1.49 x 10 ⁻¹⁸	1.60 x 10 ⁻¹⁷
NO ₂	1.72 x 10 ⁻²⁷	7.96 x 10 ⁻²⁵	1.37 x 10 ⁻²²	1.06 x 10 ⁻²⁰	4.29 x 10 ⁻¹⁹	1.09 x 10 ⁻¹⁷
NO ₂ Cl	5.49 x 10 ⁻³⁸	5.85 x 10 ⁻³⁵	2.05 x 10 ⁻³²	2.91 x 10 ⁻³⁰	2.03 x 10 ⁻²⁸	8.00 x 10 ⁻²⁷
NO ₃	1.48 x 10 ⁻⁴⁴	1.90 x 10 ⁻⁴⁰	5.32 x 10 ⁻³⁷	4.34 x 10 ⁻³⁴	1.35 x 10 ⁻³¹	1.95 x 10 ⁻²⁹
N ₂	2.51 x 10 ⁻²	2.50 x 10 ⁻²	2.50 x 10 ⁻²	2.50 x 10 ⁻²	2.50 x 10 ⁻²	2.50 x 10 ⁻²
N ₂ O	6.12 x 10 ⁻²¹	2.71 x 10 ⁻¹⁹	6.52 x 10 ⁻¹⁸	9.60 x 10 ⁻¹⁷	9.63 x 10 ⁻¹⁶	7.10 x 10 ⁻¹⁵
N ₂ O ₃	2.31 x 10 ⁻⁴⁹	3.42 x 10 ⁻⁴⁵	1.07 x 10 ⁻⁴¹	9.65 x 10 ⁻³⁹	3.26 x 10 ⁻³⁶	5.03 x 10 ⁻³⁴
N ₂ O ₄	3.08 x 10 ⁻⁶⁰	3.85 x 10 ⁻⁵⁵	7.34 x 10 ⁻⁵¹	3.05 x 10 ⁻⁴⁷	3.85 x 10 ⁻⁴⁴	1.87 x 10 ⁻⁴¹
N ₂ O ₅	1.82 x 10 ⁻⁷⁵	4.34 x 10 ⁻⁶⁹	9.82 x 10 ⁻⁶⁴	3.32 x 10 ⁻⁵⁹	2.52 x 10 ⁻⁵⁵	5.78 x 10 ⁻⁵²
N ₃	2.63 x 10 ⁻²⁹	3.10 x 10 ⁻²⁷	1.68 x 10 ⁻²⁵	4.92 x 10 ⁻²⁴	8.93 x 10 ⁻²³	1.11 x 10 ⁻²¹

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
ZrO₂(c,l)						
O	5.34 x 10 ⁻²¹	1.52 x 10 ⁻¹⁸	1.71 x 10 ⁻¹⁶	9.33 x 10 ⁻¹⁵	2.86 x 10 ⁻¹³	5.55 x 10 ⁻¹²
OH	1.11 x 10 ⁻¹²	2.98 x 10 ⁻¹¹	4.63 x 10 ⁻¹⁰	4.69 x 10 ⁻⁹	3.39 x 10 ⁻⁸	1.88 x 10 ⁻⁷
O ₂	1.17 x 10 ⁻²¹	3.77 x 10 ⁻¹⁹	4.76 x 10 ⁻¹⁷	2.82 x 10 ⁻¹⁵	9.29 x 10 ⁻¹⁴	1.90 x 10 ⁻¹²
O ₃	3.50 x 10 ⁻⁴³	9.29 x 10 ⁻³⁹	4.91 x 10 ⁻³⁵	6.83 x 10 ⁻³²	3.36 x 10 ⁻²⁹	7.14 x 10 ⁻²⁷
Zr	4.46 x 10 ⁻⁵¹	1.44 x 10 ⁻⁴⁵	5.42 x 10 ⁻⁴¹	4.01 x 10 ⁻³⁷	8.29 x 10 ⁻³⁴	6.13 x 10 ⁻³¹
Zr(OH) ₂	1.07 x 10 ⁻³³	3.53 x 10 ⁻³⁰	2.95 x 10 ⁻²⁷	8.67 x 10 ⁻²⁵	1.12 x 10 ⁻²²	7.50 x 10 ⁻²¹
Zr(OH) ₃	4.16 x 10 ⁻²⁹	2.49 x 10 ⁻²⁶	5.08 x 10 ⁻²⁴	4.55 x 10 ⁻²²	2.13 x 10 ⁻²⁰	5.91 x 10 ⁻¹⁹
Zr(OH) ₄	6.22 x 10 ⁻²³	5.62 x 10 ⁻²¹	2.41 x 10 ⁻¹⁹	5.76 x 10 ⁻¹⁸	8.71 x 10 ⁻¹⁷	9.09 x 10 ⁻¹⁶
ZrCl	1.69 x 10 ⁻⁴³	4.03 x 10 ⁻³⁹	1.74 x 10 ⁻³⁵	2.07 x 10 ⁻³²	8.94 x 10 ⁻³⁰	1.71 x 10 ⁻²⁷
ZrCl ₂	1.46 x 10 ⁻³³	1.52 x 10 ⁻³⁰	4.91 x 10 ⁻²⁸	6.53 x 10 ⁻²⁶	4.32 x 10 ⁻²⁴	1.62 x 10 ⁻²²
ZrCl ₃	1.30 x 10 ⁻²⁴	5.42 x 10 ⁻²³	1.22 x 10 ⁻²¹	1.72 x 10 ⁻²⁰	1.66 x 10 ⁻¹⁹	1.18 x 10 ⁻¹⁸
ZrCl ₄	5.52 x 10 ⁻¹⁸	1.32 x 10 ⁻¹⁷	2.78 x 10 ⁻¹⁷	5.26 x 10 ⁻¹⁷	9.14 x 10 ⁻¹⁷	1.47 x 10 ⁻¹⁶
ZrN	1.97 x 10 ⁻⁴⁹	2.08 x 10 ⁻⁴⁴	3.07 x 10 ⁻⁴⁰	1.03 x 10 ⁻³⁶	1.07 x 10 ⁻³³	4.33 x 10 ⁻³¹
ZrO	1.56 x 10 ⁻³⁷	3.28 x 10 ⁻³³	1.28 x 10 ⁻²⁹	1.39 x 10 ⁻²⁶	5.49 x 10 ⁻²⁴	9.66 x 10 ⁻²²
ZrO(OH)	1.21 x 10 ⁻³²	6.07 x 10 ⁻²⁹	7.20 x 10 ⁻²⁶	2.83 x 10 ⁻²³	4.68 x 10 ⁻²¹	3.85 x 10 ⁻¹⁹
ZrO(OH) ₂	9.79 x 10 ⁻²⁹	9.01 x 10 ⁻²⁶	2.64 x 10 ⁻²³	3.20 x 10 ⁻²¹	1.93 x 10 ⁻¹⁹	6.65 x 10 ⁻¹⁸
ZrOH	2.00 x 10 ⁻⁴²	6.69 x 10 ⁻³⁸	3.80 x 10 ⁻³⁴	5.63 x 10 ⁻³¹	2.91 x 10 ⁻²⁸	6.42 x 10 ⁻²⁶
ZrO ₂	1.09 x 10 ⁻³⁰	4.68 x 10 ⁻²⁷	4.91 x 10 ⁻²⁴	1.74 x 10 ⁻²¹	2.62 x 10 ⁻¹⁹	1.99 x 10 ⁻¹⁷
Σ P(Zr) (atm)	5.52 x 10 ⁻¹⁸	1.32 x 10 ⁻¹⁷	2.80 x 10 ⁻¹⁷	5.84 x 10 ⁻¹⁷	1.79 x 10 ⁻¹⁶	1.08 x 10 ⁻¹⁵
Σ P(Zr-O) (atm)	1.09 x 10 ⁻³⁰	4.68 x 10 ⁻²⁷	4.91 x 10 ⁻²⁴	1.74 x 10 ⁻²¹	2.62 x 10 ⁻¹⁹	1.99 x 10 ⁻¹⁷
Σ P(Zr-Cl) (atm)	5.52 x 10 ⁻¹⁸	1.32 x 10 ⁻¹⁷	2.78 x 10 ⁻¹⁷	5.26 x 10 ⁻¹⁷	9.16 x 10 ⁻¹⁷	1.48 x 10 ⁻¹⁶
Zr(2125) ^a	0 ^b	0	0	0	0	0
ZrC(3805)	0	0	0	0	0	0
ZrN(3225)	0	0	0	0	0	0
ZrO ₂ (2950)	1	1	1	1	1	1
ZrCl ₂ (995)	0	0	0	0	0	0
ZrCl ₃ (900)	0	0	0	0	0	0
ZrCl ₄ (c)	0	0	0	0	0	0

Notes: ΣP(Zr) = Sum of vapor pressures of species containing Zr, O, and H
 ΣP(Zr-O) = Sum of vapor pressures of species containing Zr and O only
 ΣP(Zr-Cl) = Sum of vapor pressures of species containing Zr and Cl only
 a = Melting point in degrees Kelvin
 b = One (1) and zero (0) represent the presence and absence of the solid phase respectively.

**CALCULATED PARTIAL PRESSURES OF SPECIES OVER METAL OXIDES IN THE
PRESENCE OF TEXACO COAL GAS MIXTURE CONTAINING 300 PPM HCl
AT 20 ATM TOTAL PRESSURE**

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
	TiO ₂ (c,l)					
C	6.26 x 10 ⁻³⁰	1.33 x 10 ⁻²⁶	3.51 x 10 ⁻²⁴	3.11 x 10 ⁻²²	1.37 x 10 ⁻²⁰	3.65 x 10 ⁻¹⁹
CCl	1.20 x 10 ⁻²⁵	2.59 x 10 ⁻²³	1.14 x 10 ⁻²¹	2.42 x 10 ⁻²⁰	3.23 x 10 ⁻¹⁹	3.05 x 10 ⁻¹⁸
CCl ₂	5.78 x 10 ⁻²⁶	2.56 x 10 ⁻²⁴	3.39 x 10 ⁻²³	2.85 x 10 ⁻²²	1.76 x 10 ⁻²¹	8.58 x 10 ⁻²¹
CCl ₃	6.05 x 10 ⁻³⁰	1.18 x 10 ⁻²⁸	8.86 x 10 ⁻²⁸	5.10 x 10 ⁻²⁷	2.34 x 10 ⁻²⁶	8.83 x 10 ⁻²⁶
CCl ₄	1.12 x 10 ⁻³³	7.10 x 10 ⁻³³	2.36 x 10 ⁻³²	7.50 x 10 ⁻³²	2.12 x 10 ⁻³¹	5.33 x 10 ⁻³¹
CH	1.35 x 10 ⁻²⁵	8.50 x 10 ⁻²³	7.59 x 10 ⁻²¹	2.55 x 10 ⁻¹⁹	4.84 x 10 ⁻¹⁸	6.15 x 10 ⁻¹⁷
CHCl	1.27 x 10 ⁻²¹	7.20 x 10 ⁻²⁰	9.74 x 10 ⁻¹⁹	7.23 x 10 ⁻¹⁸	3.86 x 10 ⁻¹⁷	1.64 x 10 ⁻¹⁶
CHCl ₂	1.35 x 10 ⁻²⁰	1.28 x 10 ⁻¹⁹	4.43 x 10 ⁻¹⁹	1.14 x 10 ⁻¹⁸	2.51 x 10 ⁻¹⁸	5.01 x 10 ⁻¹⁸
CHCl ₃	5.79 x 10 ⁻²⁴	1.71 x 10 ⁻²³	2.52 x 10 ⁻²³	3.45 x 10 ⁻²³	4.57 x 10 ⁻²³	5.89 x 10 ⁻²³
CH ₂	4.44 x 10 ⁻¹⁸	3.18 x 10 ⁻¹⁶	4.38 x 10 ⁻¹⁵	2.86 x 10 ⁻¹⁴	1.32 x 10 ⁻¹³	4.92 x 10 ⁻¹³
CH ₂ Cl	1.97 x 10 ⁻¹⁴	1.56 x 10 ⁻¹³	3.85 x 10 ⁻¹³	6.43 x 10 ⁻¹³	9.44 x 10 ⁻¹³	1.31 x 10 ⁻¹²
CH ₂ Cl ₂	1.39 x 10 ⁻¹⁵	2.28 x 10 ⁻¹⁵	1.71 x 10 ⁻¹⁵	1.14 x 10 ⁻¹⁵	7.85 x 10 ⁻¹⁶	5.69 x 10 ⁻¹⁶
CH ₂ O	5.29 x 10 ⁻⁵	1.17 x 10 ⁻⁴	1.36 x 10 ⁻⁴	1.29 x 10 ⁻⁴	1.19 x 10 ⁻⁴	1.10 x 10 ⁻⁴
CH ₃	3.34 x 10 ⁻⁸	1.93 x 10 ⁻⁷	3.07 x 10 ⁻⁷	3.05 x 10 ⁻⁷	2.75 x 10 ⁻⁷	2.49 x 10 ⁻⁷
CH ₃ Cl	5.75 x 10 ⁻⁸	5.64 x 10 ⁻⁸	2.29 x 10 ⁻⁸	7.90 x 10 ⁻⁹	2.96 x 10 ⁻⁹	1.26 x 10 ⁻⁹
CH ₄	1.40	7.80 x 10 ⁻¹	1.65 x 10 ⁻¹	2.83 x 10 ⁻²	5.61 x 10 ⁻³	1.36 x 10 ⁻³
CN	1.65 x 10 ⁻¹⁸	1.56 x 10 ⁻¹⁶	3.15 x 10 ⁻¹⁵	3.22 x 10 ⁻¹⁴	2.25 x 10 ⁻¹³	1.20 x 10 ⁻¹²
CNO	1.38 x 10 ⁻¹⁷	4.84 x 10 ⁻¹⁶	6.58 x 10 ⁻¹⁵	5.71 x 10 ⁻¹⁴	3.61 x 10 ⁻¹³	1.79 x 10 ⁻¹²
CN ₂	1.31 x 10 ⁻²⁹	5.81 x 10 ⁻²⁷	4.37 x 10 ⁻²⁵	1.39 x 10 ⁻²³	2.58 x 10 ⁻²²	3.24 x 10 ⁻²¹
CO	3.23	6.13	7.11	7.50	7.74	7.92
COCl	4.06 x 10 ⁻¹⁵	4.63 x 10 ⁻¹⁴	2.70 x 10 ⁻¹³	1.23 x 10 ⁻¹²	4.54 x 10 ⁻¹²	1.41 x 10 ⁻¹¹
COCl ₂	5.07 x 10 ⁻¹⁷	1.35 x 10 ⁻¹⁶	2.64 x 10 ⁻¹⁶	5.24 x 10 ⁻¹⁶	9.79 x 10 ⁻¹⁶	1.70 x 10 ⁻¹⁵
COHCl	4.59 x 10 ⁻¹¹	1.15 x 10 ⁻¹⁰	1.79 x 10 ⁻¹⁰	2.52 x 10 ⁻¹⁰	3.37 x 10 ⁻¹⁰	4.34 x 10 ⁻¹⁰
COOH	1.17 x 10 ⁻¹⁰	6.40 x 10 ⁻¹⁰	2.60 x 10 ⁻⁹	8.90 x 10 ⁻⁹	2.59 x 10 ⁻⁸	6.54 x 10 ⁻⁸
CO ₂	6.03	4.06	3.07	2.67	2.43	2.26
Cl	8.27 x 10 ⁻¹²	6.81 x 10 ⁻¹¹	4.45 x 10 ⁻¹⁰	2.37 x 10 ⁻⁹	1.04 x 10 ⁻⁸	3.73 x 10 ⁻⁸
ClHO	1.15 x 10 ⁻¹⁵	7.69 x 10 ⁻¹⁵	6.10 x 10 ⁻¹⁴	4.30 x 10 ⁻¹³	2.41 x 10 ⁻¹²	1.08 x 10 ⁻¹¹
ClO	5.61 x 10 ⁻²³	2.81 x 10 ⁻²¹	1.27 x 10 ⁻¹⁹	4.15 x 10 ⁻¹⁸	8.76 x 10 ⁻¹⁷	1.24 x 10 ⁻¹⁵
ClO ₂	6.67 x 10 ⁻³⁷	2.70 x 10 ⁻³⁴	1.08 x 10 ⁻³¹	2.60 x 10 ⁻²⁹	3.20 x 10 ⁻²⁷	2.10 x 10 ⁻²⁵

Species	Partial Pressure (atm)					
T(K) =	1000	1100	1200	1300	1400	1500
	TiO ₂ (c,l)					
Cl ₂	4.26 x 10 ⁻¹⁶	1.91 x 10 ⁻¹⁵	8.46 x 10 ⁻¹⁵	3.57 x 10 ⁻¹⁴	1.28 x 10 ⁻¹³	3.94 x 10 ⁻¹³
Cl ₂ O	1.29 x 10 ⁻³³	1.20 x 10 ⁻³¹	1.02 x 10 ⁻²⁹	6.19 x 10 ⁻²⁸	2.29 x 10 ⁻²⁶	5.30 x 10 ⁻²⁵
H	4.40 x 10 ⁻⁹	5.80 x 10 ⁻⁸	4.71 x 10 ⁻⁷	2.63 x 10 ⁻⁶	1.14 x 10 ⁻⁵	4.06 x 10 ⁻⁵
HCN	7.78 x 10 ⁻⁶	3.00 x 10 ⁻⁵	3.96 x 10 ⁻⁵	3.83 x 10 ⁻⁵	3.49 x 10 ⁻⁵	3.20 x 10 ⁻⁵
HCO	4.47 x 10 ⁻¹⁰	5.05 x 10 ⁻⁹	2.43 x 10 ⁻⁸	8.13 x 10 ⁻⁸	2.22 x 10 ⁻⁷	5.29 x 10 ⁻⁷
HCl	7.41 x 10 ⁻³	6.47 x 10 ⁻³	6.10 x 10 ⁻³	6.02 x 10 ⁻³	6.00 x 10 ⁻³	6.00 x 10 ⁻³
HNCO	6.08 x 10 ⁻⁷	1.35 x 10 ⁻⁶	1.74 x 10 ⁻⁶	1.94 x 10 ⁻⁶	2.08 x 10 ⁻⁶	2.21 x 10 ⁻⁶
HNO	4.19 x 10 ⁻¹⁸	1.01 x 10 ⁻¹⁶	2.15 x 10 ⁻¹⁵	3.24 x 10 ⁻¹⁴	3.42 x 10 ⁻¹³	2.64 x 10 ⁻¹²
HNO ₂	1.41 x 10 ⁻²²	3.85 x 10 ⁻²¹	1.40 x 10 ⁻¹⁹	3.93 x 10 ⁻¹⁸	7.37 x 10 ⁻¹⁷	9.45 x 10 ⁻¹⁶
HNO ₃	3.77 x 10 ⁻³⁴	4.38 x 10 ⁻³²	8.22 x 10 ⁻³⁰	1.10 x 10 ⁻²⁷	8.18 x 10 ⁻²⁶	3.49 x 10 ⁻²⁴
HO ₂	3.57 x 10 ⁻²³	2.68 x 10 ⁻²¹	2.18 x 10 ⁻¹⁹	1.19 x 10 ⁻¹⁷	3.90 x 10 ⁻¹⁶	8.10 x 10 ⁻¹⁵
H ₂	3.79	5.09	5.75	5.72	5.55	5.38
H ₂ O	4.91	3.40	3.39	3.57	3.77	3.94
H ₂ O ₂	1.50 x 10 ⁻¹⁸	2.63 x 10 ⁻¹⁷	5.98 x 10 ⁻¹⁶	1.05 x 10 ⁻¹⁴	1.29 x 10 ⁻¹³	1.14 x 10 ⁻¹²
N	2.42 x 10 ⁻²²	4.13 x 10 ⁻²⁰	3.09 x 10 ⁻¹⁸	1.22 x 10 ⁻¹⁶	2.85 x 10 ⁻¹⁵	4.40 x 10 ⁻¹⁴
NH	3.65 x 10 ⁻¹⁹	2.42 x 10 ⁻¹⁷	7.72 x 10 ⁻¹⁶	1.39 x 10 ⁻¹⁴	1.65 x 10 ⁻¹³	1.40 x 10 ⁻¹²
NH ₂	4.37 x 10 ⁻¹²	4.14 x 10 ⁻¹¹	2.45 x 10 ⁻¹⁰	1.01 x 10 ⁻⁹	3.30 x 10 ⁻⁹	9.20 x 10 ⁻⁹
NH ₂ NO ₂	8.25 x 10 ⁻³³	4.24 x 10 ⁻³¹	2.52 x 10 ⁻²⁹	1.05 x 10 ⁻²⁷	2.74 x 10 ⁻²⁶	4.69 x 10 ⁻²⁵
NH ₂ OH	5.41 x 10 ⁻¹⁶	3.27 x 10 ⁻¹⁵	1.93 x 10 ⁻¹⁴	8.90 x 10 ⁻¹⁴	3.32 x 10 ⁻¹³	1.04 x 10 ⁻¹²
NH ₃	3.39 x 10 ⁻³	2.69 x 10 ⁻³	1.89 x 10 ⁻³	1.21 x 10 ⁻³	7.98 x 10 ⁻⁴	5.52 x 10 ⁻⁴
NO	6.78 x 10 ⁻¹⁵	1.34 x 10 ⁻¹³	2.55 x 10 ⁻¹²	3.71 x 10 ⁻¹¹	3.84 x 10 ⁻¹⁰	2.93 x 10 ⁻⁹
NOCl	1.13 x 10 ⁻²³	3.11 x 10 ⁻²²	8.76 x 10 ⁻²¹	1.95 x 10 ⁻¹⁹	2.98 x 10 ⁻¹⁸	3.20 x 10 ⁻¹⁷
NO ₂	9.15 x 10 ⁻²⁶	7.47 x 10 ⁻²⁴	7.17 x 10 ⁻²²	4.83 x 10 ⁻²⁰	1.92 x 10 ⁻¹⁸	4.84 x 10 ⁻¹⁷
NO ₂ Cl	2.11 x 10 ⁻³⁶	2.95 x 10 ⁻³⁴	5.00 x 10 ⁻³²	5.99 x 10 ⁻³⁰	4.06 x 10 ⁻²⁸	1.59 x 10 ⁻²⁶
NO ₃	2.58 x 10 ⁻⁴²	2.54 x 10 ⁻³⁹	3.01 x 10 ⁻³⁶	2.01 x 10 ⁻³³	6.06 x 10 ⁻³¹	8.66 x 10 ⁻²⁹
N ₂	6.16 x 10 ⁻¹	5.38 x 10 ⁻¹	5.07 x 10 ⁻¹	5.01 x 10 ⁻¹	5.00 x 10 ⁻¹	5.00 x 10 ⁻¹
N ₂ O	4.91 x 10 ⁻¹⁹	8.29 x 10 ⁻¹⁸	1.43 x 10 ⁻¹⁶	1.95 x 10 ⁻¹⁵	1.93 x 10 ⁻¹⁴	1.42 x 10 ⁻¹³
N ₂ O ₃	1.99 x 10 ⁻⁴⁶	2.12 x 10 ⁻⁴³	2.74 x 10 ⁻⁴⁰	2.00 x 10 ⁻³⁷	6.53 x 10 ⁻³⁵	1.00 x 10 ⁻³²
N ₂ O ₄	8.70 x 10 ⁻⁵⁷	3.40 x 10 ⁻⁵³	2.02 x 10 ⁻⁴⁹	6.42 x 10 ⁻⁴⁶	7.73 x 10 ⁻⁴³	3.71 x 10 ⁻⁴⁰

Species	Partial Pressure (atm)					
	T(K) = 1000	1100	1200	1300	1400	1500
	TiO ₂ (c,l)					
N ₂ O ₅	1.69 x 10 ⁻⁷¹	5.43 x 10 ⁻⁶⁷	2.91 x 10 ⁻⁶²	7.04 x 10 ⁻⁵⁸	5.05 x 10 ⁻⁵⁴	1.15 x 10 ⁻⁵⁰
N ₃	3.19 x 10 ⁻²⁷	3.10 x 10 ⁻²⁵	1.54 x 10 ⁻²³	4.42 x 10 ⁻²²	8.00 x 10 ⁻²¹	9.91 x 10 ⁻²⁰
O	1.75 x 10 ⁻²⁰	2.16 x 10 ⁻¹⁸	1.85 x 10 ⁻¹⁶	9.43 x 10 ⁻¹⁵	2.86 x 10 ⁻¹³	5.54 x 10 ⁻¹²
OH	1.24 x 10 ⁻¹¹	1.70 x 10 ⁻¹⁰	2.19 x 10 ⁻⁹	2.12 x 10 ⁻⁸	1.52 x 10 ⁻⁷	8.40 x 10 ⁻⁷
O ₂	1.26 x 10 ⁻²⁰	7.63 x 10 ⁻¹⁹	5.54 x 10 ⁻¹⁷	2.89 x 10 ⁻¹⁵	9.29 x 10 ⁻¹⁴	1.90 x 10 ⁻¹²
O ₃	1.23 x 10 ⁻⁴¹	2.67 x 10 ⁻³⁸	6.16 x 10 ⁻³⁵	7.07 x 10 ⁻³²	3.36 x 10 ⁻²⁹	7.10 x 10 ⁻²⁷
Ti	1.14 x 10 ⁻³⁷	8.97 x 10 ⁻³³	4.45 x 10 ⁻²⁹	4.24 x 10 ⁻²⁶	1.38 x 10 ⁻²³	2.04 x 10 ⁻²¹
Ti(OH) ₂	4.32 x 10 ⁻²²	2.21 x 10 ⁻¹⁹	3.51 x 10 ⁻¹⁷	2.27 x 10 ⁻¹⁵	7.82 x 10 ⁻¹⁴	1.66 x 10 ⁻¹²
Ti(OH) ₃	5.77 x 10 ⁻¹⁸	3.85 x 10 ⁻¹⁶	1.63 x 10 ⁻¹⁴	3.89 x 10 ⁻¹³	5.89 x 10 ⁻¹²	6.19 x 10 ⁻¹¹
Ti(OH) ₄	1.17 x 10 ⁻¹⁷	2.32 x 10 ⁻¹⁶	5.21 x 10 ⁻¹⁵	8.16 x 10 ⁻¹⁴	8.91 x 10 ⁻¹³	7.10 x 10 ⁻¹²
TiCl	9.70 x 10 ⁻³²	5.89 x 10 ⁻²⁸	3.90 x 10 ⁻²⁵	7.41 x 10 ⁻²³	6.22 x 10 ⁻²¹	2.85 x 10 ⁻¹⁹
TiCl ₂	1.82 x 10 ⁻²²	3.05 x 10 ⁻²⁰	1.14 x 10 ⁻¹⁸	2.09 x 10 ⁻¹⁷	2.42 x 10 ⁻¹⁶	2.01 x 10 ⁻¹⁵
TiCl ₃	4.22 x 10 ⁻¹⁸	5.18 x 10 ⁻¹⁷	2.47 x 10 ⁻¹⁶	8.71 x 10 ⁻¹⁶	2.52 x 10 ⁻¹⁵	6.33 x 10 ⁻¹⁵
TiCl ₄	7.93 x 10 ⁻¹⁸	1.83 x 10 ⁻¹⁷	2.45 x 10 ⁻¹⁷	3.22 x 10 ⁻¹⁷	4.12 x 10 ⁻¹⁷	5.13 x 10 ⁻¹⁷
TiN	1.34 x 10 ⁻⁴⁰	9.48 x 10 ⁻³⁶	4.42 x 10 ⁻³²	4.05 x 10 ⁻²⁹	1.28 x 10 ⁻²⁶	1.85 x 10 ⁻²⁴
TiO	1.50 x 10 ⁻²⁸	9.28 x 10 ⁻²⁵	8.54 x 10 ⁻²²	2.29 x 10 ⁻¹⁹	2.63 x 10 ⁻¹⁷	1.58 x 10 ⁻¹⁵
TiO(OH)	1.87 x 10 ⁻²³	1.66 x 10 ⁻²⁰	4.41 x 10 ⁻¹⁸	4.65 x 10 ⁻¹⁶	2.46 x 10 ⁻¹⁴	7.57 x 10 ⁻¹³
TiO(OH) ₂	6.59 x 10 ⁻²⁵	2.29 x 10 ⁻²²	4.06 x 10 ⁻²⁰	3.42 x 10 ⁻¹⁸	1.54 x 10 ⁻¹⁶	4.17 x 10 ⁻¹⁵
TiOCl ₂	1.11 x 10 ⁻¹⁵	1.71 x 10 ⁻¹⁴	1.36 x 10 ⁻¹³	7.93 x 10 ⁻¹³	3.58 x 10 ⁻¹²	1.32 x 10 ⁻¹¹
TiOH	7.01 x 10 ⁻³²	7.00 x 10 ⁻²⁸	9.01 x 10 ⁻²⁵	3.05 x 10 ⁻²²	4.21 x 10 ⁻²⁰	2.95 x 10 ⁻¹⁸
TiO ₂	1.41 x 10 ⁻²³	1.33 x 10 ⁻²⁰	3.93 x 10 ⁻¹⁸	4.77 x 10 ⁻¹⁶	2.87 x 10 ⁻¹⁴	9.92 x 10 ⁻¹³
Σ P(Ti) (atm)	1.14 x 10 ⁻¹⁵	1.78 x 10 ⁻¹⁴	1.58 x 10 ⁻¹³	1.27 x 10 ⁻¹²	1.05 x 10 ⁻¹¹	8.56 x 10 ⁻¹¹
Σ P(Ti-O) (atm)	1.41 x 10 ⁻²³	1.33 x 10 ⁻²⁰	3.93 x 10 ⁻¹⁸	4.77 x 10 ⁻¹⁶	2.88 x 10 ⁻¹⁴	9.94 x 10 ⁻¹³
Σ P(Ti-Cl) (atm)	1.12 x 10 ⁻¹⁵	1.72 x 10 ⁻¹⁴	1.37 x 10 ⁻¹³	7.94 x 10 ⁻¹³	3.58 x 10 ⁻¹²	1.32 x 10 ⁻¹¹

Species	Partial Pressure (atm)					
T(K) =	1000	1100	1200	1300	1400	1500
	TiO ₂ (c,l)					
Ti(1939) ^a	0 ^b	0	0	0	0	0
TiC(3290)	0	0	0	0	0	0
TiN(c)	0	0	0	0	0	0
TiO ₂ -r(2130)	1	1	1	1	1	1
Ti ₄ O ₇ (1950)	0	0	0	0	0	0
Ti ₃ O ₅ (2050)	0	0	0	0	0	0
Ti ₂ C ₃ (2115)	0	0	0	0	0	0
TiO(2023)	0	0	0	0	0	0
TiCl ₃ (c)	0	0	0	0	0	0
TiCl ₂ (1308)	0	0	0	0	0	0
TiCl ₄ (l)	0	0	0	0	0	0
C(5000)	1	0	0	0	0	0

Notes: $\Sigma P(\text{Ti})$ = Sum of vapor pressures of species containing Ti, O, and H

$\Sigma P(\text{Ti-O})$ = Sum of vapor pressures of species containing Ti and O only

$\Sigma P(\text{Ti-Cl})$ = Sum of vapor pressures of species containing Ti and Cl only

a = Melting point in degrees Kelvin

b = One (1) and zero (0) represent the presence and absence of the solid phase respectively.

APPENDIX C: CARBON DEPOSITION BOUNDARY DIAGRAMS

Figure C-1. Carbon deposition boundary line at 500°C.

Figure C-2. Carbon deposition boundary line at 600°C.

Figure C-3. Carbon deposition boundary line at 700°C.

Figure C-4. Carbon deposition boundary line at 800°C.

Figure C-5. Carbon deposition boundary at 900°C.

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