

MARSHALL ISLANDS FILE TRACKING DOCUMENT

Record Number: 311

File Name (TITLE): The Chemical Species of the
Plumets Resulting from an Atomic Bomb

Document Number (ID): USWRDL AD-325 (c)

DATE: 5/1951

Previous Location (FROM): CIC

AUTHOR: L. R. Bunnay, et al

Additional Information: _____

OrMIbox: 18

CyMIbox: 11

2

U N C L A S S I F I E D

0060631

**U.S. NAVAL
RADIOLOGICAL DEFENSE
LABORATORY**

SAN FRANCISCO 24, CALIF.



NS 081-001
NA 520
NY 320-001
USAF 15-04-87-001

THE CHEMICAL SPECIES OF THE ELEMENTS RESULTING
FROM AN ATOMIC BOMB DETONATION IN AIR

L. R. Bunney and N. E. Ballou

RICHARD COLE

U N C L A S S I F I E D

1.
AD-325(C)

This document consists of 32 pages.
This is copy 285 of 290, Series A.

U N C L A S S I F I E D

THE CHEMICAL SPECIES OF THE ELEMENTS RESULTING
FROM AN ATOMIC BOMB DETONATION IN AIR

L. R. Bunney and N. E. Ballou

Final Report

Technical Objective AW-7

Chemistry Branch
C. R. Schwob, Head

Chemical Technology Division
E. R. Tompkins, Acting Head

U. S. NAVAL RADIOLOGICAL DEFENSE LABORATORY
San Francisco 24, California

Scientific Director
William H Sullivan

25 May 1951

U N C L A S S I F I E D

U N C L A S S I F I E D

DISTRIBUTION

Copies

NAVY

1-9 Chief, Bureau of Ships (Code 324)
 10 Chief, Bureau of Medicine and Surgery (Code 74)
 11 Chief, Bureau of Aeronautics (Code AE54)
 12 Chief, Bureau of Yards and Docks (P-312)
 13-15 Chief, Bureau of Supplies and Accounts (Code OW)
 16 Chief of Naval Research
 17 Chief of Naval Operations (Op-36)
 18 Commander, New York Naval Shipyard, Material Laboratory
 19 Director, Naval Research Laboratory
 20 Commanding Officer, Naval Unit, Army Chemical Center
 21 CO, U. S. Naval Civil Engineering, Res. & Eval. Laboratory
 22 U. S. Naval Civil Engineer Corps, Officers School
 23 Chief, Naval Air Experimental Station
 24 Naval Medical Research Institute
 25 Aviation Medical Acceleration Laboratory
 26 Commandant, U. S. Marine Corps
 27 Research and Development Board, Committee on Atomic Energy

ARMY

28 Chief of Engineers, Department of the Army
 29-30 Chief, Research and Engineering Division
 31-32 Office of Chief Signal Officer
 33 President, Army Field Forces Board No. 1, Fort Bragg
 34 CG, Philadelphia Quartermaster Department
 35 Quartermaster General, Department of the Army
 36 CO, Engineer Research and Development Laboratory
 37-38 Army Medical Service Graduate School (Stone)
 39 Radiological Division, CmlC Chemical and Radiological Laboratories
 40-41 CO, CmlC Chemical and Radiological Laboratories
 42 Operations Research Office
 43 Atomic Energy Branch (Betts)

AFSWP

44 Chief, Armed Forces Special Weapons Project
 45 AFSWP, Weapons Defense Division
 46 AFSWP, Sandia Base

AIR FORCE

47-48 Director of Research and Development DCS/D, Hq., USAF (AFDRD-RE)
 49 CG, Headquarters, Wright-Air Development Center (WCRTH-11)
 50 CG, Headquarters, Air Materiel Command (MCMTE-11)

U N C L A S S I F I E D

U N C L A S S I F I E D
DISTRIBUTION (Continued)

Copies

51-53 Wright-Patterson Air Force Base (MCREOA)
 54-58 Wright-Patterson Air Force Base (CADO-EL)
 59 Wright-Patterson Air Force Base (Nudenberg)
 60 Wright-Patterson Air Force Base (WRCDO)
 61 USAF, School of Aviation Medicine
 62 Air Research and Development Command (DCS/Research)
 63 Kirtland Air Force Base (Hooks)
 64 Commanding General, Offutt Air Force Base
 65 Eglin Air Force Base (Technical Library)

ATOMIC ENERGY COMMISSION

66 AEC, Military Applications Division
 67-74 Argonne National Laboratory
 75-79 Atomic Energy Commission, Washington
 80-83 Atomic Energy Project, Chalk River
 84 Battelle Memorial Institute
 85 Brush Beryllium Company
 86-89 Brockhaven National Laboratory
 90-93 Carbide and Carbon Chemicals Division (K-25 Plant)
 94-97 Carbide and Carbon Chemicals Division (Y-12 Area)
 98 Columbia University (Failla)
 99 Dow Chemical Company
 100-104 duPont Company
 105 H. K. Ferguson Company
 106-111 General Electric, Richland
 112 Harshaw Chemical Corporation
 113-116 Idaho Operations Office
 117-118 Iowa State College
 119 Isotopes Division (McCormick)
 120 Kellex Corporation
 121-124 Knolls Atomic Power Laboratory
 125-126 Library of Congress, Acquisition Department (Comm)
 127-129 Los Alamos Scientific Laboratory
 130 Mallinckrodt Chemical Works
 131 Massachusetts Institute of Technology (Gaudin)
 132 Massachusetts Institute of Technology (Kaufmann)
 133-135 Mound Laboratory
 136 National Advisory Committee for Aeronautics
 137 National Bureau of Standards (Huntoon)
 138 National Bureau of Standards (Library)
 139 National Research Council, Ottawa
 140-141 ANP Project

U N C L A S S I F I E D

U N C L A S S I F I E D

DISTRIBUTION (Continued)

142 New Brunswick Laboratory
143-145 New York Operations Office
146 North American Aviation, Inc.
147 Nucleonics
148-149 Oak Ridge Institute of Nuclear Studies
150-157 Oak Ridge National Laboratory (X-10 Site)
158 Patent Branch, Washington
159 RAND Corporation
160 Sandia Corporation
161 Savannah River Operations Office
162 Sylvania Electric Products, Inc.
163-237 Technical Information Service (Oak Ridge)
238-247 United Kingdom Scientific Mission (Greenhill)
248-249 U. S. Geological Survey (Nolan)
250-251 U. S. Public Health Service
252 University of California at Los Angeles
253-256 University of California Radiation Laboratory
257-258 University of Rochester
259 University of Washington
260 UT-AEC Agricultural Research Program (Hobbs)
261 Western Reserve University
262-263 Westinghouse Electric Corporation

USNRDL
264-290 USNRDL, Technical Information Division

Date issued: 2 August 1951

U N C L A S S I F I E D

U N C L A S S I F I E D

ABSTRACT

Estimates have been made of the chemical nature of the products of an atomic bomb detonation occurring in air. A discussion of the relevant data and necessary assumptions is included. Based largely on thermodynamic data, the results indicate that these products should exist mainly as the oxides. Thus, with problems such as those of contamination and decontamination in which chemical properties are a factor, the behaviors of the various elements under a variety of conditions can be predicted.

U N C L A S S I F I E D

U N C L A S S I F I E DTHE CHEMICAL SPECIES OF THE ELEMENTS RESULTING
FROM AN ATOMIC BOMB DETONATION IN AIR

L. R. Bunney and N. E. Ballou

INTRODUCTION

The chemical nature of a contaminant is of importance for studies of its contamination and decontamination behavior. This report presents an estimation of the main chemical species of the various elements to be expected from an air detonation of an atomic bomb. The reactions considered are thus mainly dry, although the possible effects of atmospheric moisture are discussed to some extent. (A similar study of the chemical nature of the products of an underwater atomic bomb detonation has been started.)

A detailed and accurate analysis is impossible owing to the lack of sufficient experimental data on the type of reactions involved, and also because much information concerning the atomic cloud is lacking at present. This report presents a best estimate based on the available data and a series of bold assumptions. The authors are at present planning experimental tests of some of the hypotheses used in this report.

The elements under consideration are the bomb materials: iron (since the composition of the steel was not accurately known, such things as small percentages of nickel, manganese, etc., were estimated from the composition of armor plate); uranium or plutonium; conventional explosive products: carbon, nitrogen, hydrogen and oxygen; and the fission products from zinc, atomic number 30, to gadolinium, atomic number 64.

The report is comprised of a discussion of the assumptions involved; a table listing the elements and their estimated predominant chemical species; a section devoted to brief outlines showing how we arrived at the data listed in the table, with reference notes; a short conclusion, in which the possible effects of nuclear reactions (not considered in the analysis) are pointed out; and a bibliography.

DISCUSSION OF ASSUMPTIONS

It is necessary for even a rough type of calculation to assume that certain relative percentages of construction material, such as iron, uranium or plutonium, and fission products are present after the detonation of an atomic bomb. It is considered that even a ten-fold error in any of these estimates would not seriously affect the conclusions in this report.

U N C L A S S I F I E D

U N C L A S S I F I E D

The analysis is limited to "high" air bursts, i.e., ones in which the actual detonation occurs at or above 500 feet from ground level, which results in no appreciable vaporization of soil material or mixing of soil with the ball of fire.¹ Such altitudes prevent rapid cooling of the ball owing to the expenditure of energy in vaporization of soil material² and, hence, equilibrium conditions are more closely approached in a given temperature range.

The volume of the vaporized bomb materials and products is an important consideration. This was estimated by a rough calculation from data on the size of the ball of fire as a function of time after detonation.¹ At one second after detonation its volume is approximately 1×10^{10} liters.

The consideration of the amount of mixing of the surrounding atmosphere, in the first ten seconds, was of the utmost importance. The data in (1) and a mathematical treatment by Taylor³ indicate that the degree of mixing should be very large, even in the first two seconds following the detonation. A rough calculation, from an application of Taylor's theory by Cohen, Hirschfelder, et al.,⁴ showed that a most conservative estimate of the amount of air mixed with the ball of fire in the first two seconds would contain 10^3 times as much O_2 as would be necessary to react all bomb material to the highest oxidation state possible. The conclusion is that the amount of air present is not a limiting factor in a reaction of the bomb materials and products, and that, of the possible chemical species of the various elements present, the oxides and nitrides should be by far the most important.

In some cases, the nitrides of the particular element were known to be unstable. As pointed out by Kelley,⁵ ZrN is the most stable of the metallic nitrides.^{6,8} Rough equilibrium calculations at $2500^\circ K$ using the data of Brewer^{7,8} indicate no appreciable amount of ZrN in equilibrium with ZrO_2 at atmospheric concentrations of N_2 and O_2 . Similar calculations for other elements involved show similar nitride concentrations at equilibrium. Of course, the equilibrium constants for the formation of oxides from nitrides in air increase rapidly with decreasing temperature. The conclusion is that the oxides are the most important chemical species present in most cases, although trace concentrations (~ 2 percent or less) of nitrides are possible in some cases. Hence, the estimates in Table 1 are not meant to preclude the possibility or even the probability of the formation of some unmentioned compounds to the extent of 2 or 3 percent. In some cases, compounds which are thought to occur only in such quantity are mentioned in the table because of our convictions of their probable presence.

General equilibrium considerations⁹ show that in most cases appreciable compound formation does not take place much above $5000^\circ K$, since above that temperature most elements exist as gaseous atoms or ions. This temperature is reached approximately one second after detonation of a nominal (20,000

U N C L A S S I F I E D

U N C L A S S I F I E D

ton TNT equivalent) atomic bomb.¹ Just below this temperature, most compounds are thought to be only diatomic in nature (i.e., only compounds of the type FeO, UO, PuO, etc., are formed), but on cooling further oxidation is achieved. In the cases of those elements for which oxides are predicted, the particular oxides resulting should be those which are thermodynamically most stable. However, it is known that in some cases the rate of reaction is slow where transitions occur between oxides of an element (e.g., $\text{Fe}_3\text{O}_4 \rightarrow \text{Fe}_2\text{O}_3$);¹¹ hence, the oxide of the element which predominantly results at room temperature should be the one which is thermodynamically stable at the lowest temperature at which equilibrium is attained fairly rapidly. Where information was lacking on such transformations, qualitative statements in reference works were interpreted in a rough quantitative way. In a few cases, the best interpretation is the existence of a mixture of two or more possible species; it is probable that the composition of the mixture would be dependent on the cooling time in significant temperature ranges, and such other factors as pressure of O_2 and particle size.

The effects of the ultraviolet radiation resulting from the detonation of an atomic bomb are considered. The available data¹ show that this type of radiation is small when the ball of fire has a temperature of about 5000°K . Below 5000°K , the amount of ultraviolet radiation decreases very rapidly, approaching zero at about 4000°K . As has been pointed out, very little compound formation is possible above 5000°K .⁹ Hence, the ultraviolet radiation is considered to have a negligible effect.

It is thought that the radiation field of the fission products, which is of longer duration than the ultraviolet radiation, would have a definite effect. This is considered in the paragraph on silver. Other compounds which undergo photoelectric decomposition would be similarly affected. However, no evidence has been found for this type of reaction in the other compounds which are considered to be possible species.

No attempt has been made to evaluate the "valence inductivity" effect reported by Selwood¹⁴ although it should be pointed out that this may be exhibited to a large extent in the fission products owing to the small particle size and large proportion of iron expected to be present.

The effects of solid solutions were not evaluated because of the lack of available data. The problem becomes quite complicated if all the possible constituents are considered. Each element has been treated individually in this report. However, the possibility of formation of compounds between basic and acidic oxides should be considered. In many cases (selenites, tellurites, germanates, stannates, arsenites, antimonites, carbonates, nitrates, silicates, phosphates, sulfites, sulfates, molybdates, and in some cases even ferrates and uranates) the formation of such compounds is thermodynamically possible.

U N C L A S S I F I E D

U N C L A S S I F I E D

The factors affecting the formation of such compounds are: concentration of the reactants; rate of cooling in the significant temperature range; amount and type of surface available; adsorption of gaseous species by condensed species; rate of formation of the compounds; and in many cases the presence or absence of appreciable amounts of water. Many of these factors are either not known at present or are not sufficiently well known to be useful in predicting the results to any reasonable order of magnitude.

General statements as to the likelihood of the formation of certain anions are included in the appropriate paragraphs in the body of this report, but the discussion of the formation of specific compounds is limited to the very few well known cases. These are to be found in the paragraph on the element which forms the cation.

Lastly, an assumption is made of strongly oxidizing conditions in air for the elements considered. In certain cases, it is thought that there is the possibility of incomplete oxidation owing to entrapment of minor elements in larger particles of major constituents. This effect is considered to be a minor one. It has been necessary in many cases to extrapolate thermodynamic data beyond the point where it is reasonably accurate, but the trends shown are felt to be significant.

U N C L A S S I F I E D

U N C L A S S I F I E D

TABLE 1

<u>Atomic No.</u>	<u>Element</u>	<u>Estimated Predominant Species</u> (Expected lesser species in parentheses)
1	Hydrogen	H ₂ O
6	Carbon	CO ₂
7	Nitrogen	N ₂ *
8	Oxygen	O ₂ **
14	Silicon	SiO ₂ or Silicates
15	Phosphorus	P ₂ O ₅ or Phosphates
16	Sulfur	SO ₂ (SO ₃) or Sulfites (Sulfates)
24	Chromium	Cr ₂ O ₃
25	Manganese	Mn ₃ O ₄
26	Iron	Fe ₃ O ₄ (Fe ₂ O ₃)
28	Nickel	NiO
29	Copper	CuO
30	Zinc	ZnO
31	Gallium	Ga ₂ O ₃
32	Germanium	GeO ₂
33	Arsenic	As ₂ O ₃
34	Selenium	SeO ₂
35	Bromine	Br ⁻ (IBr, Br ₂)
36	Krypton	Kr
37	Rubidium	RbO ₂ (RbI, RbBr, RbOH, Rb ₂ CO ₃)
38	Strontium	SrO (Sr(OH) ₂ , SrCO ₃)

* Note: Of importance to the optical properties of the ball of fire is the formation of oxides of nitrogen to the extent of roughly 100 tons in an air burst. The equilibrium concentrations of nitric oxide and nitrogen dioxide in the air are from one to five percent for temperatures between 2000°C and 5000°C; the equilibrium concentrations are negligible below 2000°C, and above 5000°C the oxides are dissociated into atoms.¹

** Note: Small amounts of ozone are probably formed to an unknown extent in an air burst of an atomic bomb.

U N C L A S S I F I E D

U N C L A S S I F I E D

<u>Atomic No.</u>	<u>Element</u>	<u>Estimated Predominant Species</u> (Expected lesser species in parentheses)
39	Yttrium	Y ₂ O ₃
40	Zirconium	ZrO ₂
41	Niobium	Nb ₂ O ₅
42	Molybdenum	MoO ₃
43	Technicium	TcO ₃
44	Ruthenium	RuO ₂
45	Rhodium	Rh ₂ O ₃ (Rh)
46	Palladium	PdO (Pd)
47	Silver	Ag (AgBr, AgI, Ag ₂ O)
48	Cadmium	CdO
49	Indium	In ₃ O ₄ (In ₂ O ₃)
50	Tin	SnO ₂
51	Antimony	Sb ₂ O ₃ (Sb ₂ O ₄)
52	Tellurium	TeO ₂
53	Iodine	I ⁻ (I ₂ , IBr)
54	Xenon	Xe
55	Cesium	CsO ₂ (CsI, CsBr, CsOH, Cs ₂ CO ₃)
56	Barium	BaO (Ba(OH) ₂ , BaCO ₃)
57	Lanthanum	La ₂ O ₃
58	Cerium	CeO ₂
59	Praseodymium	Pr ₆ O ₁₁
60	Neodymium	Nd ₂ O ₃
61	Promethium	Pm ₂ O ₃
62	Samarium	Sm ₂ O ₃
63	Europium	Eu ₂ O ₃
64	Gadolinium	Gd ₂ O ₃
92	Uranium	U ₃ O ₈
93	Neptunium	NpO ₂
94	Plutonium	PuO ₂

U N C L A S S I F I E D

U N C L A S S I F I E D

DATA AND REFERENCES

H The thermodynamic data^{6,9} indicate that the only possible species is H₂O.

C The thermodynamic data^{6,8,9} indicate that CO₂ is the only important species. CO is thermally the most stable of the carbon compounds and it is oxidized to CO₂ at lower temperatures.⁹

N
and
O Nitrogen and oxygen are considered in connection with each of the other elements. Other than the compounds mentioned in the other paragraphs, the oxides of nitrogen, nitrates and nitrites are considered to be the only possible species. The data in "Effects of Atomic Weapons"¹ indicate that there is a large quantity of NO₂ formed between 2000°K and 5000°K, but this amount would be rapidly decomposed as the temperature dropped below 2000°K.

The formation of most nitrates and nitrites is not thermodynamically possible under the pertinent conditions until the temperature drops below 1000°K. Since at this temperature the concentration of NO₂ and NO are decreasing due to decomposition and diffusion and the rate of reaction is probably quite slow, the probability of nitrates and nitrites being present as significant resulting species is considered to be very small. Hence, the nitrogen and oxygen other than that combined with the other elements is considered to be in the elemental state when at the temperature of the atmosphere.

Si There are two known oxides of silicon, SiO and SiO₂.^{7,10,11,13} SiO is only obtained by drastic reduction of SiO₂.^{7,11} SiO₂ is very stable and is the usual oxidation product of the element.^{7,13}

The data of Brewer, Bromley, Gilles and Lofgren^{7,8} indicate that the nitride should not be present to an appreciable extent.

The thermodynamic data^{7,17,20,21} indicate that the bromides and iodides should not occur to more than one percent* of the silicon.

There is a very good possibility of silicate formation, but the extent is thought to be unpredictable.

* The phrase "should not occur to more than one percent" used here and with slightly different wording subsequently only establishes an upper limit. The species may not occur at all.

U N C L A S S I F I E D

U N C L A S S I F I E D

The difference between actual silicate formation and solid solution of SiO_2 with one or more basic oxides is difficult to define. Suffice it to say then that the final resulting species is considered to be SiO_2 either in solid solution with other oxides or actually combined with basic oxides to form silicates.

P Phosphorus has three known oxides, P_2O_3 , P_2O_4 and P_2O_5 .^{10,11,13} In excess air, the lower oxides are oxidized to P_2O_5 .^{10,11,13} P_2O_4 is only produced by heating P_2O_3 in a limited amount of air.^{11,13} P_2O_3 is oxidized to P_2O_5 in excess air even at 50-60°C.¹³ P_2O_5 is stable even at 1700°K,¹³ and, hence, is concluded to be the major resulting species.

In general, the likelihood of the formation of various phosphates is considered rather small unless one brings in the effects of moisture. In that case, neutralization of the phosphoric acid formed from the P_2O_5 would give phosphates. This neutralization might be limited in extent, as far as materials resulting from the detonation are concerned, by volatility of P_2O_5 (sublimes at 347°C¹⁹), which could bring about a physical separation from many of the basic oxides. However, phosphoric acid would be formed in the presence of moisture, and neutralization by other basic compounds is possible.

The thermodynamic data^{6,12} indicate that the nitride, P_3N_5 , should not be present to an appreciable extent.

The thermodynamic data^{6,12,17,20,21} also indicate that the bromides and iodides should not be present to an appreciable extent.

S The only important oxides of sulfur are SO , SO_2 and SO_3 .^{6,10,11,13} The others need not be considered here since these are the only ones which are obtained by oxidation in air.^{10,11,13} SO is only obtained at low pressure in air.¹³ It is thought to be a possible high temperature species, but should be oxidized to SO_2 on cooling to temperatures of about 3000°-4000°C. SO_2 is the usual product of oxidation in air,^{10,11,13} although SO_3 is the thermodynamically more stable at room temperature.^{6,36} However, at temperatures (below 1000°K) at which SO_3 is more stable than SO_2 , the rate of oxidation is rather slow.^{10,11,13} The rate is speeded up by surface catalysts such as Fe_2O_3 .^{10,11,13} It is thought that a mixture of the two oxides would result in the case under consideration with SO_2 predominating, but the composition would be a function of the concentrations of the gases, amount of available catalyst, and of the rate of cooling. The low concentration favors SO_2 formation.

SO_2 and SO_3 might very well react with some of the basic oxides to give sulfites and sulfates, especially in the presence of water.

U N C L A S S I F I E D

U N C L A S S I F I E D

In general, these reactions become thermodynamically possible at about 1000°K. The situation is similar to that with other acidic oxides in that physical separation may occur to some extent and the rates of the possible reactions are not well known.

Nitrogen sulfide, the most common of the nitrogen and sulfur compounds, is endothermic and is thought to be metastable.¹³

The thermodynamic data^{6,17,20,21} indicate that the bromides and iodides should not be formed to an appreciable extent.

Cr There are three well known oxides of chromium, CrO, Cr₂O₃ and CrO₃.^{6,7,10,11,13} CrO is easily oxidized to Cr₂O₃ in air¹³ and may only be a solid solution of metal and Cr₂O₃.⁷ Cr₂O₃ is quite stable,^{6,7} and is the usual oxidation product in air.^{10,11,13} CrO₃ is decomposed at about 540°K,⁷ and about 700°K the decomposition product is Cr₂O₃.⁷ The intermediate product may be a solid solution.

The nitride, CrN, decomposes at about 1770°K. The thermodynamic data^{6,7,8} indicate that it should not be formed to an appreciable extent.

The thermodynamic data^{6,7,17,20,21} indicate that the bromides and iodides should not occur to an appreciable extent.

Mn There are four known stable oxides of manganese, MnO, Mn₃O₄, Mn₂O₃ and MnO₂.^{7,10,11,13} MnO can be readily oxidized to the other oxides in various temperature ranges.^{7,10,11,13} At room temperature, MnO goes to MnO₂ in air, if the oxide is finely divided,¹³ but no evidence is available on similar reactions for the higher oxides. MnO₂ decomposes to Mn₂O₃ at about 535°C.¹⁹ Mn₂O₃ decomposes to Mn₃O₄ at 1080°C.^{15,19} Mn₃O₄ does not seem to oxidize further on cooling. Hence, Mn₃O₄ is considered to be the probable resulting species.

The thermodynamic data^{6,7,8} indicate that the nitrides should not be present to an appreciable extent.

The bromides and iodides are indicated by the thermodynamic data^{6,7,17,20,21} not to be present to more than one percent of the manganese.

Fe There are three known stable oxides of iron, FeO, Fe₃O₄ and Fe₂O₃.^{7,10,11,13} The equilibria among these is discussed by Darken and Gurry.^{47,48} At 1400°C there is a free energy of -54,500 cal for the reaction of $2\text{Fe}_3\text{O}_4 + \frac{1}{2}\text{O}_2 \rightarrow 3\text{Fe}_2\text{O}_3$ as written.⁴⁸ FeO is easily oxidized^{7,10,11,13,47,48} and is not thought to be a possible species. The thermodynamic data^{6,7,47,48} indicate that Fe₂O₃ should be the

U N C L A S S I F I E D

U N C L A S S I F I E D

major resulting species if equilibrium is approached below 1500°K. However, the composition is dependent on the partial pressure of oxygen and the cooling time. Latimer and Hildebrand state that the rate of oxidation of Fe_3O_4 to Fe_2O_3 is slow.¹¹

The nitrides of iron are metastable⁸ and are not considered to be possible species.

The bromides and iodides are not thought to be present to an appreciable extent according to the thermodynamic data,^{6,7,17,20,21} but also are not possible to any appreciable extent because of the relatively small amounts of the halides present with respect to the amount of iron present.

The conclusion is that Fe_3O_4 should be the main species, but smaller amounts of Fe_2O_3 are possible.

Ni The only oxide of nickel known as a single pure phase is NiO .⁷ Others which vary in composition from NiO to NiO_2 are claimed,^{11,13} but are usually prepared in solution¹¹ or as surface films.¹⁴ Ephraim¹³ claims that Ni_3O_4 gives off oxygen to form NiO at about 240°C. Only NiO is preparable from the elements.^{7,11,13}

No stable nitride of nickel is known.⁸ Therefore, it is not considered to be a possible species.

The thermodynamic data^{6,7,17,20,21} indicate that the bromides and iodides should not be present to an appreciable extent.

Cu Copper has two known stable oxides, Cu_2O and CuO .^{10,11,13} When oxidized in air, the usual product is CuO ,^{10,11,13} which decomposes to Cu_2O and oxygen, on heating to about 1026°C in air.^{15,19} However, on cooling, Cu_2O is oxidized back to CuO .

The nitrides of copper are metastable^{6,8} and are not considered to be possible species.

The diiodide is not a possible species, since it is not stable.¹⁷ The dibromide is indicated by the thermodynamic data^{6,7,17,20,21} to be a possible species. The monobromide and monoiodide are, also, possible. Thermodynamic considerations^{6,7,17,20,21} show that altogether they should not be present to more than one percent of the copper.

Zn Zinc is readily oxidized in air to ZnO , the only known oxide.^{10,11}

Zinc nitride, Zn_3N_2 , is metastable⁸ and hence is not considered to be a possible species.

U N C L A S S I F I E D

U N C L A S S I F I E D

The data of Brewer^{17,20} indicate that with concentration considerations the bromides and iodides are not possible to more than one percent of the total zinc present.

Ga Ga_2O_3 is the most stable oxide and the oxidation product of the metal in air.^{6,10,11} Ga_2O is known, but is unstable with respect to Ga_2O_3 and gallium metal.¹¹

The thermodynamic data^{6,8,12} lead to the conclusion that GaN should not be present to a greater extent than one percent of the total amount of gallium.

The thermodynamic data^{6,17,20} indicate that it is not possible for more than one percent of the total gallium present to occur as the bromides or iodides.

Ge GeO and GeO_2 are known; germanium and GeO are readily oxidized to GeO_2 in air.^{10,11,13}

The nitride, Ge_3N_4 , is metastable and, hence, should not occur.

It is felt that, because of the considerations mentioned in the Discussion, germanates could not be a very important species for this element, although it is a possible one in a few cases.

Rough equilibria data^{6,17,20,22} indicate that the bromides or iodides should not be present to a greater extent than one percent of the germanium.

As As_2O_3 and As_2O_5 are the two known oxides of arsenic.^{10,11,13} Although As_2O_5 is thermodynamically stable at room temperature, it decomposes to As_2O_3 and O_2 at 588°K.¹⁹ When the element is burnt in air, fairly pure As_2O_3 results.^{10,11}

The nitride, AsN, has a heat of formation of between +7 and +35 kilocalories per mole.^{6,18} It is not stable⁸ and is not considered to be a possible species.

As_2O_5 is not thermodynamically stable above 588°K; thus, combination with other oxides is probably slow owing to the low temperatures required. As_2O_3 is quite volatile (sublimes at 193°C) and, hence, might be physically separated from other oxides. Most arsenites (particularly those of iron) decompose at low temperatures. Therefore, the probability of arsenite or arsenate formation is considered to be very small. The presence of appreciable amounts of moisture would increase the probability of such reactions, but the extent is difficult to predict.

U N C L A S S I F I E D

U N C L A S S I F I E D

The bromides and iodides should not be present to more than one percent of the arsenic.^{6,17,20,21}

Se SeO_2 is the only known oxide of selenium which is thermodynamically stable under ordinary conditions.^{6,10,11,13}

Selenium nitride, Se_4N_4 , explodes at 200°C ,^{15,19} and hence is not thought to be a possible species.

Selenites of heavy metals decompose at rather low temperatures¹⁶ and, while those of the alkali and alkaline earth metals are possible, it is felt that concentration considerations preclude the possibility of their formation to an appreciable extent.

The thermodynamic data^{6,17,20} indicate that less than one percent of the selenium present should occur as bromides and iodides.

Br The case of bromine is complicated somewhat by the fact that many of the bromides of the elements involved in this discussion are not stable at temperatures at which the corresponding oxides are.^{6,7,12,17} It is also felt that much of the bromide formation would be prevented by the much larger concentration of O_2 (and hence the oxide would be formed in many cases in preference to the bromide). Furthermore, all oxides of bromine are unstable at ordinary temperatures.^{6,10,11}

It appears that the bromine will to some extent react with elements with which it can form bromides (e.g., Rb and Cs), with a distribution among the elements which is very difficult to predict.

It also seems quite likely that a small portion will not react in this manner and will cool out in the elementary state. In this connection, it should be pointed out that IBr is thermodynamically more stable than either Br_2 or I_2 .¹⁷ Therefore, since there is a similar situation with iodine, some of the mixed halogen (IBr) should result.

In the special case of the reaction with silver, which is thermodynamically possible because of the comparative instability of Ag_2O ,^{6,17} it is thought that much of the halide formed would be decomposed by light and gamma radiation.

It is felt that addition compounds of the type MObR (where M stands for any divalent metal) or any other oxyhalide are either too unstable to be significant,¹⁰ or the rate of formation is too slow to form an appreciable amount.³⁵

Kr Krypton, because of its lack of chemical reactivity^{10,11,24} is concluded to be in the elemental state.

U N C L A S S I F I E D

U N C L A S S I F I E D

Rb

Rubidium presents one of the more complicated cases considered in this discussion thus far. There are four known oxides of rubidium, Rb_2O , Rb_2O_2 , Rb_2O_3 , RbO_2 (Rb_2O_4), as well as possible suboxides.^{7,10,11,13} The suboxides are only prepared under conditions that are not possible in the situation under consideration.¹¹ Rb_2O_2 has only been prepared by treating liquid ammonia solutions of the metal with oxygen.¹³ Since RbO_2 is the product obtained by ignition in air,^{10,13} it is felt that it would be the chief product in the case under discussion. The alkali metals have a greater tendency to form higher oxides with increasing atomic number;¹³ hence, in rubidium the tendency is very great. In excess oxygen, it should readily oxidize to RbO_2 .¹³

Rubidium nitride, Rb_3N , is decomposed above 688°K ,⁸ and hence should not be a possible species.

RbO_2 decomposes at rather low temperatures,⁷ as do the other oxides of rubidium,^{7,15,19,23} whereas the bromide and iodide are quite stable at high temperatures²⁰ (above 3000°K). This leads to the conclusion that the bromide and iodide should be important species in the case of rubidium. The iodide should be more important than the bromide because iodine is present to about twice the extent of bromine in the time available for reaction.²² Since there is enough halogen to react with only about one-half the alkali metals,²² the latter will also form their oxides.

In the cases of Rb, Cs, Sr, and Ba, the possibility of formation of hydroxide, bicarbonate, and carbonate should be considered.

Appreciable amounts of moisture and CO_2 are usually present in the atmosphere. Water vapor usually comprises about one percent of the air,¹⁹ while CO_2 makes up on the order of 0.03 - 0.05 percent.¹¹

These amounts are such that the formation of hydroxides and carbonates are thermodynamically possible^{6,7,12,52} at temperatures of the order of 1000°K and bicarbonates at about 400°K . However, it should be pointed out that the rates of reaction to produce these compounds are not well known. Also, high temperature forms of oxides which are very unreactive (e.g., "dead burnt" CaO and MgO) are quite numerous.¹³

For these reasons, the exact resultant species of these elements are almost impossible of prediction. They may also vary with length of time following the burst.

Sr

Strontium is known to have only two oxides in the dry state, SrO and SrO_2 .^{10,11,13} SrO_2 is only prepared under high O_2 pressure and

U N C L A S S I F I E D

U N C L A S S I F I E D

decomposes at 488°K to SrO.⁷ Hence, it is not a possible species.

Strontium nitride, Sr₃N₂, decomposes at temperatures at which SrO is stable in air.^{7,8} Consequently, it is thought that the nitride would not be present to greater than one percent of the strontium.

The data of Brewer^{7,17,20,21} shows that the halides should not be present to more than one percent of the strontium.

For discussion of the possible formation of hydroxides, carbonates, and bicarbonates, see the paragraph on rubidium.

Y The only known oxide of yttrium is Y₂O₃.^{10,24,37}

Rough equilibrium calculations from the data of Brewer^{7,8} indicate that the nitride, YN, should not be present to the extent of one percent of the yttrium, if conditions approach equilibrium at temperatures at which Y and Y₂O₃ are condensed phases (2500°K).^{1,8,21,23} In addition, calculations show that the oxide is stable at temperatures at which YN is dissociated.^{7,8}

Similar calculations for the bromides and iodides^{7,17,20,21} indicate that they should not be possible to more than one percent of the yttrium.

Zr ZrO₂ is the only known oxide of zirconium.^{7,10,13}

The possibility of ZrN formation is covered in the preliminary discussion in this report. In addition, the thermodynamic data^{7,8,21,23} indicate that, if equilibrium is approached at 2500°K, no appreciable amount of ZrN is present.

The thermodynamic data^{7,17,20,21,23} indicate that, if equilibrium is approached at 2000°K, the bromides and iodides should not be present to an appreciable extent.

Nb Niobium has three stable oxides, NbO, NbO₂ and Nb₂O₅.^{7,10,24} Nb₂O₃ is doubtful⁷ and, if preparable, is relatively unstable compared to the other oxides. Ignition in air of the metal or of any of the lower oxides gives Nb₂O₅.²⁴ Brewer's data⁷ indicate that Nb₂O₅ is stable above 1500°K. Niobates are considered possible, but only to a very minor extent.

NbN, the nitride, should not be present to an appreciable extent from the indications of the thermodynamic data.^{7,8,23}

U N C L A S S I F I E D

U N C L A S S I F I E D

The iodide is known to react with atmospheric oxygen to form Nb_2O_5 ,²⁴ and hence is not a possible species. The bromide is also thought to be unstable at high temperature in air with respect to Nb_2O_5 and bromine.

Mo

MoO_2 and MoO_3 are the two known stable oxides of molybdenum.^{7,10} Mo_2O_3 has been claimed by two groups of investigators and later denied by one of them. Another group failed to find evidence of Mo_2O_3 .⁷ The thermodynamic data indicate that of the two, MoO_3 is the more stable up to a temperature of about 2000°K.^{6,7} MoO_2 is oxidized to MoO_3 by the oxygen of the air at temperatures below about 1500°K.^{6,7,24}

Molybdates are considered possible, but only to a very small extent.

The nitride, Mo_2N , is not very stable and should decompose near 1000°K.⁸ Hence, it is not thought to be a possible species.

The bromides and iodides of molybdenum are not stable above 1000°K.²⁰ Hence, they are not thought to be possible species.

Tc

Technetium presents a rather unique problem inasmuch as its basic chemistry has not been studied to an extent that would give much indication of its most stable compounds. According to the early investigators of the chemical properties of technetium, it resembles rhenium much more than manganese in its chemical behavior.^{25,26,27,28}

Reviews on rhenium^{24,29} indicate that it has a very wide variety of valence states, but the heptavalent state is the most stable.

Two groups of workers^{30,33,34} indicate the existence of Tc_2S_7 as a normal sulfide precipitate in acid solution. Inghram, Hess and Hayden³¹ state that for some mass spectrometer work they received a sample of NH_4TcO_4 and obtained peaks corresponding to TcO^+ , TcO_2^+ , and TcO_3^+ in the work. Fried³² indicates the existence of NH_4TcO_4 . In later work³⁴ it was shown that a hexavalent state of technetium exists and that TcO_4^- is not as easily reduced as MnO_4^- . In the latter experiment, no compound analogous to MnO_2 was discovered on reduction. The indications of the work mentioned above are that the oxides of technetium are possibly TcO , Tc_3O_4 , Tc_2O_3 , TcO_2 and Tc_2O_7 with TcO , TcO_3 and Tc_2O_7 most probable. The latest work, that of Fried and Hall,⁴⁹ shows that TcO_3 is the volatile oxide which was previously thought to be Tc_2O_7 by most workers. Indications seem to favor the formation of TcO_3 in the case under discussion, although this needs verification. Technetates may also be possible species.

U N C L A S S I F I E D

U N C L A S S I F I E D

No work has been done with the nitrides, bromides or iodides, but it is thought that, as with manganese, they would not be as stable as the oxides under the considered conditions.

Ru Ruthenium has three well-defined oxides, Ru_2O_3 , RuO_2 and RuO_4 .^{10,24} RuO does not appear to exist.^{10,11,24} RuO_2 is obtained on heating the finely divided metal in air.^{10,11,24} RuO_4 appears to decompose to RuO_2 at about 100°C.^{10,13,19} The conclusion is that RuO_2 is the most probable oxide and, since the metal is readily oxidized in air, the most probable species. However, Ru_2O_3 is also possible.¹³

No nitride of ruthenium is known and hence is not considered to be a possible species.^{8,13}

The bromides and iodides are rather easily decomposed and, according to Brewer's data,^{20,21} should not be present to an appreciable extent.

Rh Five oxides of rhodium are known, Rh_2O , RhO , Rh_2O_3 , RhO_2 and RhO_3 .^{10,13,24} RhO_3 and RhO_2 are readily decomposed by heat^{10,15,19,24} and are not thought to be possible species. Assuming reasonable entropies, as in the method of Brewer,^{7,17,23} the thermodynamic data^{6,12} indicate that Rh_2O_3 is substantially more stable than Rh_2O and RhO at almost all temperatures at which they exist. This is born out by the dissociation temperatures under one atmosphere of O_2 given by Mellor¹⁰ for the three oxides, Rh_2O at 1127°C, RhO at 1121°C and Rh_2O_3 at 1113°C. Mellor also states that Rh_2O_3 is the product of oxidation in air of the finely divided metal between 600°C and 1000°C. It would appear that Rh_2O_3 should result almost entirely if the cooling rate in the significant temperature range (i.e., the temperature range at which reaction becomes possible for rhodium under conditions found in AED) is fairly slow. The element itself is also possible, but in the finely divided state expected it should be oxidized.

As in the case of ruthenium, the nitride is not known^{8,13} and is not considered possible.

The bromides and iodides are rather easily decomposed^{10,17,20,21} and are not thought to be present to an appreciable extent.

Pd The only stable oxides of palladium are PdO and PdO_2 .^{10,11,24} PdO_2 is not very stable and decomposes to the monoxide on heating to about 200°C. PdO_2 has never been formed by heating the metal in air.¹⁰ Various claims for the existence of Pd_2O have been disproven by showing that the product was a mixture of PdO and the metal.¹⁰

U N C L A S S I F I E D

U N C L A S S I F I E D

The nitride is not known^{8,13} and is not considered to be a possible species.

The bromides and iodides are rather easily decomposed^{10,17,20,21} and are not thought to be present to an appreciable extent.

There is a very good possibility that the metal itself occurs, because of the relatively small thermodynamic stability of PdO.^{6,12} However, in the very finely divided state expected, it is thought that PdO would be the predominant species, although metallic palladium is also expected to some extent. The composition of the mixture would depend on the rate of cooling of the metal. If the cooling is fairly rapid, palladium metal should be the predominant species.

Ag

Two oxides of silver are known, Ag₂O and Ag₂O₂. Ag₂O₂ is not very stable and decomposes a little above 100°C.^{15,19} Ag₂O is also rather unstable and does not become thermodynamically feasible^{6,12} until the temperature is about 200°C. It is the oxide which is formed when the metal is heated to 200°C for a long time.¹³

Silver nitride, AgN₃, explodes¹⁵ and is thought to be an azide not preparable from the elements and hence is not a possible species. No stable nitride is known.⁸

The bromide and iodide of silver are stable^{17,20,21} and are definitely possible species. However, they are photosensitive^{10,11,13} as is Ag₂O. It is thought, therefore, that they would be considerably decomposed by the sunlight and gamma-rays from the fission products.

The conclusion is that the main product should be metallic silver with small amounts of the bromide, iodide and oxide.

Cd

CdO is the only known oxide of cadmium. It is readily obtained by oxidizing the metal in air.^{11,13}

As with zinc, cadmium nitride is metastable⁸ and is not thought to be a possible species.

The bromide, but not the iodide, is shown to be a possible species by the data of Brewer,^{17,20,21} but not until low temperatures are reached. There is a slightly greater possibility of the bromide and iodide being formed by means of formation of the monovalent halides at high temperatures with subsequent disproportionation to the divalent halides and the metal. In any event, it is thought that they will not be present to more than two or three percent of the cadmium present.

U N C L A S S I F I E D

U N C L A S S I F I E DIn

There are three known oxides of indium, InO , In_2O_3 and In_3O_4 .^{10,17,24} InO is readily oxidized to In_2O_3 in air.^{10,11} In_2O_3 is the product in air oxidation at temperatures up to 850°C .^{10,24} At temperatures above 850° the product is In_3O_4 , which is analogous to Fe_3O_4 .^{10,11,24} No information on the rate of transformation from In_3O_4 to In_2O_3 on cooling could be found.

The nitride, InN , is metastable⁸ and is not considered to be a possible species.

The thermodynamic data^{6,17,20,21} indicate that the bromides and iodides should not be present to more than one percent of the indium.

Our conclusion is that a mixture of In_2O_3 and In_3O_4 should result with In_3O_4 predominating.

Sn

Only two oxides of tin are known, SnO and SnO_2 .^{10,11,13} SnO_2 is the usual product of the oxidation in air.^{10,11,13} SnO burns when heated in air.^{10,11} SnO_2 is stable below 1400°K .^{15,19}

Stannates may be possible, but it is thought that they should not be important.

No stable nitride of tin is known⁸ and, hence, it is not considered to be a possible species.

The thermodynamic data^{6,17,20,21} indicate that the bromides and iodides should not be present to an appreciable extent.

Sb

There are three known stable oxides of antimony, Sb_2O_3 , Sb_2O_4 and Sb_2O_5 .^{10,11,13} Sb_2O_5 loses oxygen at about 400°C .^{15,19} to form Sb_2O_4 which, in turn, loses oxygen at about 1000°C .^{15,19} to form Sb_2O_3 , which is very stable.³⁶ Latimer and Hildebrand¹¹ state the ignition products of the element in air to be Sb_2O_3 with some Sb_2O_4 .

Antimonites and antimonates may also be possible, but, as in other cases, the probability is thought to be rather small. Concentration considerations in the few known cases, the lack of knowledge concerning some possible compounds, and the ease of decomposition of others lead to this conclusion.

No stable nitride of antimony is known.⁸ Therefore, a nitride is not considered to be a possible species.

The thermodynamic data^{6,12,17,20,21} indicate that the bromides and iodides should not be present to an appreciable extent.

U N C L A S S I F I E D

U N C L A S S I F I E D

The conclusion is that the resulting species will be a mixture of Sb_2O_3 and a smaller amount of Sb_2O_4 .

Te There are three known oxides of tellurium, TeO , TeO_2 and TeO_3 .^{10,11,24} Te and TeO are easily oxidized in air to TeO_2 .^{10,24} TeO_3 readily decomposes on heating to TeO_2 and oxygen.^{10,13,24}

The nitride, Te_3N_4 , is probably endothermic, but in any case would not be very stable.⁸ It is not considered to be a possible species.

Tellurites are even less stable than selenites¹⁶ and are not expected to an appreciable extent (cf. selenium).

The thermodynamic data^{6,17,20} indicate that the bromides and iodides should not occur to an appreciable extent.

I The considerations in the case of iodine are so similar to those of bromine that only the differences will be mentioned here (cf. bromine).

Iodine does have one thermodynamically stable oxide, I_2O_5 , which is formed from the elements.²⁰ However, it is unstable above $570^\circ K$ and is not considered to occur to more than one percent of the iodine present.

The iodides are even less stable than the bromides^{6,12,20} and the proportion expected to occur in elemental form would be larger than with bromine.

Xe Xenon, as with krypton, is concluded to be in the elemental state because of its lack of chemical reactivity.^{10,11,24}

Cs The considerations for cesium are almost identical with those of rubidium (cf. rubidium references). The conclusions are also the same.

Ba Two stable oxides of barium are known, BaO and BaO_2 .^{6,7,10,11,13} Ba_2O is also known as is BaO_2 .¹³ Ba_2O is doubtful and, if it exists, is easily oxidized to BaO or to BaO_2 .¹³ BaO_4 decomposes at rather low temperatures to BaO_2 .¹³ BaO_2 decomposes to BaO at about $700^\circ C$ in air.^{7,13} BaO is very stable^{6,7} and is considered to be the most probable species.

Barium nitride, Ba_3N_2 , decomposes at about $1270^\circ K$.⁸ The thermodynamic data^{6,7,8} indicate that it should not be present to an appreciable extent.

U N C L A S S I F I E D

U N C L A S S I F I E D

The thermodynamic data^{6,7,17,20,21} indicate that the bromide and iodide would not be present to more than one percent of the barium.

For discussion of the possible formation of hydroxides, carbonates, and bicarbonates, see the paragraph on rubidium.

La La_2O_3 is the only known oxide of lanthanum.^{10,11,24,37} The thermodynamic data^{6,7,8,23} indicate that the nitride, LaN , should not be present to more than one percent of the lanthanum.

Similar calculations for the bromides and iodides^{6,7,17,20,21,23} indicate that they should not be present to more than one percent of the lanthanum.

Ce Cerium has two known oxides, Ce_2O_3 and CeO_2 .^{7,10,24,37} The usual ignition product of cerium is CeO_2 .^{10,24,37} Ce_2O_3 is easily oxidized to CeO_2 .^{10,24,37} Hence, CeO_2 is considered to be the most probable species.

The nitride, CeN , is indicated by the thermodynamic data^{6,7,8,23} not to be present to more than one percent of the cerium.

Similarly, the data^{6,7,17,20,21,23} indicate that the bromides and iodides should not be present to more than one percent of the cerium.

Pr Two well-defined oxides of praseodymium are known, Pr_2O_3 and PrO_2 .^{10,24,37} In addition to these, the most common product of oxidation in air is usually formulated as Pr_6O_{11} .^{10,24,37} although this is possibly a solid solution of Pr_2O_3 and PrO_2 . The decomposition of Pr_6O_{11} to Pr_2O_3 occurs above 1000°K .^{7,37,38} The oxide takes up O_2 at room temperature if oxidized slightly above Pr_2O_3 .⁵¹

No data are available on the nitride, although it is thought that its stability should be slightly less than that of the cerium nitride. If that is true, the data^{6,7,8,23} indicate that the nitride should not be present to more than one percent of the praseodymium.

The thermodynamic data^{6,7,17,20,21} indicate that the bromides and iodides should not be present to more than one percent of the praseodymium. Asprey and Cunningham's data³⁸ indicate Pr_6O_{11} as the major species.

Nd The only known oxide of neodymium is Nd_2O_3 .^{7,10,24,37}

No data are available for the nitride, but an estimation similar to that made for praseodymium indicates that the nitride would not be present to more than one percent of the neodymium.

U N C L A S S I F I E D

U N C L A S S I F I E D

The thermodynamic data^{6,7,17,20,21} indicate that the bromides and iodides should not be present to more than one percent of the neodymium.

Pm There is very little information available on promethium. However, it is thought that the similarity of the rare earths^{13,24} gives a good basis for estimating that the product would be Pm_2O_3 , since the sesquioxide is the expected species for neodymium and samarium, (cf. neodymium and samarium) the neighboring elements.

Sm Sm_2O_3 is the only known oxide of samarium. The metal is easily oxidized in air, as are the other rare earth elements.^{7,10,13,24,37}

No data are available for the nitride, but an estimation, as with praseodymium and neodymium, indicates it to be present to no more than one percent of the samarium.

The thermodynamic data^{7,17,20,21} indicate that the bromides and iodides should not be present to more than one percent of the samarium.

Eu The only known oxide of europium is Eu_2O_3 .^{10,13,23,24}

No data are available on the nitride, but estimations as with the other rare earth elements indicate that it should not be present to more than one percent of the europium.

The thermodynamic data^{7,17,20,21} indicate that the bromides and iodides should not be present to more than one percent of the europium.

Gd The only known oxide of gadolinium is Gd_2O_3 .^{10,13,23,24}

No data are available on the nitride, but extrapolation of the estimations mentioned in the previous members of the rare earth elements indicates that the nitride should not be present to more than one percent of the gadolinium.

The thermodynamic data^{7,17,20,21} indicate that the bromides and iodides should not be present to more than one percent of the gadolinium.

U There are four known oxides of uranium, UO , UO_2 , U_3O_8 and UO_3 .^{7,10,11,37,39} The usual product of ignition in air is U_3O_8 .^{10,37,39} UO and UO_2 are easily oxidized in air.^{7,23,37,39,40} U_3O_8 decomposes to UO_2 at about 2000°K .^{23,40} UO_3 decomposes to U_3O_8 between 800° and 900°K .³⁹ From these facts, U_3O_8 is considered to be the most probable species.

U N C L A S S I F I E D

U N C L A S S I F I E D

The nitrides are not thought to be present to more than one percent of the uranium according to the thermodynamic data.^{6,7,8,13}

The thermodynamic data^{6,7,20,21,23,39,50} indicate that the bromides and iodides should not be present to an appreciable extent.

Our conclusion is that the most important species for uranium should be U_3O_8 with a much smaller amount of UO_3 being possible.

Np Two oxides of neptunium are known, NpO_2 and Np_2O_5 ,^{37,41,42,43} Np_2O_5 is also claimed.⁴³ Oxides higher than NpO_2 are prepared with difficulty.^{37,43} NpO_2 is the product of ignition in air of the element under ordinary conditions.^{37,41,42,43}

No data are available on the nitrides, but by analogy with uranium^{23,39} no nitride is thought to be present to more than one percent of the neptunium.

The data of Brewer, Bromley, Gilles and Lofgren⁴⁴ indicate that the bromide and iodide should not be present to more than one percent of the neptunium.

Pu Plutonium has only one known stable oxide, PuO_2 .^{37,43,45,46} Pu_2O_3 has been prepared, but only with great difficulty.⁴¹

Only one estimate of the thermodynamic data on the nitride is available.⁴⁵ This indicates that the nitride should not be an important species.

The data available^{45,46} also indicate that the bromides and iodides should not be important species. Considerations of relative concentrations indicate that they are not possible to any appreciable extent.

CONCLUSION

The foregoing estimates indicate that, under the temperature and concentration conditions resulting from an atomic bomb detonation in air, the chemical states of the products are mainly the oxides. The rare gases are, of course, uncombined, and nitrogen is largely left as N_2 ; silver remains predominantly as the metal, and the halogens exist mainly as the halides.

It should be pointed out that no consideration has been given in the foregoing report to the nuclear reactions which take place in the fission products. No adequate data seem to be available at the present time on the effects of such reactions on the chemical species of the radioactive

U N C L A S S I F I E D

U N C L A S S I F I E D

nuclides. However, it seems very probable that the effect would be a very important one.

To illustrate the point in question, let us consider the reaction $\text{Rb}^{89}\text{O}_2 \rightarrow \text{Sr}^{89}\text{O}_2$. The daughter atoms are not produced in sufficient quantities at high temperatures to allow significant thermal decomposition of Sr^{89}O_2 . That is, the majority of Sr^{89} atoms are produced by radioactive decay from Rb^{89} and should occur as Sr^{89}O_2 , not as Sr^{89} , as would be estimated if the Sr^{89} had been produced at high temperatures. However, this is based on the supposition that the nuclear disintegration does not have a large effect on the crystal structure in which the decaying atom exists. This is not necessarily so, for it is quite probable that the disintegration will have a marked effect on the structure. This problem has not yet been investigated sufficiently for a definite prediction of the effects.

Further complications are introduced when a chain of radioactive decays is followed, e.g., $\text{Rb}^{97} \rightarrow \text{Sr}^{97} \rightarrow \text{Y}^{97} \rightarrow \text{Zr}^{97} \rightarrow \text{Nb}^{97} \rightarrow \text{Mo}^{97}$. Obviously, the concentration of a final chemical species of Mo^{97} (even without considering the effects of the disintegrations) would be dependent on the chemical species of the original and each subsequent nucleus, the possible reactions involved and their rates of reaction, and the half-lives of the disintegrations.

Hence, it is not possible for us to say that all of an element will occur in a predicted species or group of species, since part of an element present at any time may be the result of radioactive decay of another or several other elements.

Approved by: William H Sullivan *WHS*
Scientific Director

U N C L A S S I F I E D

U N C L A S S I F I E D

BIBLIOGRAPHY

1. "The Effects of Atomic Weapons," prepared under the direction of the Los Alamos Scientific Laboratory of the U. S. Atomic Energy Commission, 1950, U. S. Government Printing Office, Washington 25, D. C.
2. J. O. Hirschfelder, R. Kamm, J. Magee, N. Sugarman, Atomic Energy Commission Report, LAMS-277, 20 August 1945.
3. G. I. Taylor, Atomic Energy Commission Report, LA-236, 15 March, 1945.
4. S. T. Cohen, J. O. Hirschfelder, M. Hull, J. L. Magee, Atomic Energy Commission Report, LA-550, 9 April 1946.
5. K. K. Kelley, private communication, September, 1950.
6. "Selected Values of Chemical Thermodynamic Properties," edited by F. D. Rossini, National Bureau of Standards, 31 March 1950.
7. L. Brewer, Atomic Energy Commission Report, UCRL-104, July, 1948.
8. L. Brewer, L. A. Bromley, P. W. Gilles and N. L. Lofgren, National Nuclear Energy Series, Div. IV, Vol. 19B, Paper 4, "Chemistry and Metallurgy of Miscellaneous Materials: Thermodynamics," edited by L. L. Quill, McGraw-Hill Book Company, 1950.
9. W. M. Latimer, Atomic Energy Commission Declassified Report, MDDC-1462, 10 September 1947.
10. J. W. Mellor, "A Comprehensive Treatise on Inorganic and Theoretical Chemistry," Longmans, Green and Company, 1922-1937.
11. W. M. Latimer and J. H. Hildebrand, "Reference Book of Inorganic Chemistry," the Macmillan Company, 1940.
12. F. R. Bichowsky and F. D. Rossini, "The Thermochemistry of the Chemical Substances," Reinhold Publishing Company (1936).
13. F. Ephraim, "Inorganic Chemistry" (edited by P. C. L. Throne and E. R. Roberts), Nordeman Publishing Company (1943).
14. P. W. Selwood, J. Am. Chem. Soc. 70, 883, 1948.
15. N. A. Lange, "Handbook of Chemistry," Handbook Publishers, Inc. (1946).
16. G. R. Waitkins and C. W. Clark, Chem. Rev. 36, 239 (1945).

U N C L A S S I F I E D

U N C L A S S I F I E D

17. L. Brewer, L. A. Bromley, P. W. Gilles, and N. L. Lofgren, National Nuclear Energy Series, Div. IV, Vol. 19B, Paper 6, "Chemistry and Metallurgy of Miscellaneous Materials: Thermodynamics," edited by L. L. Quill, McGraw-Hill Book Company, 1950.
18. S. Soto, Chemical Abstracts 33, 2406 (1939).
19. "Handbook of Chemistry and Physics," 30th Edition, C. D. Hodgman, editor, Chemical Rubber Publishing Company (1946).
20. L. Brewer, National Nuclear Energy Series, Div. IV, Vol. 19B, Paper 7, "Chemistry and Metallurgy of Miscellaneous Materials: Thermodynamics," edited by L. L. Quill, McGraw-Hill Book Company, 1950.
21. L. Brewer, National Nuclear Energy Series, Div. IV, Vol. 19B, Paper 3, "Chemistry and Metallurgy of Miscellaneous Materials: Thermodynamics," edited by L. L. Quill, McGraw-Hill Book Company, 1950.
22. H. F. Hunter and N. E. Ballou, Naval Radiological Defense Laboratory Report, ADC-65, February, 1949.
23. L. Brewer, Atomic Energy Commission Report, CC-672, 15 May 1943.
24. B. S. Hopkins, "Chapters in the Chemistry of the Less Familiar Elements," Stipes Publishing Company, 1940.
25. Gmelin's Handbook, System Numbers 69 and 70, Verlag Chemie, 1941.
26. C. Perrier and E. Segre, J. Chem. Phys. 5, 712 (1937).
27. C. Perrier and E. Segre, J. Chem. Phys. 7, 155 (1939).
28. G. T. Seaborg and E. Segre, Phys. Rev. 55, 808 (1939).
29. J. G. F. Druce, "Rhenium," Cambridge University Press, 1948.
30. E. E. Motta, G. E. Boyd and Q. V. Larson, Atomic Energy Commission Declassified Report, MDDC-1430, 1947.
31. M. G. Inghram, D. C. Hess, Jr., and A. J. Hayden, Atomic Energy Commission Declassified Report, MDDC-1460, 1947.
32. S. Fried, Atomic Energy Commission Declassified Report, MDDC-1513, 1947.
33. G. W. Parker, J. Reed and J. W. Rush, Atomic Energy Commission Declassified Report, AECD-2043, 1948.

U N C L A S S I F I E D

U N C L A S S I F I E D

34. G. E. Boyd, Q. V. Larson and E. E. Motta, Atomic Energy Commission Declassified Report, AECD-2151, 1948.
35. P. Pierron, Bull. Soc. Chem. France 6, 1054 (1939).
36. S. Glasstone, "Thermodynamics for Chemists," D. Von Nostrand Company, Inc., 1947.
37. D. M. Gruen and J. J. Katz, Atomic Energy Commission Declassified Report, AECD-1892, 1948.
38. L. B. Asprey and B. B. Cunningham, Atomic Energy Commission Report, UCRL-329, April, 1949.
39. L. Brewer, L. A. Bromley, P. W. Gilles, and N. L. Lofgren, Atomic Energy Commission Declassified Report, MDDC-1543, September, 1945.
40. D. M. Gillies, Atomic Energy Commission Declassified Report, MDDC-647, June, 1946.
41. S. Fried and N. R. Davidson, Atomic Energy Commission Declassified Report, MDDC-1332, July, 1947.
42. L. B. Magnusson and T. J. LaChapelle, National Nuclear Energy Series, Div. IV, Vol. 14B, Paper 1.7, "The Transuranium Elements," edited by G. T. Seaborg, J. J. Katz and W. M. Manning, McGraw-Hill Book Company, 1949.
43. L. Brewer, Atomic Energy Commission Declassified Report, AECD-1899, February, 1948.
44. L. Brewer, L. A. Bromley, P. W. Gilles and N. L. Lofgren, Atomic Energy Commission Declassified Report, CN-3306, October, 1945.
45. L. Brewer, L. A. Bromley, P. W. Gilles and N. L. Lofgren, Atomic Energy Commission Report, BC-88, December, 1945.
46. T. E. Phipps, R. L. Seifert, and O. C. Simpson, Atomic Energy Commission Report, CN-3223, September, 1945.
47. L. S. Darken and R. W. Gurry, J. Am. Chem. Soc. 67, 1398 (1945).
48. L. S. Darken and R. W. Gurry, J. Am. Chem. Soc. 68, 798 (1946).
49. S. Fried and N. F. Hall, Atomic Energy Commission Report, ANL-4469, June, 1950.

U N C L A S S I F I E D

U N C L A S S I F I E D

50. H. A. Young and H. G. Reiber, Atomic Energy Commission Declassified Report, MDDC-1729, December, 1947.
51. R. Gher, G. L. Bushey, and L. F. Audrieth, Office of Naval Research Report, N6ORI-71-C.T.#7, 1 June 1950.
52. W. M. Latimer, "Oxidation Potentials," Prentice-Hall, Inc. 1938.

U N C L A S S I F I E D

UNCLASSIFIED