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Phase Relations in the CaO–IrO_2–Ir System in Air

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The equilibrium phase relations for the CaO–IrO_2–Ir system were determined in air using the quenching technique. The system contains three stable compounds $4CaO \cdot IrO_2$, $2CaO \cdot IrO_2$, and $CaO \cdot IrO_2$; they dissociate to an oxide phase, Ir metal, and oxygen at 1240, 1170, and 1135°C, respectively. A metastable form of $CaO \cdot IrO_2$ occurs at temperatures between 900 and 1100°C. Indexed X-ray diffraction powder patterns of all compounds are given.

1. Introduction

This study was initiated as part of a general program of phase equilibrium investigations involving the alkaline earth and other oxides with the Pt-group metal oxides (*1–3*). These systems have practical importance since Pt-group metals are used extensively for container materials and other high temperature applications. Presented here are equilibrium relationships of the condensed phases in the system CaO–IrO_2–Ir in air.

2. Experimental Procedure

Specimens were prepared from 0.4 g batches of various combinations of calcium carbonate and IrO_2, each having a purity of at least 99.6%. Calculated amounts of each end member, corrected for ignition loss, were weighed to the nearest milligram. Each batch was thoroughly hand mixed and calcined in a muffle furnace at a minimum temperature of 800°C, or heated directly at the temperature of interest. Specimen containers were open gold tubes and open or welded platinum tubes; no apparent reaction occurred with the various oxide samples. Portions of each calcined batch were refired in a platinum alloy wire-wound quench furnace at various temperatures for different periods of time, and quenched in ice water or air. Temperatures in the quench furnace were measured with a Pt–Pt, 10% Rh calibrated thermocouple. All furnace temperatures[1] are considered accurate to ±5°C. The precision of the measurements was estimated to be ±2°C.

Equilibrium was assumed when the X-ray pattern showed no change after successive heat treatments. The stability of a compound was established by heating first above and then below the dissociation temperature. Stable compounds always reformed from the dissociation products; if prolonged heating failed to reform the phase, it was assumed to be metastable, forming only on heating. All specimens were examined by X-ray diffraction at room temperature with a high-angle-recording Geiger counter diffractometer and Ni-filtered Cu radiation. The scanning rate was 1/4° 2θ/min. Unit cell dimensions were refined by a least-squares computer program[2] and estimated accurate to at least 2 in the last decimal place.

3. Results and Discussion

The equilibrium phase diagram in air, Fig. 1, was constructed from the data in Table I. Oxygen reaction lines are dashed, and *A* through *E* indicate tie lines. The three phase triangular areas with listed temperatures represent invariant situations where three condensed phases coexist in equilibrium with oxygen. The oxygen reaction lines connect compositions on the CaO–IrO_2 join and the final compositions attained on dissociation of the oxide mixtures. It should be emphasized that the dissociation products are condensed phases always in equilibrium with oxygen.

Key Words: CaO:IrO_2 compounds, CaO–IrO_2–Ir system, dissociation, equilibrium, phase relations.

[1] This scale (IPTS 1968) applies to all temperatures listed in this paper.

[2] H. T. Evans Jr., D. E. Appleman, and D. S. Handwerker, Amer. Crystal. Assoc. Annual Meeting, Cambridge, MA Program, 43–43.

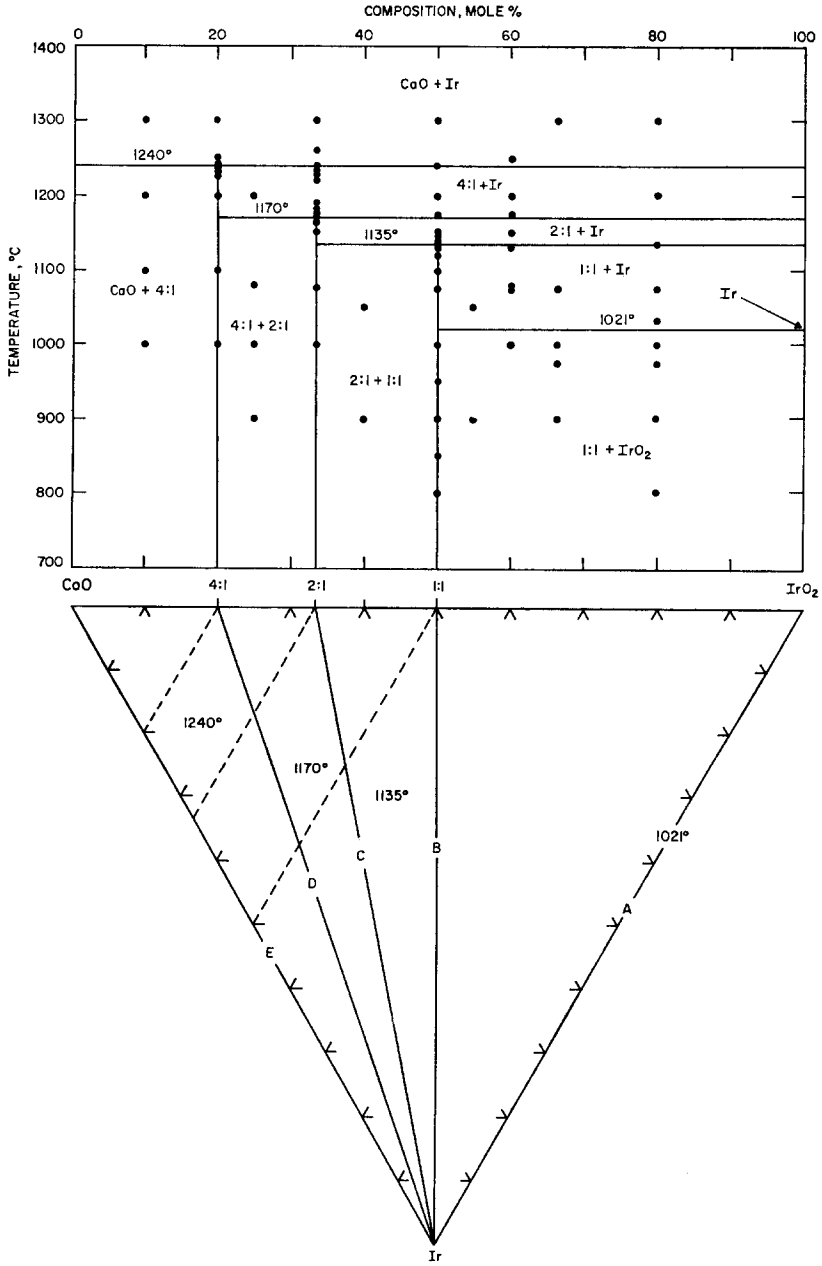

FIG. 1. Phase equilibrium diagram for the CaO–IrO_2–Ir System in Air. Compositions and temperatures of experiments. Oxygen reaction lines are dashed. *A* through *E* indicate tie lines for given temperatures: $A = 1021°C$; $1021°C < B < 1135°C$; $1135°C < C < 1170°C$; $1170°C < D < 1240°C$; $E = >1240°C$.

The binary-type phase diagram in the top portion of Fig. 1 is a projection of certain elements of the three dimensional ternary system CaO–IrO_2–Ir on a two dimensional plane figure; it represents a composite of the CaO–Ir and CaO–IrO_2 systems. As the temperature is increased, the compositions of the solid phases change by an apparent oxygen loss to those indicated by the CaO–Ir join. Illustrating a dissociation as a type of phase transition or decomposition in which vapor phase is ignored gives a simple binary representation of the ternary phase relations. This method of representation has been used by other investigators and is discussed in detail (*1*, *4*).

TABLE I

EXPERIMENTAL DATA FOR COMPOSITIONS IN THE CaO–IrO_2–Ir SYSTEM

Composition		Heat Treatment[a]			
CaO	IrO_2	Previous[e]	Final	X-ray diffraction analyses[b]	Remarks
Mol%	Mol%	°C-hr	°C-hr		
90	10		1000-72	$2CaO·IrO_2$+CaO	
		1000-72	1000-20	$2CaO·IrO_2$+CaO	
		1000-72,1000-20	1100-96	$CaO+4CaO·IrO_2+2CaO·IrO_2$	nonequilibrium
		1000-72,1000-20	1200-18[c]	$CaO+4CaO·IrO_2$	
		1000-72,1000-20	1300-2	CaO,Ir	
80	20		1000-72	$2CaO·IrO_2$+CaO	
		1000-72	1000-20	$2CaO·IrO_2$+CaO	
		1000-72,1000-20,1200-20	1000-144	$4CaO·IrO_2$	
		1000-72,1000-20	1100-96	$2CaO·IrO_2+CaO+4CaO·IrO_2$	nonequilibrium
		1000-72,1000-20	1200-1	$4CaO·IrO_2$+unidentified phase	Quenched in ice water; unidentified phase probably a hydrate
		1000-72,1000-20	1200-18[c]	$4CaO·IrO_2$+CaO	
		1000-72,1000-20,1300-2	1200-20	$4CaO·IrO_2$	$4CaO·IrO_2$ formed from CaO+Ir
		1000-72,1000-20	1225-2	$4CaO·IrO_2$	
		1000-72,1000-20	1230-2	$4CaO·IrO_2$	
		1000-72,1000-20	1235-2	$4CaO·IrO_2$	
		1000-72,1000-20	1240-2	$4CaO·IrO_2$+CaO+Ir	
		1000-72,1000-20	1250-2	$CaO+4CaO·IrO_2$+Ir	nonequilibrium
		1000-72,1000-20	1300-2	CaO+Ir	
75	25		1000-20	$2CaO·IrO_2$+CaO	
		1000-20	1000-22	$2CaO·IrO_2$+CaO	
		1000-20,1000-22	1080-18[c]	$2CaO·IrO_2$+CaO	
		1000-20,1000-22	1200-3	$4CaO·IrO_2+2CaO·IrO_2$+CaO	nonequilibrium
66.6	33.3		1000-18	$2CaO·IrO_2$+CaO	
		1000-18	1000-18	$2CaO·IrO_2$	
		1000-18,1000-18,1300-2	1000-96	$2CaO·IrO_2$	$2CaO·IrO_2$ formed from CaO+Ir
		1000-18,1000-18	1075-20	$2CaO·IrO_2$	
		1000-18,1000-18	1075-120[c]	$2CaO·IrO_2$	
		1000-18,1000-18	1075-360[c]	$2CaO·IrO_2$	
		1000-18,1000-18	1165-18	$2CaO·IrO_2$	
		1000-18,1000-18	1170-19	$2CaO·IrO_2+4CaO·IrO_2$	
		1000-18,1000-18	1190-18	$2CaO·IrO_2+4CaO·IrO_2$+Ir+CaO	nonequilibrium
		1000-18,1000-18	1210-2	$2CaO·IrO_2+4CaO·IrO_2$+CaO	nonequilibrium
		1000-18,1000-18	1220-2	$2CaO·IrO_2+4CaO·IrO_2$+CaO	nonequilibrium
		1000-18,1000-18	1220-96	$4CaO·IrO_2+2CaO·IrO_2$+Ir	nonequilibrium
		1000-18,1000-18	1225-2	$2CaO·IrO_2+4CaO·IrO_2$+CaO	nonequilibrium
		1000-18,1000-18	1230-2	$2CaO·IrO_2+4CaO·IrO_2$+Ir+CaO	nonequilibrium
		1000-18,1000-18	1240-2	$4CaO·IrO_2$+CaO+Ir	
		1000-18,1000-18	1260-2	CaO+Ir+$4CaO·IrO_2$	nonequilibrium
		1000-18,1000-18	1300-2	CaO+Ir	
60	40		900-18	$2CaO·IrO_2+IrO_2$	
		900-18	1050-192	$2CaO·IrO_2$+Ir	
50	50		800-18	$2CaO·IrO_2+IrO_2$	
		1000-18,1000-19,1300-2	800-96	$CaO·IrO_2+2CaO·IrO_2+IrO_2$	nonequilibrium
		800-18	850-18	$2CaO·IrO_2+IrO_2$	
			900-1	$2CaO·IrO_2$+M-$CaO·IrO_2$+$CaO·IrO_2$	nonequilibrium
		800-18,850-18	900-20	$2CaO·IrO_2$+M-$CaO·IrO_2+IrO_2+CaO·IrO_2$	nonequilibrium
		1000-18,1000-19,1300-2	900-24	$CaO·IrO_2+2CaO·IrO_2$	$CaO·IrO_2$ formed from CaO+Ir; trace amount of $2CaO·IrO_2$
			950-2	M-$CaO·IrO_2$+$CaO·IrO_2$	nonequilibrium
		800-18,850-18,900-20	950-120	$CaO·IrO_2$+M-$CaO·IrO_2$	nonequilibrium
			1000-1	M-$CaO·IrO_2$+$CaO·IrO_2$	nonequilibrium
			1000-2	M-$CaO·IrO_2$+$CaO·IrO_2$	nonequilibrium
			1000-3	$CaO·IrO_2$+M-$CaO·IrO_2$	nonequilibrium
		1000-20[d],1000-22[d]	1000-18[d]	M-$CaO·IrO_2$+$CaO·IrO_2+2CaO·IrO_2$	nonequilibrium
			1000-18	M-$CaO·IrO_2$+$2CaO·IrO_2+IrO_2$	nonequilibrium
		1000-18,1000-19,1300-2	1000-19	$CaO·IrO_2+2CaO·IrO_2$	M-$CaO·IrO_2$ failed to form from CaO+Ir
			1000-19	$CaO·IrO_2$+M-$CaO·IrO_2$	nonequilibrium
			1000-19	$CaO·IrO_2$+M-$CaO·IrO_2$	slow cooled; nonequilibrium
		1000-18	1000-19	M-$CaO·IrO_2+2CaO·IrO_2+CaO·IrO_2$	nonequilibrium
			1000-20[d]	M-$CaO·IrO_2+CaO·IrO_2+2CaO·IrO_2$	nonequilibrium

TABLE I—*continued*

Composition		Heat Treatment[a]			
CaO	IrO_2	Previous[e]	Final	X-ray diffraction analyses[b]	Remarks
Mol%	Mol%	°C-hr	°C-hr		
50	50	1000-20[d]	1000-22[d]	M-$CaO{\cdot}IrO_2$+$CaO{\cdot}IrO_2$+$2CaO{\cdot}IrO_2$	nonequilibrium
		800-18,850-18,900-20,			
		950-120	1075-18	$CaO{\cdot}IrO_2$+$2CaO{\cdot}IrO_2$+M-$CaO{\cdot}IrO_2$	nonequilibrium
		800-18,850-18,900-20,			
		950-120	1075-18[c]	$CaO{\cdot}IrO_2$+$2CaO{\cdot}IrO_2$+M-$CaO{\cdot}IrO_2$	nonequilibrium
		1000-18,1000-19	1075-20	M-$CaO{\cdot}IrO_2$+$CaO{\cdot}IrO_2$+$2CaO{\cdot}IrO_2$	nonequilibrium
		1000-18,1000-19	1075-120[c]	$CaO{\cdot}IrO_2$+$2CaO{\cdot}IrO_2$	trace amount of $2CaO{\cdot}IrO_2$
		1000-18,1000-19,1200-2	1075-360	$CaO{\cdot}IrO_2$+$2CaO{\cdot}IrO_2$	M-$CaO{\cdot}IrO_2$ failed to form from $2CaO{\cdot}IrO_2$+Ir
		1000-18,1000-19	1100-3	M-$CaO{\cdot}IrO_2$+$CaO{\cdot}IrO_2$+$2CaO{\cdot}IrO_2$	nonequilibrium
		800-18,850-18,			
		900-20,950-120	1100-18	$CaO{\cdot}IrO_2$+M-$CaO{\cdot}IrO_2$+$2CaO{\cdot}IrO_2$	nonequilibrium
		1300-2	1100-19	$2CaO{\cdot}IrO_2$+Ir+$CaO{\cdot}IrO_2$	nonequilibrium
		800-18,850-18,			
		900-20,950-120	1120-2	$CaO{\cdot}IrO_2$+$2CaO{\cdot}IrO_2$	trace amount of $2CaO{\cdot}IrO_2$
		800-18,850-18,			
		900-20,950-120	1130-2	$CaO{\cdot}IrO_2$+$2CaO{\cdot}IrO_2$	trace amount of $2CaO{\cdot}IrO_2$
		800-18,850-18,			
		900-20,950-120	1135-2	$CaO{\cdot}IrO_2$+$2CaO{\cdot}IrO_2$+Ir	
		800-18,850-18,			
		900-20,950-120	1140-2	$CaO{\cdot}IrO_2$+$2CaO{\cdot}IrO_2$Ir	nonequilibrium
		800-18,850-18,			
		900-20,950-120	1150-2	$2CaO{\cdot}IrO_2$+$CaO{\cdot}IrO_2$+Ir	nonequilibrium
		800-18,850-18,			
		900-20,950-120	1175-2	$2CaO{\cdot}IrO_2$+Ir	
		800-18,850-18,			
		900-20,950-120	1200-2	$2CaO{\cdot}IrO_2$+Ir	
		1000-18,1000-19	1240-2	$4CaO{\cdot}IrO_2$+Ir+CaO	
		1000-18,1000-19	1300-2	Ir+CaO	
45	55		900-18	M-$CaO{\cdot}IrO_2$+IrO_2+$2CaO{\cdot}IrO_2$	nonequilibrium
		900-18	1050-192	M-$CaO{\cdot}IrO_2$+$CaO{\cdot}IrO_2$	nonequilibrium
40	60		1000-20	M-$CaO{\cdot}IrO_2$+IrO_2+$CaO{\cdot}IrO_2$	nonequilibrium
		1000-20	1000-22	M-$CaO{\cdot}IrO_2$+IrO_2+$CaO{\cdot}IrO_2$	nonequilibrium
		1000-20,1000-22	1075-360[c]	$CaO{\cdot}IrO_2$+IrO_2+M-$CaO{\cdot}IrO_2$	trace amount of M-$CaO{\cdot}IrO_2$
		1000-20,1000-22	1080-18[c]	$CaO{\cdot}IrO_2$+M-$CaO{\cdot}IrO_2$+IrO_2	nonequilibrium
		1000-20,1000-22	1150-20[c]	$CaO{\cdot}IrO_2$+IrO_2+M-$CaO{\cdot}IrO_2$	trace amount of M-$CaO{\cdot}IrO_2$
		1000-20,1000-22	1200-2[c]	$CaO{\cdot}IrO_2$+IrO_2+M-$CaO{\cdot}IrO_2$	nonequilibrium
		1000-20,1000-22	1250-20	$4CaO{\cdot}IrO_2$+Ir+CaO	nonequilibrium
25	75	1000-18,1000-19	900-3	IrO_2+M-$CaO{\cdot}IrO_2$	nonequilibrium
			975-52	M-$CaO{\cdot}IrO_2$+IrO_2+$CaO{\cdot}IrO_2$	nonequilibrium
			1000-18	IrO_2+M-$CaO{\cdot}IrO_2$	nonequilibrium
		1000-18	1000-19	M-$CaO{\cdot}IrO_2$+IrO_2+$CaO{\cdot}IrO_2$	nonequilibrium
		1000-18,1000-19	1075-20	$CaO{\cdot}IrO_2$+M-$CaO{\cdot}IrO_2$+Ir	nonequilibrium
		1000-18,1000-19	1075-120[c]	$CaO{\cdot}IrO_2$+IrO_2	
		1000-18,1000-19	1300-2	Ir+CaO	
20	80		900-3	IrO_2+M-$CaO{\cdot}IrO_2$	nonequilibrium
			900-18	IrO_2+M-$CaO{\cdot}IrO_2$+$CaO{\cdot}IrO_2$	nonequilibrium
			975-240	IrO_2+M-$CaO{\cdot}IrO_2$+$CaO{\cdot}IrO_2$	nonequilibrium
			1000-4	IrO_2+M-$CaO{\cdot}IrO_2$	nonequilibrium
		900-18	1030-4	M-$CaO{\cdot}IrO_2$+$CaO{\cdot}IrO_2$+Ir	nonequilibrium
		900-18,1300-2	1075-19	Ir+$CaO{\cdot}IrO_2$+$2CaO{\cdot}IrO_2$	$CaO{\cdot}IrO_2$ formed from Ir+CaO
		900-18	1135-4	M-$CaO{\cdot}IrO_2$+$CaO{\cdot}IrO_2$+Ir	nonequilibrium
		900-18	1200-21	$4CaO{\cdot}IrO_2$+Ir	
		900-18	1300-2	Ir+CaO	

a All specimens were heat treated in open platinum tubes and air quenched unless otherwise indicated. All temperatures listed applied to (IPTS 1968).

b Phases identified are given in order of the relative amount present at room temperature; M-$CaO{\cdot}IrO_2$ = metastable $CaO{\cdot}IrO_2$ probably a metastable phase in air at atmospheric pressure.

c Sealed platinum tube container; quenched in ice water.

d Open gold tube container; air quenched.

e No entry under "Previous" column indicates the specimen received no prior heat treatment.

Tables II and III list the indexed X-ray powder patterns for each binary phase in the CaO–IrO_2 system. Dissociation temperatures of the stable phases are indicated by Fig. 1.

This system is somewhat similar to the SrO–IrO_2 system (*1*) since both systems have three stable compounds (4:1, 2:1, 1:1) in air. The 4:1 compounds of both systems have hexagonal (rhombo-

Table II.

X-Ray Diffraction Powder Data for $4CaO \cdot IrO_2$ and $2CaO \cdot IrO_2$

(CuKα radiation)[a]

$4CaO \cdot IrO_2$[b]				$2CaO \cdot IrO_2$[c]			
	d(Å)				d(Å)		
hkl	obs	calc	I/I_1	hkl	obs	calc	I/I_1
110	4.667	4.665	71	110	4.709	4.710	100
012	4.612	4.610	73	200	4.079	4.079	4
202	3.282	3.279	42	001	3.193	3.195	10
113	2.921	2.919	21	210	3.083	3.084	2
300	2.693	2.693	100	300	2.718	2.720	67
122	2.682	2.683	23	111	2.643	2.644	86
104	2.652	2.652	53	220	2.355	2.355	22
220	2.3323	2.3326	19	310	2.262	2.263	2
024	2.3053	2.3052	61	211	2.217	2.219	8
131	2.1980	2.1977	16	301	2.071	2.071	15
312	2.0818	2.0814	65	400	2.0395	2.0397	3
214	2.0669	2.0667	79	221	1.8960	1.8958	36
223	1.9791	1.9795	41	320	1.8714	1.8718	3
042	1.9012	1.9008	25	410	1.7804	1.7804	16
410	1.7634	1.7633	49	321	1.6148	1.6150	2
134	1.7509	1.7513	29	002	1.5981	1.5975	8
116	1.7367	1.7368	47	330	1.5701	1.5702	12
404	1.6394	1.6396	8	411	1.5556	1.5552	34
413	1.5948	1.5951	8	112	1.5130	1.5129	10
330	1.5549	1.5550	40	331	1.4095	1.4092	8
324	1.5466	1.5469	48	302	1.3773	1.3774	11
422	1.4735	1.4734	18	600	1.3601	1.3598	6
226	1.4599	1.4596	21	222	1.3222	1.3221	5
152	1.4052	1.4050	9	520	1.3064	1.3065	5
054	1.4009	1.4005	19	601	1.2511	1.2512	3
018	1.3828	1.3830	10	521	1.2095	1.2093	8
600	1.3469	1.3468	22	412	1.1892	1.1890	6
244	1.3416	1.3413	22	332	1.1199	1.1198	4
208	1.3259	1.3258	19	441	1.1049	1.1050	3
137	1.3043	1.3043	2	710	1.0808	1.0807	3
520	1.2937	1.2938	12	113	1.0389	1.0388	3
342	1.2928	1.2926	11	602	1.0357	1.0355	4
514	1.2893	1.2891	13	630	1.0280	1.0279	4
416	1.2833	1.2833	29	711	1.0237	1.0237	5
128	1.2756	1.2753	10	522	1.0114	1.0113	3
612	1.2036	1.2035	9	631	0.9785	0.9785	3
434	1.2009	1.2007	10	223	0.9704	0.9704	3
318	1.1898	1.1895	5	413	0.9140	0.9140	4
048	1.1529	1.1526	3				
532	1.1308	1.1306	2				
164	1.1285	1.1283	5				
238	1.1192	1.1189	8				
1,0,10	1.1124	1.1121	3				
710	1.0704	1.0702	2				
704	1.0678	1.0675	25				
624	1.0410	1.0406	4				
428	1.0338	1.0333	3				
419	1.0184	1.0184	6				
158	1.0093	1.0089	2				

[a] d-interplanar spacing, I/I_1 - relative intensity

[b] X-ray pattern obtained from specimen heat treated at 1230°C for 2 hrs. Indexing based on hexagonal cell with a=9.330 and c=11.228Å.

[c] X-ray pattern obtained from specimen treated at 1075° for 20 hrs. Indexing based on hexagonal cell with a=9.421 and c=3.195Å.

hedral) symmetry, and appear similar in structure. The $4SrO \cdot IrO_2$ has been reported to have the K_4CdCl_6-type structure (*5*). By analogy the X-ray pattern of $4CaO \cdot IrO_2$ was indexed with a hexagonal (rhombohedral) cell, $a = 9.330$ Å and $c = 11.228$ Å. However, the 2:1 and 1:1 compounds in the present system differ in symmetry and have no apparent similarity to the corresponding stable compounds in the SrO–IrO_2 system. Babel, Rudorff, and Tschopp (*6*) reported a hexagonal structure for $2CaO \cdot IrO_2$. Our hexagonal cell with $a = 9.421$ Å and $c = 3.195$ Å, is in good agreement.

A structure for $CaO \cdot IrO_2$ (1:1) was proposed by Rodi and Babel (*7*). Our orthorhombic cell with $a = 3.145$ Å, $b = 9.857$ Å, and $c = 7.296$ Å, is essentially the same.

We detected a phase that appears to be a metastable $CaO \cdot IrO_2$ (M–1:1) compound[3] in air. It exists from about 900 to 1100°C, always in combination with other phases, usually the stable 1:1 compound. All attempts to produce a single phase were unsuccessful. Table III gives powder X-ray

[3] This composition yielded the greatest quantity of the phase.

Table III.

X-Ray Diffraction Powder Data for $CaO \cdot IrO_2$ and Metastable $CaO \cdot IrO_2$

(CuKα radiation)[a]

$CaO \cdot IrO_2$[b]				Metastable $CaO \cdot IrO_2$[c]			
	d(Å)				d(Å)		
hkl	obs	calc	I/I_1	hkl	obs	calc	I/I_1
020	4.927	4.928	69	101	3.860	3.863	78
002	3.645	3.648	44	020	3.832	3.836	43
110, 031	2.994	2.996, 2.996	56	111	3.449	3.450	2
022	2.930	2.932	100	002	2.792	2.793	25
				121	2.721	2.722	100
111	2.771	2.771	3				
040	2.464	2.464	24	200	2.673	2.673	24
112	2.314	2.315	41	022	2.259	2.258	10
130	2.271	2.272	41	220	2.193	2.193	8
131	2.1691	2.1691	9	202	1.932	1.931	30
				040	1.918	1.918	15
042	2.0417	2.0420	12				
132	1.9286	1.9285	41	103	1.758	1.759	8
113	1.8886	1.8882	4	222	1.725	1.725	14
004	1.8237	1.8240	16	141	1.718	1.718	16
024	1.7105	1.7106	10	301	1.6978	1.6978	6
				123	1.5983	1.5986	12
150	1.6704	1.6703	13				
060	1.6426	1.6428	3	042	1.5808	1.5811	8
200	1.5720	1.5724	10	321	1.5530	1.5525	19
114	1.5578	1.5580	19	142	1.5170	1.5162	3
211, 152	1.5190	1.5187, 1.5187	20	213	1.4979	1.4985	2
				242	1.3613	1.3609	8
220, 062	1.4984	1.4980, 1.4980	18				
044	1.4665	1.4661	11	143	1.2965	1.2962	4
202	1.4443	1.4440	5	341	1.2714	1.2712	3
134	1.4227	1.4223	13	224	1.1779	1.1781	3
222	1.3857	1.3857	14				
240	1.3258	1.3255	5				
170	1.2856	1.2852	3				
242	1.2460	1.2458	3				
080	1.2324	1.2321	9				
251	1.2126	1.2122	6				
204	1.1911	1.1909	4				
026	1.1808	1.1806	5				
082	1.1677	1.1673	3				
224	1.1579	1.1576	3				
116	1.1269	1.1267	5				
065	1.0910	1.0910	2				
262	1.0847	1.0846	6				
244	1.0725	1.0723	8				
174	1.0508	1.0506	3				
056	1.0349	1.0349	2				
084	1.0213	1.0210	3				

[a] d-interplanar spacing, I/I_1 - relative intensity.

[b] X-ray pattern obtained from specimen heat treated at 950°C for 120 hrs. Indexing based on orthorhombic cell with a=3.145, b=9.857, and c=7.296 Å.

[c] X-ray pattern obtained from specimen heat treated at 950°C for 2 hrs. Indexing based on orthorhombic cell with a=5.346, b=7.672, and c=5.587Å.

diffraction data for the M–1 : 1 compound indexed as an orthorhombic perovskite cell with $a = 5.346$ Å, $b = 7.672$ Å, and $c = 5.587$ Å. It appears to be similar to other orthorhombic perovskites like $CaO \cdot TiO_2$ (*8*) and high pressure $SrO \cdot IrO_2$ (*9*).

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