The Crystal Structure of $AuAl_2$.

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While the binary alloys of *Cu Ag* and *Au* with other metals have been shown, especially by Westgren and Phragmen, to have many features in common, the compound $AuAl_2$ appears to be of an exceptional nature; for this reason an account of its crystal structure is of interest.

$AuAl_2$ is formed by the reaction of the elements in the liquid phase with the evolution of considerable heat; it solidifies at the unusually high temperature 1060° (Au melts at 1063°) to a crystalline purple solid. The present material assays 78.10% *Au* (calculated for $AuAl_2$, 78.52% *Au*) and is of density 7.60. A powder photograph was taken in *Mo* radiation in a camera of radius 13 cm. The lines indicate a face-centered cubic structure with $a = 6.00 \pm .02$, $Z = 4$, calculated density 7.66. The absence of all reflections with mixed indices shows that *Au* is in 4b of Wyckoff's notation. While the *Al* atoms cannot be located with the same certainty, the agreement between observed intensities and those calculated for the CaF_2 structure (*Al* in 8c) is satisfactory (Table I). On the contrary the placing of *Al* in 8h

Table I. Powder photograph of $AuAl_2$.

h k l	*a*	Intensity obs.	Intensity calc.	*h k l*	*a*	Intensity obs.	Intensity calc.	*h k l*	*a*	Intensity obs.	Intensity calc.
111	5.99	5	20	440	6.01	3	20	731, 553	6.00	5	55
200	5.97	1	7	531	6.02	5	47	800	—	0	6
220	5.98	10	38	600, 442	6.01	2	16	733	6.00	1	16
311	5.99	9	41	620	6.01	4	35	644, 820	—	0	20
222	5.98	3	7	533	6.01	4	21	660, 822	6.00	2	35
400	5.98	4	15	622	6.00	1	12	555, 751	6.01	2	34
331	5.98	7	33	444	6.00	w	10	662	—	0	9
420	6.02	4	17	551, 711	6.00	4	38	840	6.02	w	20
422	5.99	7	48	640	—	0	12	911, 753	6.00	2	39
511, 333	6.01	6	37	642	6.01	5	55				

Values in the third column are visual estimates; those in the fourth column are proportional to H. F^2 as calculated from the *F* curves of James and Brindley (Z. Krist. 78, 470. 1931).

(pyrite structure), or in 8g, or a statistical distribution of *Au* and *Al* over three face centered lattices beginning in 000, $\pm \frac{1}{4}\frac{1}{4}\frac{1}{4}$, would lead to serious conflicts with the observed intensities of reflections 331, 420 and 422; the CaF_2 structure may therefore be accepted as correct.

With this structure the distance *Au-Al* is 2.58 or considerably less than the sum of the radii of the atoms 2.87. The volume per atom, 17.8 A^3, is greater than that found in *Au*, 16.9, or in *Al* metal, 16.5. The ratio valence

electrons/atoms or 7/3 is greater than those characteristic of the more common β, γ or ε phases. The only intermetallic compounds heretofore described as having the CaF_2 structure are Mg_2Si, Mg_2Pb and Mg_2Sn. These compounds seem to have at least some of the peculiarities noted in $AuAl_2$.

Summary: The purple compound $AuAl_2$ has most probably the CaF_2 structure with $a = 6.00$.

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On the High Temperature Modification of *CsCl*.

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Three powder photographs *CsCl* were taken in *Mo* radiation at different temperatures. The lattice constants, reliable to about .02 A, are: at 25° $a = 4.09$, distance *Cs—Cl* $d = 3.54$, volume $V = 68$; at a temperature below the transition at 460° $a = 4.20$, $d = 3.64$, $V = 74$; at a temperature above the transition there is present a cubic phase having the *NaCl* structure with $a = 7.08$, $d = 3.54$, $V = 79$. Thus on heating through the transition, d decreases by about 3%, a figure that has been observed in a number of similar instances; V increases as in the corresponding transitions in the ammonium and rubidium halides, and thus as with these substances the transition temperature will increase with increasing pressure.

The foregoing is in agreement with the recently reported work of Wagner and Lippert[1]), who found $a = 7.10$ for the *NaCl* cubic phase.

Powder lines of *CsCl* at 500°.

hkl	a	Intensity	*hkl*	a	Intensity
111	7.15	5	400	7.08	1[2])
200	7.10	5	331	absent	
220	7.08	5	420	7.06	1
311	7.09	2	422	7.08	0.5
222	7.09	3[2])			

There is no experimental work on the question whether *CsBr* and *CsI* have similar transitions. By analogy to the *Rb* halides it would be predicted that *CsBr* and *CsI* would invert, if at all, at a higher temperature than *CsCl* at any given pressure; in fact some photographs of mine show the absence of any inversion in *CsBr* and *CsI* at a temperature above the transition temperature of *CsCl*. With the ammonium halides the reverse order is found, the iodide having the lowest transition temperature at any given pressure.

Summary: — At 500° *CsCl* has the *NaCl* structure with $a = 7.08$.

1) G. Wagner, L. Lippert, Z. physik. Chem. **21** B, 471. 1933.

2) Coincidence with a reflection from the heating coil.

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