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Interatomic distances in the γ-phase compound Ag_5Zn_8.*

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The refinement of crystallographic parameters for the γ-phase compound Ag_5Zn_8 has been undertaken by least-squares analyses of powder and single-crystal diffraction photographs prepared with copper X-radiation; these parameters have been used to calculate interatomic distances in this compound.

The sample was prepared by heating stoichiometric quantities of metallic silver and zinc in a sealed quartz tube to about 650° C. Loss of zinc by distillation was checked by weighing the ingot, and was found to be negligible. Powder photographs, prepared in a Straumanis-type Philips camera, were measured with a steel rule and analyzed by a least-squares method (Shoemaker, Marsh, Ewing & Pauling, 1952); the resultant cell constant for the cubic unit cell is

$$a_0 = 9{\cdot}3407 \pm 0{\cdot}0003 \text{ Å}$$
$$(\lambda = 1{\cdot}54050 \text{ Å for Cu } K\alpha_1;\ 1{\cdot}54434 \text{ for } K\alpha_2),$$

where the uncertainty is the calculated standard deviation. This is in good agreement with the value 9·327 kX. (9·344 Å) reported by Westgren & Phragmén (1925) for a sample containing a slight excess of zinc.

A small single crystal was isolated from the ingot and was oriented by Laue photography. Multiple-film Weissenberg photographs were prepared for the equator and first six layer lines, the axis of rotation being the a axis. Thus, all of the reflections within the sphere of copper radiation were checked; of the total of 112 independent reflections, 92 were actually observed. The space group was confirmed as being T_d^3–$I\bar{4}3m$, as first reported by Bradley & Thewlis (1926). Three successive least-squares refinements of the five atomic positional parameters were performed, all of the observed reflections being included in the calculations. Since the space group is non-centrosymmetric, the minimization was performed on $(F_o^2 - F_c^2)$ values. The starting parameters were those reported by Bradley & Gregory (1931) for the compound Cu_5Zn_8, and the weighting scheme was similar to that of Shoemaker *et al.* (1952). In the final least-squares adjustment, the maximum shift in any parameter was 0·003 Å.

The resultant atomic parameters and the standard deviations (with the starting parameters listed in parentheses) are:

8 Zn_I in 8(*c*) a, a, a; ..., with $a = 0{\cdot}1120 \pm 0{\cdot}0012$ (0·110).
8 Ag_I in 8(*c*) b, b, b; ..., with $b = 0{\cdot}8240 \pm 0{\cdot}0006$ (0·828).
12 Ag_{II} in 12(*e*) $c, 0, 0$; ..., with $c = 0{\cdot}3551 \pm 0{\cdot}0008$ (0·355).
24 Zn_{II} in 24(*g*) d, d, e; ..., with $d = 0{\cdot}3130 \pm 0{\cdot}0008$ (0·313), $e = 0{\cdot}0331 \pm 0{\cdot}0010$ (0·036).

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The final calculated F values, which included an empirical temperature factor with $B = 0{\cdot}58$ Å^2, yielded an R factor of 0·098 for the 92 observed reflections.

In Table 1 there are listed, for each type of atom, the number and kind of neighboring atoms together with the corresponding interatomic distances and standard deviations. If these interatomic distances are used to calculate bond numbers n and valences according to Pauling's theory (Pauling, 1947, 1949), the resulting valences for the various kinds of atoms are:

Table 1. *Atomic distances in* Ag_5Zn_8

Atom	Neighbor		Distance (Å)	S.d.	n
Ag_I	Ag_{II}	(3)	2·864	0·005	0·47
(1·328 Å)	Zn_I	(3)	2·820	0·011	0·36
	Zn_{II}	(3)	2·663	0·010	0·67
	Zn_{II}	(3)	2·721	0·010	0·53
Ag_{II}	Ag_I	(2)	2·864	0·005	0·47
(1·340 Å)	Ag_{II}	(1)	2·707	0·015	0·90
	Zn_I	(2)	2·710	0·006	0·57
	Zn_{II}	(2)	2·682	0·011	0·65
	Zn_{II}	(4)	2·966	0·007	0·22
	Zn_{II}	(2)	2·978	0·011	0·21
Zn_I	Ag_I	(3)	2·820	0·011	0·36
(1·223 Å)	Ag_{II}	(3)	2·710	0·006	0·57
	Zn_I	(3)	2·959	0·032	0·14
	Zn_{II}	(3)	2·755	0·023	0·31
Zn_{II}	Ag_I	(1)	2·663	0·010	0·67
(1·229 Å)	Ag_I	(1)	2·721	0·010	0·53
	Ag_{II}	(1)	2·682	0·011	0·65
	Ag_{II}	(2)	2·966	0·007	0·22
	Ag_{II}	(1)	2·978	0·011	0·21
	Zn_I	(1)	2·755	0·023	0·31
	Zn_{II}	(4)	2·771	0·004	0·30

Ag_I, 6·0; Ag_{II}, 5·5; Zn_I, 4·1; Zn_{II}, 4·0.

The standard deviations in the bond distances lead to an estimated probable error of about 0·2 units in the calculated valences. The single-bond radii corresponding to these valences are given in parentheses below each type of atom in Table 1; these radii were the ones used to calculate the bond numbers n.

References

Bradley, A. J. & Gregory, C. H. (1931). *Phil. Mag.* (7), **12**, 143.
Bradley, A. J. & Thewlis, J. (1926). *Proc. Roy. Soc.* A, **112**, 678.
Pauling, L. (1947). *J. Amer. Chem. Soc.* **69**, 542.
Pauling, L. (1949). *Proc. Roy. Soc.* A, **196**, 23.
Shoemaker, D. P., Marsh, R. E., Ewing, F. J. & Pauling, L. (1952). *Acta Cryst.* **5**, 637.
Westgren, A. & Phragmén, G. (1925). *Phil. Mag.* (6), **50**, 311.