

Acta Cryst. (1954). **7**, 781

The crystal structures of SrCd, BaCd, SrHg and BaHg. By RICCARDO FERRO, *Chemical Institute of Genoa University, Genoa, Italy*

(Received 9 August 1954)

SrCd, BaCd, SrHg and BaHg have been prepared by electric melting of the various metals in pure iron vessels, followed by heating to 950° C. and slow cooling (in about 100 hr.) to room temperature. None of the metals used was below 99.9% purity.

The alloys obtained are brittle (especially those with cadmium) and, particularly the amalgams, easily alterable in air; therefore it is necessary to handle them under inert gas.

The micrographic appearance, although difficult to observe owing to the reactivity of the samples, agrees with the hypothesis of the existence of only one phase for the 1:1 composition.

The amalgams were analysed by treating them with HCl, collecting the mercury on a Gooch crucible and precipitating the SrSO₄ or BaSO₄ from the filtrate. The alloys with cadmium, after dissolution in HCl, were first treated with H₂SO₄ to precipitate SrSO₄ or BaSO₄ and then the cadmium in the filtrate was determined as CdSO₄. The tested samples had the following compositions:

SrCd: Cd % 57.0₅ (56.19 theor.);
BaCd: Cd % 45.1₀ (45.01 theor.);
SrHg: Hg % 70.8₁ (69.60 theor.);
BaHg: Hg % 60.2₂ (59.36 theor.).

The specific gravity was checked by filling the pycnometer (under vacuum) with rectified benzene which had been dehydrated on sodium and potassium.

The alloys were examined by X-rays (Cu K α radiation) using the powder method. The positions and intensities of the reflexions were in accordance with a CsCl-type cubic structure. The constants are shown in Table 1.

It is interesting to compare these data with those of

Table 1. *Structure data for A Cd and A Hg Compounds*
(All distances are in kX. units.)

AB	a_0	A-B distance	$r_A + r_B$	Specific gravity	
				Calc.	Meas.
SrCd	4.003	3.476	3.56	5.15	5.06
BaCd	4.207	3.643	3.66	5.54	5.69
SrHg	3.922	3.396	3.59	7.88	7.77
BaHg	4.125	3.572	3.69	7.95	7.90
Differences between interatomic distances					
		3.572 - 3.396 = 0.176	3.396 - 3.248 = 0.148		
		(Ba-Hg) (Sr-Hg)	(Sr-Hg) (Ca-Hg)		
		3.643 - 3.467 = 0.176	3.467 - 3.317 = 0.150		
		(Ba-Cd) (Sr-Cd)	(Sr-Cd) (Ca-Cd)		

CaCd ($a_0 = 3.830$ kX.) and CaHg ($a_0 = 3.751$ kX.) (Iandelli, 1949), and to observe how the interatomic distances vary, as regards the various cadmium compounds, in perfect correspondence with those of the amalgams. Finally it is useful to note the resemblance with rare earths, of which the following isostructural compounds are known: LaCd, CeCd, PrCd (Iandelli & Botti, 1937); LaHg, CeHg, PrHg and NdHg (Iandelli & Ferro, 1951).

References

- IANDELLI, A. (1949). *R. C. Semin. Fac. Sci. Univ. Cagliari*, **19**, 1.
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Acta Cryst. (1954). **7**, 781

Crystallographic data on some diester phosphate compounds.* By J. SCANLON and R. L. COLLIN, *Cancer Research Institute, New England Deaconess Hospital, Boston 15, Massachusetts, U.S.A.*

(Received 16 July 1954)

In the course of a structural investigation into simple compounds related to the nucleic acids we have obtained preliminary crystallographic data on several diester phosphates.

Dibenzyl phosphates

Crystals of silver dibenzyl phosphate were supplied by Dr E. G. Heineman of Harvard University. The silver salt was converted to the free acid by acidification with dilute sulfuric acid and then extracted with chloroform. The chloroform solution was evaporated slowly to give crystals of dibenzyl phosphoric acid.

* This work was aided by U.S. Atomic Energy Contract AT(30-1)-901 with the New England Deaconess Hospital, Boston 15, Massachusetts, U.S.A.

Diethyl phosphate salts

Excess silver oxide was added to a solution of diethyl chlorophosphate (kindly supplied by Victor Chemical Works) and allowed to stand for about four hours at 60° C. with occasional stirring. The precipitate of silver chloride and the excess silver oxide were filtered off and the solution of silver diethyl phosphate was then titrated with a dilute solution of the appropriate chloride (e.g. cupric chloride) until no more silver chloride precipitated. This was filtered and the solution of the salt (e.g. cupric diethyl phosphate) was concentrated by vacuum distillation and then dried by evaporation at room temperature.

Further crystallizations were carried out to obtain good crystals for X-ray work. Cupric diethyl phosphate was crystallized from chloroform and magnesium diethyl phosphate from a mixture of ethyl alcohol and ethyl

Table 1. *Crystallographic data*

Compound	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	α	β	γ	Space group	Density (g.cm. ⁻³)		<i>n</i>
								obs.	calc.	
Silver dibenzyl phosphate	14.5	5.77	9.03	—	112° 50'	—	<i>P</i> ₂ ₁ or <i>P</i> ₂ ₁ / <i>m</i>	> 1.595	1.83	2
Dibenzyl phosphoric acid	12.7	5.72	28.6	—	136° 35'	—	<i>P</i> ₂ ₁ / <i>c</i>	1.30	1.30	4
Cupric diethyl phosphate	5.02	14.9	14.2	129° 12'	92° 24'	91° 42'	<i>P</i> ₁ or <i>P</i> ₁ $\bar{1}$	1.51	1.45	2
Silver diethyl phosphate	20.3	14.4	5.88	—	—	—	<i>P</i> <i>ccn</i>	> 1.495	2.01	8
Zinc diethyl phosphate	22.1	8.07	9.15	—	96° 45'	—	<i>Cc</i> or <i>C</i> ₂ / <i>c</i>	1.54	1.50	4
Magnesium diethyl phosphate	22.3	8.02	9.33	—	97° 10'	—	<i>Cc</i> or <i>C</i> ₂ / <i>c</i>	1.35	1.35	4

acetate with a small amount of water. Zinc and silver diethyl phosphate were crystallized from water. All crystallizations were carried out by slow evaporation at room temperature. The possibility that these crystals contain solvent of crystallization has not been excluded.

Mo *K* α and Cu *K* α precession photographs, both zero- and upper-level, were used to obtain the crystallographic

data in Table 1. Densities were determined by the sink-or-float method with appropriate liquid mixtures.

The magnesium and zinc salts appear isomorphous and the investigation of their crystal structure is proceeding. Neither compound gives a piezoelectric test and thus the space group is probably *C*₂/*c*.

Acta Cryst. (1954). **7**, 782

Simplified formula for calculating interplanar spacings in the rhombohedral system. By

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(Received 12 July 1954)

It is apparently not common knowledge that the formula (*International Tables*, 1935) for calculating interplanar spacings in the rhombohedral system:

$$\frac{a^2}{d^2} = \frac{\cos^2 \alpha/2}{\sin \alpha/2 \cdot \sin 3\alpha/2} \times [(h^2 + k^2 + l^2) - (1 - \tan^2 \alpha/2)(hk + kl + lh)]$$

can be simplified by the use of half-angle formulas. When this is done, the coefficient of the bracket becomes

$$\frac{1 + \cos \alpha}{1 + \cos \alpha - 2 \cos^2 \alpha}$$

This is an advantage because one has to look up only one trigonometric function instead of three.

One can make a similar but trivial simplification of the tangent term.

Reference

International Tables for the Determination of Crystal Structures (1935). Berlin: Borntraeger.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the British Co-editor (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).

Dictionary of Values of Molecular Constants

The editors have received a copy of Volume I of the above publication. This work is to contain the numerical values of quantities such as the energies, coefficients and charges of the electron levels in a large number of molecules of interest to chemists. The values have been gathered together by Dr Daudel in Paris and Prof. Coulson in Oxford. Both the valence-bond approximation of Pauling and the molecular-orbital approximation of Hund, Mulliken and Lennard-Jones have been used, so that comparisons are possible. When complete the dictionary will consist of approximately four volumes, each containing some 50–100 pages. A limited number of copies are available. Enquiries should be addressed to Dr R. Daudel,

Centre de Chimie Théorique de France, 5 avenue de l'Observatoire, Paris VI, France.

Publicaciones del Departamento de Cristalografía y Mineralogía

The editors have received Parts 1 and 2 (October 1953 and May 1954) of Volume 1 of the above new publication. Each part contains about 55 small pages and carries some six articles in the fields of morphology, crystal chemistry, structure analysis and instrumentation. Abstracts are in English and the articles in Spanish. All enquiries should be addressed to the Department of Crystallography and Mineralogy, University of Barcelona, Spain.