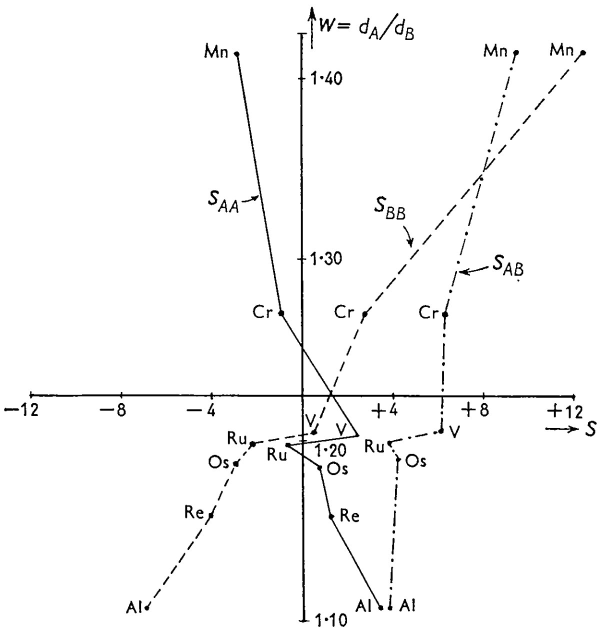

Fig. 1. Plot of S_{AA}, S_{BB} and S_{AB} against $W = d_A/d_B$ for Laves phases of the C_{14} type with zirconium as the 'A' component.

——— S_{AA}; - - - - S_{BB}; —·—·— S_{AB}.

Raynor. Aluminium appears to fit very well into this scheme and since chemically aluminium differs considerably from all other metals in this set, the importance of geometrical factors in the formation of the C_{14} phase seem to be over-riding.

The author would like to thank Mr F. J. Spooner and Mr D. K. Thomas of the Physics Branch, R.M.C.S., for their assistance in computation and film measurement and also Mr H. D. Mallon of the Metallurgy Branch, R.M.C.S., for the preparation and examination of micrographs of $ZrAl_2$. The friendly advice and guidance of Dr J. Adam, A.E.R.E., Harwell is gratefully acknowledged. This paper is published by permission of the Dean of the Royal Military College of Science.

References

Adam, J. (1954). *J. Sci. Instrum.* **31**, 131.

Berry, R. L. & Raynor, G. V. (1953). *Acta Cryst.* **6**, 178.

Klug, H. P. & Alexander, L. E. (1954). *X-ray Diffraction Procedures*, p. 155. New York: Wiley.

Lees, C. S. (1955). *J. Sci. Instrum.* **32**, 17.

McPherson, D. J. & Hanson, M. (1954). *Trans. Amer. Soc. Metals*, **46**, 354.

Acta Cryst. (1959). **12**, 662

Transition Element—Rare Earth Compounds with the Cu_5Ca Structure

By J. H. Wernick and S. Geller

Bell Telephone Laboratories, Inc., Murray Hill, New Jersey, U.S.A.

(*Received* 26 *January* 1959 *and in revised form* 11 *March* 1959)

A number of new B_5A compounds, with A a rare earth or yttrium and B a transition element, Co, Ni, or Cu, having the Cu_5Ca structure, have been prepared. In most of the compounds, the interatomic distances are normal. However, Ce appears to have a valence substantially greater than three. Also, in Co_5Pr, Pr appears to have a valence slightly greater than three.

Introduction

In the course of a continuing study of the magnetic and structural properties of intermetallic compounds between rare earth and transition metals, a number of new compounds with the Cu_5Ca structure have been made. Some of the results of magnetic measurements have already been reported by Nesbitt *et al.* (1959). It is the purpose of this paper to report on the crystallographic investigations of these new compounds.

Experimental

Stoichiometric amounts of the constituents were melted by induction heating in fused Al_2O_3 or quartz crucibles in an argon atmosphere.* The compounds appear to melt congruently as they form readily from the melt.

X-ray powder photographs were taken with Cr $K\alpha$ radiation and a Straumanis type Norelco camera (114·6 mm. diameter). Observed and calculated interplanar spacings are shown in Table 1.

These compounds, B_5A, belong to space group $P6/mmm(D_{6h}^1)$ with A in (a): 0, 0, 0, $2B_{\text{I}}$ in (c): $\pm(\frac{1}{3}, \frac{2}{3}, 0)$, and $3B_{\text{II}}$ in (g): $\frac{1}{2}, 0, \frac{1}{2}$, $0, \frac{1}{2}, \frac{1}{2}$, $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$.

---

* All of the rare earth elements, except Pr (99·9+%), and Y were of 99+% purity. Co and Ni 99·9+%; Cu 99·999%. The Nd was kindly supplied to us by Dr F. H. Spedding.

Table 1. *Powder diffraction data for B_5A compounds*

Cr *Kα* radiation

hk·l	Co_5Y d obs	Co_5Y d calc	Co_5Ce d obs	Co_5Ce d calc	Co_5Pr d obs	Co_5Pr d calc	Co_5Nd d obs	Co_5Nd d calc	Co_5Gd d obs	Co_5Gd d calc	Co_5Dy d obs	Co_5Dy d calc	Co_5Er d obs	Co_5Er d calc
10·0	4.229	4.268	N.O.	4.263	N.O.	4.34	N.O.	4.353	N.O.	4.308	4.212	4.266	4.172	4.231
00·1	N.O.*	3.992	3.997	4.026	3.95	3.99	N.O.	3.975	N.O.	3.973	3.979	3.989	3.967	4.002
10·1	2.902	2.915	2.918	2.926	2.92	2.94	2.926	2.935	2.901	2.920	2.899	2.914	2.891	2.907
11·0	2.450	2.464	2.452	2.461	2.49	2.50	2.501	2.513	2.475	2.487	2.454	2.463	2.432	2.443
20·0	2.128	2.134	2.124	2.131	2.17	2.17	2.169	2.176	2.143	2.154	2.127	2.133	2.108	2.115
11·1	2.092	2.097	2.096	2.100	2.11	2.12	2.119	2.124	2.099	2.108	2.088	2.096	2.077	2.085
00·2	1.992	1.996	2.012	2.013	1.99	2.00	1.985	1.988	1.980	1.986	1.994	1.994	1.996	2.001
20·1	1.877	1.882	1.880	1.884	1.90	1.91	1.901	1.909	1.887	1.895	1.878	1.881	1.862	1.870
10·2	1.798	1.808	N.O.	1.820	N.O.	1.81	N.O.	1.808	N.O.	1.804	N.O.	1.807	N.O.	1.809
21·0	1.598	1.613	1.607	1.611	N.O.	1.64	1.662	1.645	1.600	1.628	1.609	1.612	1.591	1.599
11·2	1.550	1.551	1.557	1.558	1.56	1.56	1.558	1.559	1.549	1.552	1.549	1.550	1.546	1.548
21·1	1.495	1.496	1.495	1.496	1.52	1.52	1.518	1.520	1.505	1.507	1.494	1.495	1.482	1.485
20·2	1.457	1.458	1.463	1.463	1.47	1.47	1.467	1.468	1.459	1.460	1.456	1.457	1.452	1.454
30·0	1.421	1.423	1.420	1.421	1.45	1.45	N.O.	1.451	1.433	1.436	1.420	1.422	1.408	1.410
30·1	1.338	1.340	1.339	1.340	1.36	1.36	1.362	1.363	1.349	1.350	1.338	1.339	1.329	1.330
00·3	N.O.	1.331		1.342	1.33	1.33	N.O.	1.325	N.O.	1.324	N.O.	1.330	N.O.	1.334
10·3	1.270	1.270	1.279	1.280	1.27	1.27	1.267	1.268	1.265	1.266	1.270	1.269	1.272	1.272
21·2	1.254	1.255	N.O.	1.258		1.27		1.267	1.257	1.259	1.253	1.254	N.O.	1.249
22·0	1.252	1.252	1.231	1.231	1.25	1.25	1.257	1.257	1.243	1.244	1.232	1.232	1.221	1.221
31·0	N.O.	1.184	N.O.	1.182	N.O.	1.20	N.O.	1.207	N.O.	1.195	N.O.	1.183	1.171	1.173
22·1	N.O.	1.177	1.178	1.177	1.19	1.19	N.O.	1.198	1.185	1.187	N.O.	1.177	N.O.	1.168
11·3	1.171	1.171		1.178	1.17	1.17	1.172	1.172	1.169	1.169	1.170	1.170	1.171	1.171
30·2	1.158	1.158	1.160	1.161				1.172	1.164	1.164	1.158	1.158	1.153	1.153
31·1					1.15	1.15	1.155	1.155						
20·3														

hk·l	Cu_5Y d obs	Cu_5Y d calc	Cu_5Nd d obs	Cu_5Nd d calc	Cu_5Gd d obs	Cu_5Gd d calc	Ni_5Y d obs	Ni_5Y d calc	Ni_5La d obs	Ni_5La d calc
10·0	4.270	4.316	N.O.	4.420	N.O.	4.346	4.16	4.22	4.311	4.341
00·1	N.O.	4.117	N.O.	4.107	N.O.	4.117	N.O.	3.97	N.O.	3.984
10·1	2.961	2.979	2.995	3.009	2.977	2.989	2.88	2.89	2.926	2.935
11·0	2.479	2.492	2.544	2.552	2.500	2.509	2.43	2.44	2.497	2.506
20·0	2.148	2.158	2.203	2.210	2.175	2.173	2.11	2.11	2.167	2.171
11·1	2.124	2.132	2.163	2.168	2.141	2.143	2.07	2.08	2.117	2.122
00·2	2.052	2.059	2.048	2.054	2.055	2.059	1.98	1.98	1.990	1.992
20·1	1.903	1.912	1.940	1.946	1.917	1.922	1.86	1.86	1.902	1.906
10·2	1.854	1.858	N.O.	1.862	N.O.	1.860	N.O.	1.80	1.809	1.811
21·0	1.634	1.631	N.O.	1.671	N.O.	1.643	1.59	1.60	N.O.	1.641
11·2	1.584	1.587	1.598	1.600	1.590	1.592	1.54	1.54	1.560	1.560
21·1	1.512	1.517	1.545	1.548	1.525	1.526	1.48	1.48	1.515	1.517
20·2	1.487	1.490	1.503	1.504	1.494	1.494	1.45	1.45	1.467	1.468
30·0	1.434	1.440	N.O.	1.473	N.O.	1.449	1.41	1.41	1.446	1.447
30·1	1.356	1.358	1.385	1.387	1.367	1.367	1.33	1.33	N.O.	1.360
00·3	N.O.	1.372	N.O.	1.369	N.O.	1.372		1.32	N.O.	1.328
10·3	1.307	1.308	N.O.	1.308	1.309	1.309	1.26	1.26	1.271	1.270
21·2	1.277	1.279	N.O.	1.296	N.O.	1.284	1.24	1.24	N.O.	1.267
22·0	1.246	1.246	1.276	1.276	1.255	1.255	1.22	1.22	1.253	1.253
31·0	N.O.	1.197	N.O.	1.226	1.204	1.205	N.O.	1.17	N.O.	1.204
22·1	N.O.	1.193	N.O.	1.219	N.O.	1.200	N.O.	1.17	N.O.	1.195
11·3	1.202	1.202	1.206	1.207	1.204	1.204	1.16	1.16	1.174	1.174
30·2	1.179	1.179	1.198	1.197	1.185	1.185	1.15	1.15		1.171
31·1	N.O.	1.150	1.174	1.175	1.158	1.157			1.153	1.153
20·3	1.159	1.158	1.164	1.164		1.160				

hk·l	Ni_5Ce d obs	Ni_5Ce d calc	Ni_5Pr d obs	Ni_5Pr d calc	Ni_5Nd d obs	Ni_5Nd d calc	Ni_5Gd d obs	Ni_5Gd d calc	Ni_5Dy d obs	Ni_5Dy d calc	Ni_5Er d obs	Ni_5Er d calc	Ni_5Er I calc
10·0	N.O.	4.222	4.264	4.293	N.O.	4.285	N.O.	4.243	N.O.	4.217	N.O.	4.205	0.15
00·1	N.O.	4.010	3.954	3.980	N.O.	3.977	3.953	3.973	3.943	3.969	3.944	3.966	0.48
10·1	2.889	2.907	2.910	2.919	2.908	2.915	2.884	2.900	2.874	2.890	2.874	2.885	3.44
11·0	2.426	2.437	2.473	2.479	2.466	2.474	2.439	2.450	2.424	2.435	2.422	2.428	1.99
20·0	2.103	2.111	2.142	2.147	2.138	2.143	2.116	2.121	2.100	2.108	2.097	2.103	2.07
11·1	2.077	2.083	2.099	2.104	2.098	2.101	2.080	2.085	2.066	2.075	2.066	2.071	5.87
00·2	1.998	2.005	1.987	1.990	1.987	1.988	1.982	1.987	1.977	1.985	1.979	1.983	1.57
20·1	1.863	1.868	1.887	1.889	1.886	1.886	1.868	1.871	1.854	1.862	1.855	1.858	0.27
10·2	N.O.	1.811	1.802	1.806	N.O.	1.804	N.O.	1.799	N.O.	1.796	N.O.	1.794	0.04
21·0	1.594	1.596	N.O.	1.623	1.601	1.620	1.592	1.604	1.583	1.594	1.583	1.590	0.04
11·2	1.548	1.548	1.550	1.552	1.550	1.550	1.542	1.543	1.535	1.538	1.535	1.536	1.12
21·1	1.481	1.483	1.500	1.503	1.500	1.500	1.486	1.487	1.475	1.479	1.474	1.475	1.15
20·2	1.453	1.454	1.459	1.459	1.457	1.457	1.449	1.450	1.443	1.445	1.441	1.443	1.74
30·0	1.406	1.407	1.430	1.431	1.427	1.428	1.413	1.414	1.402	1.406	1.401	1.402	0.54
30·1	1.327	1.328	1.346	1.347	1.344	1.344	1.331	1.332	1.323	1.325	1.322	1.322	2.78
00·3	N.O.	1.337	N.O.	1.327	N.O.	1.326	N.O.	1.324		1.323		1.322	0.04
10·3	1.274	1.274	1.268	1.268	1.266	1.266	1.265	1.264	1.262	1.262	1.262	1.261	0.73
21·2	N.O.	1.248	N.O.	1.258	N.O.	1.256	N.O.	1.248	N.O.	1.243	1.240	1.240	0.11
22·0	1.219	1.219	1.239	1.239	1.237	1.237	1.225	1.225	1.217	1.217	1.214	1.214	3.97
31·0	1.172	1.171	N.O.	1.191	N.O.	1.188	N.O.	1.177	1.169	1.170	N.O.	1.166	0.13
22·1	N.O.	1.166	N.O.	1.183	N.O.	1.181	N.O.	1.170	N.O.	1.164	1.161	1.161	0.87
11·3	1.172	1.172	1.170	1.170	1.168	1.168	1.165	1.165	1.163	1.163		1.161	9.44
30·2	1.152	1.152	1.162	1.162	1.160	1.160	1.152	1.152	1.148	1.147			
31·1													
20·3													

*N.O. = Not Observed

Because the intensities of the reflections on the powder photographs of the different compounds are similar*, relative intensities were computed only for Ni_5Er (Table 1) for Cr *Kα* radiation. Also, powder intensities of Ni_5Er were measured with a Norelco diffractometer using Cu *Kα* radiation. In the calculation of intensities, the atomic scattering factors of Thomas & Umeda (1957) were used. These were corrected for dispersion using the values given by Templeton & Dauben (1950).

Although there are some discrepancies between the calculated and observed intensities (Table 2) for Ni_5Er, there is little doubt that the most probable structure is that given; the discrepancies may be caused, to a large extent, by preferred orientation. Further corro-

Table 2. *Calculated and observed intensities for* Ni_5Er

Cu *Kα* radiation

hk·l	I_o	I_c	*hk·l*	I_o	I_c
10·0	0·26	0·35	10·3	0·62	0·51
00·1	0·85	0·99	21·2	N.O.	0·08
10·1	5·80	7·31	22·0	1·68	1·74
11·0	3·34	4·29	31·0	N.O.	0·03
20·0	4·09	4·48	22·1	1·89	1·72
11·1	10·00	12·65	11·3		
00·2	3·44	3·36	30·2	0·70	0·69
20·1	0·70	0·50	31·1	0·73	0·76
10·2	N.O.*	0·11	20·3		
21·0	N.O.	0·08	40·0	0·49	0·44
11·2	1·99	1·90	22·2	2·20	2·22
21·1	1·74	1·77	40·1	0·78	0·62
20·2	2·64	2·43	21·3		
30·0	0·65	0·68	30·3	1·17	1·15
30·1	2·66	2·63	10·4		
00·3					

* N.O. = Not observed.

Table 3. *Crystallographic data for the B_5A compounds**

	a_0 (Å)	c_0 (Å)	c_0/a_0	Volume (Å)^3	Calculated density g.cm.$^{-3}$
Co_5Y	4·928	3·992	0·810	83·96	7·58
Co_5Ce	4·922	4·026	0·818	84·46	8·54
Co_5Pr	5·01	3·99	0·796	86·73	8·34
Co_5Nd	5·026	3·975	0·791	86·96	8·38
Co_5Gd	4·974	3·973	0·799	85·12	8·80
Co_5Dy	4·926	3·988	0·810	83·80	9·05
Co_5Er	4·885	4·002	0·819	82·70	9·27
Ni_5Y	4·88	3·97	0·814	81·87	7·75
Ni_5La	5·013	3·984	0·795	86·70	8·28
Ni_5Ce	4·875	4·010	0·823	82·53	8·72
Ni_5Pr	4·958	3·980	0·803	84·73	8·51
Ni_5Nd	4·948	3·977	0·804	84·32	8·61
Ni_5Gd	4·899	3·973	0·811	82·58	9·05
Ni_5Dy	4·869	3·969	0·815	81·49	9·29
Ni_5Er	4·856	3·966	0·817	80·99	9·44
Cu_5Y	4·984	4·117	0·826	88·56	7·62
Cu_5Nd	5·104	4·107	0·805	92·65	8·27
Cu_5Gd	5·018	4·117	0·820	89·78	8·77

* All lattice constants are within ±0·005 Å except for Co_5Pr and Ni_5Y (±0·01 Å).

---

* The effects of dispersion are, however, observable.

Table 4. *Interatomic distances in the B_5A compounds*

B	A	B_{II}–B_{II} (Å)	B_{II}–B_I (Å)	B_I–A B_I–B_I (Å)	B_{II}–A (Å)	Average B_{II}–B (Å)	$CN(12)$ distances from B elements (Å)
Co	Y	2·46	2·45	2·85	3·17	2·46 $\left\{\begin{array}{l}+0{\cdot}05\\-0{\cdot}02\end{array}\right.$	2·51
	Ce	2·46	2·46	2·84	3·18		
	Pr	2·51	2·46	2·89	3·20		
	Nd	2·51	2·46	2·90	3·20		
	Gd	2·49	2·45	2·87	3·18		
	Dy	2·46	2·45	2·84	3·17		
	Er	2·44	2·45	2·82	3·11		
Ni	Y	2·44	2·43	2·82	3·15	2·45 $\left\{\begin{array}{l}+0{\cdot}06\\-0{\cdot}02\end{array}\right.$	2·49
	La	2·51	2·46	2·89	3·20		
	Ce	2·44	2·45	2·81	3·11		
	Pr	2·48	2·45	2·86	3·18		
	Nd	2·47	2·45	2·86	3·17		
	Gd	2·45	2·44	2·83	3·15		
	Dy	2·43	2·43	2·81	3·14		
	Er	2·43	2·43	2·80	3·13		
Cu	Y	2·49	2·51	2·88	3·23	2·52 ±0·03	2·56
	Nd	2·55	2·53	2·95	3·28		
	Gd	2·51	2·52	2·90	3·25		

boration was obtained from oscillation and precession photography of a single crystal chip of Ni_5Er.

Crystallographic data for the B_5A compounds are listed in Table 3. Five of these compounds have been reported by other authors. The lattice constants (Table 3) of Ni_5Gd, Ni_5Ce, and Ni_5Pr are in reasonably good agreement with those reported by Endtner & Klemm (1943), Nowotny (1942), and Vogel & Fülling (1947) respectively. Those of Ni_5La differ significantly from the values, $a = 4{\cdot}962$, $c = 4{\cdot}008$ Å, obtained by Nowotny (1942); those of Co_5Ce differ significantly from the values, $a = 4{\cdot}955$, $c = 4{\cdot}055$ Å, reported by Heumann (1948).

Discussion

The interatomic distances in the Cu_5Ca-type compounds are given in Table 4. The average nearest neighbor, B_{II}–B_I, distances, approximately $CN(10)$, compare favorably with $CN(12)$ distances (Table 4) obtained from elemental Co, Ni, and Cu. The A–B distances are also indicative of metallic-type bonding.

For compounds having the same B atom, the variation in c_0 is very small; i.e., the change in A atom (Ce excluded*) causes a significant change only in the size of the a-axis (Table 3). Examination of the structure leads to the conclusion that the A atoms do not interact at all in the c_0 axis direction; the arrangement of B atoms need only be modified in the basal planes to accommodate atoms A of different size.

The variations of the volume of the unit cells with atomic number of the rare earth atom are shown in Fig. 1. It is seen from this plot (see also Table 3) that the Ce atom in these compounds has a smaller size than would be expected if it were acting trivalently. A somewhat similar situation has been observed in Ce–Th alloys by Weiner, Freeth & Raynor (1957) who suggested that Ce^{4+} ions are created on adding Ce to Th by loss of the $4f$ electron to the conduction band. Support for these conclusions were obtained by Bates & Newmann (1958) who proposed that the Ce ions are resonating between Ce^{3+} and Ce^{4+} states, and that on the average a proportion of the Ce atoms may be considered to have no $4f$ electrons.

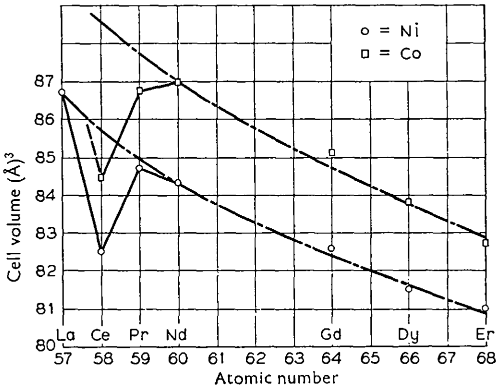

Fig. 1. The variation of cell volume with atomic number of the rare earth element.

It is known that Pr forms a number of complex oxides indicating that Pr also has more than one stable valence state. It appears that at least in Co_5Pr (Fig. 1), the $4f$ electrons in Pr may spend part of their time in orbitals outside the $4f$ shell, and that on the average, the Pr ion in this compound has less than two $4f$ electrons.

Further investigations of the magnetic properties of these compounds will be described later. It is hoped also to obtain some single crystals of some of these suitable for neutron diffraction studies.

---

* As shown later in this series of compounds, Ce behaves differently from the other rare earths.

We wish to thank R. G. Treuting for the use of his IBM 704 programs for calculation of spacings and intensities; W. J. Romanow for his aid with the calculations; D. Dorsi for making the compounds; C. E. Miller for taking the photographs; and L. C. Lovell for measuring some of the films.

References

Bates, L. F. & Newmann, M. M. (1958). *Proc. Phys. Soc.* **72**, 465, 345.

Endtner, F. & Klemm, W. (1943). *Z. anorg. Chem.* **252**, 64.

Heumann, T. (1948). *Nachr. Wiss. Göttingen*, **1**, 21.

Nesbitt, E. A., Wernick, J. H. & Corenzwit, E. (1959). *J. Appl. Phys.* **30**, 365.

Nowotny, H. (1942). *Z. Metallk.* **34**, 247.

Templeton, D. H. & Dauben, C. H. (1950). *Acta Cryst.* **3**, 261.

Thomas, L. H. & Umeda, K. (1957). *J. Chem. Phys.* **26**, 293.

Vogel, R. from investigations of Fülling, W. (1947). *Metallforschung*, **2**, 97.

Weiner, R. T., Freeth, W. E. & Raynor, G. V. (1957). *J. Inst. Met.* **86**, 185.

Acta Cryst. (1959). **12**, 665

Die Bestimmung genauer Schweratomparameter in isomorphen azentrischen Kristallen

Von W. Hoppe*

MRC-Unit for Molecular Biology, Cavendish Laboratory, University Cambridge, Cambridge, England

Eingegangen am 11. *November* 1958, *revidiert* 24. *Februar* 1959

The determination of accurate heavy atom parameters in acentric crystals is discussed in this paper.

(A) There are two possibilities for the determination of coordinates using all measured intensities:

(1) Correlation functions. The correlation functions are modulated by the structure of the crystal, thus disturbing the determination of the heavy atom coordinates. The influence of the crystal structure is discussed using convolution principles for the following correlation functions constructed with the observed structure factors F of the protein, F_1 of its heavy atom derivative, and f_1 of the heavy atoms only:

$$\begin{aligned}&C\text{-function (coefficients } \varDelta_1\varDelta_2;\ \varDelta_1 = \{|F_1|^2-|F|^2\})\,,\\ &C'\text{-function (coefficients } A_1A_2;\ A_1 = \{|F_1|^2-|F|^2-f_1^2\}/2f_1)\,,\\ &C''\text{-function (coefficients } \varphi_1\varphi_2;\ \varphi_1 = A_1/|F|)\,,\\ &C'''\text{-function (coefficients } W_1W_2;\ W_1 = \{|F_1|^2-|F|^2-f_1^2\}\,.\end{aligned}$$

It is shown that pseudocentres of symmetry particulary disturb the determination. The calculation of the composing convolution structures in a special case (myoglobin) suggests that the structure of protein crystals is quite suitable for the use of correlation functions. An error theory, based on the Gaussian error distribution law, is given. Examples of the correlation functions (in the case of myoglobin) have been calculated.

(2) In the special case of one heavy atom in the asymmetric unit a determination of the heavy atom parameters with a simultaneous elimination of the influence of the crystal structure is in principle possible.

(B) In case preliminary coordinates of the heavy atom parameters and of the phases of the acentric crystal have been determined, modified refinement methods are possible (namely difference Fourier synthesis and least-squares refinement of the heavy atom parameters).

Die erste, nach der Methode des multiplen isomorphen Ersatzes berechnete azentrische Projektion eines azentrischen Kristalles (Hämoglobin) wurde von Blow (1957) bestimmt; vor kurzem gelang es Kendrew (1958) eine dreidimensionale Fouriersynthese eines Eiweisskristalles (Myoglobin) mit einer Auflösung von 6 Å zu rechnen, welche die Anordnung der Peptidketten und den Ort der Hämingruppe zeigte.

Nach der Theorie des multiplen isomorphen Ersatzes müssen zunächst die Schweratomparameter bestimmt werden, wobei es nötig ist, diese Parameter auf irgend einen Punkt im nicht zentrosymmetrischen Proteingitter zu beziehen. Im Falle der erwähnten Myoglobinstruktur (Raumgruppe $P2_1$) ist eine Schraubenachse entlang b ausgebildet, in welche man aus

---

* Gast aus dem Physikal. chem. Institut der T. H. München, München, Deutschland.