

beim Durchgang durch das Anthrazen-Kristall verlieren und die die diffusen Flecken bilden, von einer Grössenordnung von weniger als e.V.-Dezimalen ist. Darum kann unser Filter bei Anwendung auf das Elektronenbeugungsdiagramm diese diffusen Flecken nicht zum Verschwinden bringen, denn seine Auflösung übersteigt nicht 3 e.V.

Wir haben mit dem Filter die drei auf einer Platte aufgenommenen Photographien erhalten (Fig. 3).

Wir sehen, dass die durch gestreute und inkohärente Elektronen verursachten diffusen Flecken aus dem Beugungsdiagramm des Anthrazen verschwunden und nur die v. Laue'schen Flecken geblieben sind.

Hiermit wollen wir beweisen, dass die diffusen Flecken nicht von Elektronen, die Energie an thermische Schwingungen verlieren, hervorgerufen werden.

Die Photographien sind auf ein und derselben Platten und mit Diagrammen durch dasselbe Einkristall gemacht worden. Die Schwierigkeiten, diese Photographien zu erhalten, waren sehr gross, was auf die Unstabilität der Anthrazeneinkristalle zurückzuführen ist, denn es sublimiert sich im Vakuum spontan und noch schneller, wenn es mit Elektronen beschossen wird. Darum mussten die Belichtungszeiten kürzer

sein, sodass in der Photographie Fig. 3(c) die Aufnahme schwächer ist.

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Short Communications

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The structures of ZrGe₂, HfSi₂ and HfGe₂* By J. F. SMITH and D. M. BAILEY, *Institute for Atomic Research and Department of Chemistry, Iowa State College, Ames, Iowa, U.S.A.*

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The structure parameters for ZrGe₂, HfSi₂ and HfGe₂ have been determined from X-ray diffraction patterns taken from single crystals. The crystal class and lattice parameters have been reported for ZrGe₂ by Wallbaum (1944) and for HfSi₂ by Post, Glaser & Moskowitz (1954) on the basis of powder diffraction patterns. The present work with single crystals confirms these results. In addition, layer-line symmetry and characteristic extinctions indicate that all three of the compounds belong in the space group $D_{2h}^{17}-Cmcm$. Comparison of observed and calculated intensities indicates that the compounds are isostructural. Three sets of fourfold positions are occupied. All three sets are of the type: $\pm(0, y, \frac{1}{4})$, $(\frac{1}{2}, \frac{1}{2} + y, \frac{1}{4})$. The values for the structure parameters are given in Table 1 together with values obtained by Schachner, Nowotny & Kudielka (1954) for ZrSi₂. Calculated and observed structure factors are shown in Table 2. The reliability factor, $R = \frac{|F_o| - |F_c|}{|F_o|}$, was

Table 1. Structure parameters for some isostructural AB₂ compounds

	These data (ZrGe ₂ , HfSi ₂ , HfGe ₂)	Schachner <i>et al.</i> (ZrSi ₂)
<i>y</i> (Zr or Hf)	0.106	0.108
<i>y</i> _I (Si or Ge)	0.750	0.750
<i>y</i> _{II} (Si or Ge)	0.441	0.439

found to be 0.12 for ZrGe₂, 0.11 for HfSi₂, and 0.08 for HfGe₂. The intensity measurements were taken with Cu K α radiation while using a Weissenberg unit and a Geiger-Müller tube detector.

Precision lattice parameters were also determined for each of the three compounds. Data for the ZrGe₂ and HfGe₂ parameters were obtained through use of a self-focusing back-reflection powder camera and were refined by Cohen's (1935, 1936) method. Because of a limited amount of sample, the precision lattice constants of HfSi₂ were obtained through use of a back-reflection Weissenberg camera and an extrapolation method. The lattice parameters are shown in Table 3. The precision

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Table 2. *Calculated and observed structure factors*

ZrGe ₂			HfGe ₂			HfSi ₂		
<i>hkl</i>	<i>F_o</i>	<i>F_c</i>	<i>OkL</i>	<i>F_o</i>	<i>F_c</i>	<i>OkL</i>	<i>F_o</i>	<i>F_c</i>
060	178	-236	040	116	-110	020	55	80
080	71	65	060	299	-310	040	137	-182
0,10,0	56	-48	080	134	125	060	180	-214
0,12,0	57	38	0,10,0	< 45	-29	080	126	123
0,14,0	133	-116	0,12,0	< 45	44	0,10,0	123	122
0,16,0	84	87	0,14,0	192	-196	0,12,0	—	-3
0,18,0	62	63	0,16,0	110	61	0,14,0	202	-174
110	17	6	0,18,0	72	115	0,16,0	—	-3
130	111	-100	021	171	-173	0,18,0	106	116
150	98	-92	041	< 45	11	021	215	-217
170	67	65	061	239	239	041	81	-72
190	163	170	081	195	182	061	193	194
1,11,0	104	96	0,10,1	118	-108	081	179	172
1,13,0	76	-67	0,12,1	246	-235	0,10,1	78	-85
1,15,0	123	-109	0,14,1	80	-70	0,12,1	196	-195
1,17,0	39	-31	002	333	-386	0,14,1	66	-38
200	239	233	022	< 45	-19	0,16,1	123	131
260	185	-187	062	265	252	002	299	-280
280	35	54	082	108	-107	022	94	-41
2,10,0	39	-43	0,10,2	< 45	39	042	160	145
2,14,0	119	-106	0,12,2	< 45	-46	062	187	177
330	78	-67	0,14,2	170	181	082	110	-105
350	81	-66	023	128	126	0,10,2	108	-101
370	50	50	043	< 45	-19	0,12,2	—	3
390	126	135	063	185	-178	023	165	150
3,11,0	84	72	083	145	-142	043	62	52
3,13,0	65	-57	0,10,3	93	88	063	148	-145
400	175	192	0,12,3	176	199	083	144	-133
460	127	-135	0,14,3	47	60	0,10,3	61	-68
480	40	42	004	266	268	0,12,3	158	164
4,10,0	17	-31	024	< 45	7	004	182	198
			044	< 45	-17	024	—	30
			064	184	-185	044	96	-107
						064	121	-128
						084	70	81

Table 3. *Precision lattice parameters*

Compound	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)
ZrGe ₂	3.7893	14.975	3.7606
HfSi ₂	3.677	14.550	3.649
HfGe ₂	3.8154	15.004	3.7798

Table 4. *Interatomic distances in AB₂ compounds*

Atom*	Neigh- bor	No. of Neigh- bors	Distance	Distance	Distance
			in ZrGe ₂	in HfGe ₂	in HfSi ₂
A	B _{II}	4	2.76 Å	2.77 Å	2.68 Å
	B _I	2	2.86	2.87	2.78
	B _I	2	2.87	2.88	2.79
	B ₂	2	3.10	3.13	3.02
	A	2	3.69	3.70	3.58
B _I	B _I	4	2.67	2.69	2.59
	A	2	2.86	2.87	2.78
	A	2	2.87	2.88	2.79
	B _{II}	2	3.42	3.43	3.32
	B _{II}	2	3.43	3.44	3.33
B _{II}	A	4	2.76	2.78	2.68
	B _{II}	2	2.58	2.59	2.51
	B _I	2	3.42	3.43	3.32
	B _I	2	3.43	3.44	3.33
	A	2	3.10	3.13	3.02

* A: Zr or Hf; B_I: Ge or Si; B_{II}: Ge or Si.

lattice parameters and the structure parameters were used to compute the interatomic spacings shown in Table 4.

An estimate of the heats of formation of these three compounds as -40 to -45 kcal./mol. was made on the basis of the volume contraction occurring during compound formation from the pure elements. The method of approximation is described by Kubaschewski & Evans (1951). The measured lattice parameters of the compound and of the pure elements were used to calculate the volume contraction. These estimates are probably reliable to within 20% since a similar estimate for ZrSi₂ gives ΔHf = -43 kcal./mol. while Robins & Jenkins (1955) measured -36 kcal./mol.

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