

and calculated σ_c (Table 1) suggest that some bound-levels contribute considerably to the thermal cross sections. A quantitative estimate of the bound-level parameters which are not discussed by previous authors is made here with the following assumptions. Firstly, average level parameters for the isotope or element in the virtual state are used for the bound-level resonances (Egelstaff, 1959). Secondly, only one bound-level is assigned for the even-even nuclei, since their level spacing near the binding energy is expected to be roughly 20 to 75 eV from the statistical hypothesis (Bollinger, 1960) and 70 to 110 eV from the virtual-level spacings. The bound-levels for ^{174}Hf , ^{176}Hf , ^{178}Hf and ^{180}Hf are then computed to meet the observed σ_c , as, $-E_0 = 2.335$, 13.21, 34.05 and 10.17 eV, respectively. Here, the reduced neutron width for ^{176}Hf is taken as 10.7 mV, an average of those for ^{174}Hf , ^{178}Hf and ^{180}Hf . On the other hand, a number of bound-levels may be expected for ^{177}Hf and ^{179}Hf , because of their mean spacings, 3.58 and 4.17 eV, respectively. In order to estimate a maximum possible value for the b'' term, the major contributing resonance parameters of ^{177}Hf , (L_n and gL_n in mV) at 1.10 and 2.38 eV, are taken as (64, 1.0) and (58, 4.5), respectively. Although these are insignificantly different from Igo & Landon's data (1956), deduction in the resultant σ_c of 364.9 barns may be substantially meaningful. The statistically averaged bound levels in a range 0 to -110 eV are then assigned to $-E_0 = 6.40 + 3.58n$ eV for ^{177}Hf and $1.64 + 4.17n$ eV for ^{179}Hf , where n is a non-negative integer. Correspondingly, the coherent scattering amplitudes were computed including the bound-level effect (Table 1). The reaction nuclear radius to meet the observed amplitude is 0.93×10^{-12} cm. This is close to 0.99×10^{-12} cm of the cloudy crystal-ball model with a diffuse spherical potential but is deviated considerably from 0.78×10^{-12} cm of the one with a deformed potential or the strong interaction model (Chase, Wilets & Edmonds, 1958).

The calculated σ_c of natural hafnium, 63.9 barns at 0.0717 eV, with the bound-level contribution, reduces to a self-consistent value of 11.4 barns for the total scattering cross section at 0.0717 eV. The isotropic disorder-scattering cross section of the element is calculated as

1.04 barns and the multiple scattering cross section of the hafnium sample used in the present work (0.005 mm in average diameter) is estimated as about 1 barn (Atoji, 1961). Hence, the spin incoherent scattering cross section should be less than two barns, a reasonable value for ^{177}Hf and ^{179}Hf . In our discussion, relatively large experimental errors in σ_c and the radiation widths are not rigorously treated and an experimental verification similar to that of Peterson & Smith (1962) is not presented. Nevertheless, it may well be concluded that the imaginary part of the scattering amplitude of natural hafnium can be neglected in diffraction study at sub-cadmium neutron energies.

References

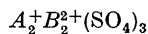
- ATOJI, M. (1961). *J. Chem. Phys.* **35**, 1950.
 BACON, G. E. (1962). *Neutron Diffraction*. 2nd ed. Oxford: Clarendon Press.
 BOLLINGER, L. M. (1960). *Nuclear Spectroscopy*. Part A, p. 424. New York: Academic Press.
 CHASE, D. M., WILETS, L. & EDMONDS, A. R. (1958). *Phys. Rev.* **110**, 1080.
 EGELSTAFF, P. A. (1959). *Phys. Rev.* **115**, 182.
 ESCH, L. J. (1960). Reactor Technology Report No. 15, Physics, Report No. KAPL-2000-12, Knolls Atomic Power Laboratory.
 HANS, H. S. & SEHGAL, M. L. (1958). *Indian J. Phys.* **32**, 276.
 IGO, G. & LANDON, H. H. (1956). *Phys. Rev.* **101**, 726.
 ITKIN, I. (1962). *Analysis of the Neutron Capture Cross Section and Resonance Integral of Hafnium*. Report No. WAPD-TM-324, Bettis Atomic Power Laboratory.
 KRIESSMAN, C. J. & CALLEN, H. B. (1954). *Phys. Rev.* **94**, 837.
 PETERSON, S. W. & SMITH, H. G. (1962). *J. Phys. Soc. Japan*, **17**, Supplement B-II, 335.
 POMERANCE, H. (1952). *Phys. Rev.* **88**, 412.
 RAYNE, J. A. & KEMP, W. R. G. (1956). *Phil. Mag.* **1**, (8) 918.
 SIDHU, S. S., HEATON, L. & ZAUBERIS, D. D. (1956). *Acta Cryst.* **9**, 607.
 WOLCOTT, N. M. (1957). *Phil. Mag.* **2**, (8) 1246.

Acta Cryst. (1964). **17**, 1088

(NH₄)₂Mn₂(SeO₄)₃, Ein Doppelselenat mit Langbeinitstruktur. Von K. KOHLER* und W. FRANKE, Freie Universität Berlin, Mineralogisches Institut, Berlin-Lichterfelde West, Germany

(Eingegangen am 12. Februar 1964)

Aus der Gruppe der isomorphen Doppelsulfate



(A = K, Rb, NH₄, Cs, Tl; B = Mg, Ca, Mn, Fe, Co, Ni, Zn, Cd)

sind durch die Arbeiten von Gattow & Zemmann (1958) bisher 26 Verbindungen bekannt. Die Strukturuntersuchung durch Zemmann & Zemmann (1957) führte zur

Raumgruppe $P2_13$ (T^4) (kubisch). Entsprechende Doppelselenate sind noch nicht beschrieben.

Durch thermischen Abbau von $(\text{NH}_4)_2\text{Mn}(\text{SeO}_4)_2 \cdot 6\text{H}_2\text{O}$ bei 100 °C und 20 Torr-H₂O-Dampfdruck erhielten wir ein äquimolares Gemisch von $(\text{NH}_4)_2\text{Mn}_2(\text{SeO}_4)_3$ mit Ammoniumselenat. Nach Extraktion mit absolutem Alkohol lag das reine Doppelselenat vor. Die kubische Indizierung des Pulverdiagramms ergab eine Gitterkonstante von $a_0 = 10,53_3$ Å. d -Werte und relative Intensitäten der Tabelle 1 wurden einer Zählrohr-Diffraktometer-Aufnahme mit Fe $K\alpha$ -Strahlung entnommen. Ein Vergleich der Intensitätsverhältnisse und der systemati-

* Herr Privatdozent Dr Kurt Kohler verstarb am 29. Januar 1964 nach kurzer schwerer Krankheit im Alter von 44 Jahren.

schen Auslöschungen mit den entsprechenden Daten des Ammonium-Mangan-Doppelsulfates zeigte, dass beide Verbindungen isotyp sind. $(\text{NH}_4)_2\text{Mn}_2(\text{SeO}_4)_3$ hat also Langbeinitstruktur.

Tabelle 1. *d*-Werte und relative Intensitäten von $(\text{NH}_4)_2\text{Mn}_2(\text{SeO}_4)_3$

<i>d</i>	<i>I</i> / <i>I</i> ₀	<i>hkl</i>	<i>d</i>	<i>I</i> / <i>I</i> ₀	<i>hkl</i>
6,12	38	111	1,954	9	520
4,71	6	210	1,924	5	521
4,30	81	211	1,834	16	522
3,72	10	220	1,807	4	530
3,51	13	221	1,782	5	531
3,33	100	310	1,733	4	610
3,17	17	311	1,709	19	611
2,922	14	320	1,665	3	620
2,817	53	321	1,645	5	621
2,635	1	400	1,626	7	541
2,556	7	410	1,570	11	630
2,357	9	420	1,553	6	631
2,299	6	421	1,505	5	632
2,150	7	422	1,461	1	640
2,110	2	430	1,448	6	720/641
2,067	14	510	1,433	5	721/633
2,028	2	511	1,371	6	731/553

Die Verbindung bildet eine lückenlose Reihe von Mischkristallen mit $(\text{NH}_4)_2\text{Mn}_2(\text{SO}_4)_3$, die Gitterkonstan-

Tabelle 2. *Gitterkonstanten von $(\text{NH}_4)_2\text{Mn}_2(\text{SeO}_4, \text{SO}_4)_3$ in Abhängigkeit vom SeO_4 -Gehalt*

<i>a</i> ₀	SeO_4
10,19 ₂ Å	0,0 mol. %
10,26 ₅	23,5
10,33 ₃	46,3
10,46 ₅	82,0
10,53 ₃	100,0

ten der Mischkristalle entsprechen der Vegardschen Regel, wie anhand von Tabelle 2 überprüft werden kann.

Die Mischkristalle Doppelsulfat-Doppelselenat wurden nach dem oben angegebenen Verfahren, thermischer Abbau mit nachfolgender Extraktion mit Alkohol, aus entsprechenden Mischkristallen von $(\text{NH}_4)_2\text{Mn}(\text{SeO}_4)_2 \cdot 6\text{H}_2\text{O}$ mit $(\text{NH}_4)_2\text{Mn}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ hergestellt.

Die Mischkristalle der Hexahydrate sind kongruent löslich, auch durch Entwässerung und Extraktion wird das Verhältnis SeO_4/SO_4 nicht geändert.

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Literatur

GATTOW, G. & ZEMANN, J. (1958). *Z. anorg. Chem.* **293**, 233.

ZEMANN, A. & ZEMANN, J. (1957). *Acta Cryst.* **10**, 409.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the General Secretary of the International Union of Crystallography (D. W. Smits, Rekencentrum der Rijksuniversiteit, Grote Appelstraat 11, Groningen, The Netherlands). Publication of an item in a particular issue cannot be guaranteed unless the draft is received 8 weeks before the date of publication.

International Union of Crystallography

Professor I. Fankuchen

The Executive Committee of the Union and the Editorial Board of *Acta Crystallographica* have learned with sorrow of the death on 28 June of Professor I. Fankuchen, for many years Co-editor of the journal. His health had not been good for some years, but he continued his full scientific and editorial activity till a few days before his death.

An obituary notice will appear in a later issue of *Acta Crystallographica*.

Pittsburgh Diffraction Conference

The annual Pittsburgh Diffraction Conference will be held at Mellon Institute, Pittsburgh, Pennsylvania, from 4 to 6 November 1964. Sessions will be devoted to instrumentation, metals and alloys, and structures, with special sessions on extinction, low-energy electron diffraction and small-angle scattering. Professor W. H. Zachariasen of the University of Chicago will be the guest speaker for the Thursday evening meeting. A placement service will be available. Further information can be

obtained from Dr W. M. Biagas, Crucible Steel Company, P. O. Box 7257, Pittsburgh, Pennsylvania 15213, U.S.A.

Fifty Years of X-ray Diffraction

A second, final printing of this book has been completed by the publishers, N.V.A. Oosthoek's Uitgevers Mij., Domstraat 11-13, Utrecht, The Netherlands. It is available directly from the publishers, or through Polycrystal Book Service, G.P.O. Box 620, Brooklyn 1, N.Y., U.S.A., or from any bookseller, at the price of 40 Netherlands Guilders (at present rate of exchange £ 4 or \$ 11.25). The text of this second printing is the same as that of the first, but a name index and a sheet of the principal errata have been added. Owners of the original printing can obtain the name index and the errata sheet (together 16 pages, format 16 × 24 cm) free of charge by sending their request, which should be accompanied by an international reply coupon (DFI. 0-50, 1 s. or \$ 0.15), to either the publishers or Polycrystal Book Service.

Accuracy in X-ray Analysis

The X-ray Analysis Group of The Institute of Physics and The Physical Society announces that it is arranging