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Research and Development Report

GROUP IV AND V TRANSITION METAL
RICH CHALCONIDE X-RAY POWDER
DIFFRACTION DATA

by

H. F. Franzen, J. G. Smeggil, and
B. R. Conard

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GROUP IV AND V TRANSITION METAL-RICH
CHALCONIDE X-RAY POWDER DIFFRACTION DATA

H. F. Franzen, J. G. Smeggil, and B. R. Conard

ABSTRACT

Guinier powder diffraction data are tabulated for the following metal-rich chalconide compounds: Ti_2S , Ti_2Se , Zr_2S , Zr_2Se , Hf_2S , Hf_2Se , HfSe , Nb_{21}S_8 , Nb_2Se , Ta_2S , and Ta_6S .

SUMMARY

Several new metal-rich chalcogenide compounds have recently been prepared.⁽¹⁾ The purpose of this report is to provide diffraction data obtained from these compounds so that their identification in powdered samples might be more easily performed.

All data, except for the data of Hf_2S , were collected using a Guinier powder diffraction camera operated at room temperature. Monochromatic CuK_{α_1} radiation, filtered by Ni was used. KCl was employed as an internal standard, $a = 6.2930\text{\AA}$.⁽²⁾ For Hf_2S a Debye-Scherrer camera was used with CuK_{α} radiation, filtered by Ni.

The lattice parameters reported in the tables which follow were obtained by a least-squares treatment⁽³⁾ of the powder diffraction data. The tables list the indices, observed intensity, and observed and calculated values of $\sin^2\theta$, 2θ and d for each reflection.

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2. P. G. Hambling, Acta Cryst., 6 , 98, 1953.
3. D. E. Williams, Lattice Constants Refinement Program, IS-1052, Iowa State University of Science and Technology, Ames, Iowa, 1964.

Table 1. Guinier X-ray data for Ti_2S^* , orthorhombic, $a = 11.367$, $b = 14.060$, $c = 3.326 \text{ \AA}$

hkl	I/I_0	$\sin^2 \theta (\text{obs}) \times 10^5$	$\sin^2 \theta (\text{calc}) \times 10^5$	$2\theta (\text{obs})$	$2\theta (\text{calc})$	$d(\text{obs})$	$d(\text{calc})$
400	1	7332	7345	31.42	31.45	2.845	2.842
221	1	8388	8398	33.67	33.69	2.660	2.658
301	60	9498	9493	35.90	35.89	2.499	2.500
311	10	9807	9797	36.50	36.48	2.460	2.461
141	50	10621	10621	38.04	38.04	2.363	2.363
060	10	10799	10804	38.37	38.38	2.344	2.343
350	100	11636	11636	39.89	39.89	2.258	2.258
510	5	11793	11776	40.17	40.14	2.243	2.245
331	100	12202	12196	40.89	40.88	2.205	2.206
520	5	12697	12680	41.75	41.72	2.162	2.163
051	60	12860	12866	42.03	42.04	2.148	2.147
151	5	13319	13325	42.81	42.82	2.111	2.110
421	50	13888	13906	43.76	43.79	2.067	2.066
170	10	15179	15167	45.86	45.84	1.977	1.978
540	10	16272	16278	47.58	47.59	1.909	1.909
501	5	16817	16843	48.42	48.46	1.878	1.877
511	20	17820	17800	48.94	48.91	1.825	1.826
002	60	21457	21450	55.19	55.18	1.663	1.663

* In the list above the line 241 does not appear. That is because it superimposes on a KCl standard line.

$$\sin^2 \theta (241, \text{Ti}_2\text{S}) = 0.11978$$

$$\sin^2 \theta (220, \text{KCl}) = 0.11985$$

Ta 2. Guinier X-ray data for Ti_2Se , orthorhombic, $a = 11.743$, $b = 14.517$, $c = 3.4566 \text{ \AA}$

hkl	I/I ₀	$\sin^2\theta(\text{obs})$ $\times 10^5$	$\sin^2\theta(\text{calc})$ $\times 10^5$	$2\theta(\text{obs})$	$2\theta(\text{calc})$	d(obs)	d(calc)
220	1	2848	2845	19.44	19.43	4.562	4.564
140	5	4924	4935	25.64	25.67	3.471	3.467
320	10	4988	4996	25.82	25.84	3.448	3.445
011	10	5242	5246	26.47	26.48	3.364	3.363
101	8	5402	5394	26.88	26.86	3.314	3.316
240	1	6218	6227	28.88	28.90	3.089	3.087
330	1	6401	6405	29.31	29.32	3.045	3.046
211	15	6981	6967	30.64	30.61	2.915	2.918
410	8	7173	7164	31.07	31.05	2.876	2.878
031	8	7510	7501	31.82	31.79	2.810	2.812
221	30	7798	7812	32.43	32.46	2.758	2.756
301	20	8828	8838	34.57	34.59	2.592	2.591
311	30	9118	9118	35.15	35.15	2.551	2.551
231	30	9218	9218	35.35	35.35	2.537	2.537
141	30	9890	9901	36.66	36.68	2.449	2.448
060	10	10152	10137	37.16	37.13	2.417	2.419
350	18	10908	10908	38.57	38.57	2.332	2.332
510	10	11575	11580	38.78	38.81	2.320	2.318
241	100	11181	11192	39.07	39.09	2.304	2.302
331	100	11369	11369	39.41	39.41	2.284	2.284
440			11391		39.45		2.282
151	20	12437	12431	41.30	41.29	2.184	2.185
421	30	12972	12977	42.22	42.23	2.139	2.138

Table 2: continued

hkl	I/I _o	$\sin^2\theta$ (obs) x 10 ⁵	$\sin^2\theta$ (calc) x 10 ⁵	2 θ (obs)	2 θ (calc)	d(obs)	d(calc)
530 } 341 }	20	1331.9	13290 13343	42.81	42.76 42.85	2.113	2.111 2.109
360	10	13991	14009	43.93	43.96	2.059	2.058
170	25	14228	14222	44.32	44.31	2.042	2.043
540	15	15255	15261	45.98	45.99	1.972	1.972
511	20	16015	16002	47.18	47.16	1.925	1.926
180	18	18466	18446	50.90	50.87	1.792	1.793
002	70	19867	19861	52.94	52.93	1.728	1.728
461	10	21990	21983	55.93	55.92	1.643	1.643
631	5	23017	22988	57.34	57.30	1.606	1.607

Ta 3. Guinier X-ray powder data for Zr_2S , $a = 12.322 \pm 0.003$, $b = 15.359 \pm 0.004$, $c = 3.508 \pm 0.001$ Å

hkl	I/I ₀	$\sin^2\theta(\text{obs})$ $\times 10^5$	$\sin^2\theta(\text{calc})$ $\times 10^5$	$2\theta(\text{obs})$	$2\theta(\text{calc})$	d(obs)	d(calc)
140	5	4362	4415	24.11	24.26	3.688	3.666
111	10	5477	5462	27.07	27.03	3.291	3.296
400	10	6261	6252	28.98	28.96	3.078	3.081
410	5	6521	6504	29.59	29.55	3.016	3.020
420	2	7268	7259	31.28	31.26	2.857	2.859
221	50	7391	7391	31.55	31.55	2.833	2.833
250	10	7849	7849	32.54	32.54	2.749	2.749
301	50	8344	8340	33.58	33.57	2.667	2.667
430	30	8529	8514	33.96	33.93	2.637	2.640
311	30	8602	8587	34.11	34.08	2.626	2.629
060	25	9092	9052	35.10	35.02	2.554	2.560
141	60	9244	9234	35.40	35.38	2.533	2.535
321	10	9350	9345	35.61	35.60	2.519	2.520
350	40	9797	9807	36.48	36.50	2.461	2.460
510	30	10016	10021	36.90	36.91	2.434	2.433
241	100	10407	10407	37.64	37.64	2.388	2.388
331	90	10610	10600	38.02	38.00	2.365	2.366
260		10610	10616	38.02	38.03	2.365	2.364
520	25	10767	10777	38.31	38.33	2.347	2.346
051	50	11121	11110	38.96	38.94	2.310	2.311
411	10	11347	11325	39.37	39.33	2.287	2.289
151	5	11502	11497	39.65	39.64	2.271	2.272
530	35	12070	12031	40.66	40.59	2.217	2.221
421		12070	12076	40.66	40.67	2.217	2.217
450	25	12564	12541	41.52	41.48	2.173	2.175
360		12564	12570	41.52	41.53	2.173	2.173

Table 3 : continued

hkl	I/I ₀	$\sin^2\theta(\text{obs})$ $\times 10^5$	$\sin^2\theta(\text{calc})$ $\times 10^5$	2 $\theta(\text{obs})$	2 $\theta(\text{calc})$	d(obs)	d(calc)
170	20	12720	12715	41.79	41.78	2.160	2.160
540	30	13779	13791	43.58	43.60	2.075	2.074
511	30	14830	14843	45.30	45.32	2.000	1.999
630	15	16317	16330	47.65	47.67	1.907	1.906
180	15	16479	16485	47.90	47.91	1.897	1.897
280	5	17667	17660	49.71	49.70	1.833	1.833
470	10	18588	18575	51.08	51.06	1.787	1.787
002	50	19224	19279	52.04	52.09	1.756	1.754
631	10	21128	21150	54.73	54.76	1.676	1.675
290	20	21939	21939	55.86	55.86	1.644	1.644
660	20	23091	23120	57.44	57.48	1.603	1.602
721	40	24962	24977	59.95	59.97	1.542	1.541
191	30	25561	25584	60.74	60.77	1.524	1.523
731	25	26203	26234	61.58	61.62	1.505	1.504
571	30	26913	26913	62.50	62.50	1.485	1.485
661	30	27980	27940	63.87	63.82	1.456	1.457
062	20	28341	28333	64.33	64.32	1.447	1.447
391	20	28719	28711	64.81	64.80	1.437	1.438
352	30	29083	29083	65.27	65.27	1.428	1.428
512	20	29305	29305	65.55	65.55	1.423	1.423

Table 4. Gunier X-ray powder data for Zr_2Se , $a = 12.640 \pm 0.003$, $b = 15.797 \pm 0.003$, $c = 3.602 \pm 0.001 \text{ \AA}$

hkl	I/I_0	$\sin^2 \theta (\text{obs})$ $\times 10^5$	$\sin^2 \theta (\text{calc})$ $\times 10^5$	$2\theta (\text{obs})$	$2\theta (\text{calc})$	$d (\text{obs})$	$d (\text{calc})$
211	5	6294	6299	29.06	29.07	3.070	3.069
221	10	7016	7012	30.72	30.71	2.908	2.909
301	30	7910	7915	32.67	32.68	2.739	2.738
311	30	8162	8152	33.20	33.18	2.696	2.698
060	30	8563	8558	34.03	34.02	2.632	2.633
141	70	8759	8749	34.43	34.41	2.603	2.604
321	15	8863	8868	34.64	34.65	2.587	2.587
350	30	9289	9284	35.49	35.48	2.527	2.528
510	40	9534	9524	35.97	35.95	2.495	2.496
241	100	9859	9854	36.60	36.59	2.453	2.454
520	30	10232	10237	37.31	37.32	2.408	2.407
051	60	10514	10519	37.84	37.85	2.375	2.375
421	50	11469	11469	39.59	39.59	2.274	2.274
540	30	13083	13089	42.41	42.42	2.130	2.129
511	20	14082	14094	44.08	44.10	2.053	2.052
180	15	15582	15587	46.50	46.51	1.951	1.951

∞

Table 5. Debye-Scherrer X-ray data for Hf_2S , hexagonal, $a = 11.7882$, $c = 3.3736 \text{ \AA}$

hkl	I/I_0	$\sin^2 \theta$ (obs) $\times 10^5$	$\sin^2 \theta$ (calc) $\times 10^5$	2θ (obs)	2θ (calc)	d(obs)	d(calc)
001	50	514	516	26.21	26.26	3.396	3.390
100	50	698	698	30.64	30.64	2.914	2.914
101	100	1205	1206	40.62	40.64	2.218	2.217
002	40	2022	2023	53.44	53.46	1.712	1.712
110	25	2092	2093	54.44	54.45	1.683	1.683
111	10	2597	2599	61.28	61.30	1.511	1.510
102	40	2718	2719	62.84	62.86	1.477	1.477
200	10	2788	2791	63.74	63.78	1.458	1.458
201	25	3296	3296	70.07	70.07	1.341	1.341
112	35	4117	4110	79.83	79.75	1.200	1.201
003	10	4535	4541	84.66	84.73	1.143	1.143
202	10	4803	4805	87.74	87.76	1.111	1.111
210	10	4878	4885	88.60	88.68	1.102	1.102
103	40	5241	5239	92.76	92.74	1.064	1.064
211	35	5385	5372	94.42	94.27	1.049	1.051
300	10	6256	6252	104.55	104.50	0.974	0.974
113	15	6615	6615	108.84	108.84	0.947	0.947
301	10	6756	6759	110.56	110.60	0.937	0.937
221	30	6875	6875	112.02	112.02	0.929	0.929
203	35	7309	7308	117.50	117.49	0.901	0.901
004	20	8047	8048	127.55	127.56	0.858	0.858
302	30	8265	8265	130.77	130.77	0.847	0.847
220	10	8336	8338	131.85	131.85	0.843	0.843

Table 5: Continued

hkl	I/I ₀	$\sin^2 \theta$ (obs) $\times 10^5$	$\sin^2 \theta$ (calc) $\times 10^5$	2θ (obs)	2θ (calc)	d(obs)	d(calc)
104	40	8744	8742	138.49	138.45	0.823	0.824
221	15	8841	8840	140.19	140.17	0.819	0.819
310	20	9029	9031	143.69	143.73	0.810	0.810
213	80	9389	9388	151.38	151.35	0.795	0.795
311	70	9530	9532	154.96	155.01	0.789	0.789

Ta 6. Guinier X-ray data for Hf_2Se , hexagonal, $a = 12.260$, $c = 3.4502 \text{ \AA}$

hkl	I/I_0	$\sin^2\theta(\text{obs})$ $\times 10^5$	$\sin^2\theta(\text{calc})$ $\times 10^5$	$2\theta(\text{obs})$	$2\theta(\text{calc})$	$d(\text{obs})$	$d(\text{calc})$
002	1	1582	1580	14.45	14.44	6.129	6.128
00 4	10	6320	6316	28.12	29.11	3.064	3.065
100	10	6651	6647	29.89	29.88	2.987	2.988
10 1	80	7043	7039	30.78	30.77	2.902	2.903
102	70	8238	8224	33.36	33.33	2.764	2.767
10 3	100	10211	10200	37.27	37.25	2.411	2.412
10 4	75	12948	12960	42.18	42.20	2.190	2.189
006	15	14203	14209	44.28	44.29	2.044	2.043
110	50	19916	19937	53.01	53.04	1.726	1.725

Table 7. Guinier X-ray powder data for HfSe, hexagonal, $a = 3.5008$, $c = 3.6059 \text{ \AA}$.

hkl	I/I _o	$\sin^2\theta$ (obs) $\times 10^5$	$\sin^2\theta$ (calc) $\times 10^5$	2θ (obs)	2θ (calc)	d(obs)	d(calc)
001	40	4567	4564	24.68	24.67	3.604	3.605
100	90	6401	6456	29.31	29.44	3.044	3.031
101	100	11028	11017	38.79	38.77	2.319	2.321
002	50	18250	18250	50.58	50.58	1.803	1.803
110	75	19355	19362	52.20	52.21	1.751	1.750
102	60	24693	24706	59.59	59.61	1.550	1.550

Table 8. Guinier X-ray data for Nb₂₁S₈, tetragonal, a = 16.836, c = 3.352 Å

hkl	I/I ₀	sin ² θ (obs) x 10 ⁵	sin ² θ (calc) x 10 ⁵	2θ (obs)	2θ (calc)	d (obs)	d (calc)
350	10	7097	7115	30.90	30.94	2.891	2.888
231	5	8014	8000	32.89	32.86	2.721	2.723
260	5	8383	8373	33.66	33.64	2.660	2.662
141	5	8853	8838	34.62	34.59	2.589	2.591
170	80	10450	10466	37.72	37.75	2.383	2.381
501	100	10519	10514	37.85	37.84	2.375	2.375
521	70	11363	11352	39.40	39.38	2.285	2.286
370	10	12150	12139	40.80	40.78	2.210	2.211
800	1	13408	13397	42.96	42.94	2.104	2.105
451	1	13876	13864	43.74	43.72	2.068	2.069
820	1	14179	14234	44.24	44.33	2.045	2.042
480	1	16732	16745	48.29	48.31	1.883	1.882
002	10	21136	21128	54.74	54.73	1.675	1.676
590	1	22214	22185	56.24	56.20	1.634	1.635
132	1	23179	23216	57.56	57.61	1.600	1.599

Table 9. Guinier X-ray data for Nb₂Se, monoclinic, a = 13.995, b = 3.429, c = 9.306 Å, β = 92.04°

hkl	I/I ₀	$\sin^2\theta(\text{obs})$ $\times 10^5$	$\sin^2\theta(\text{calc})$ $\times 10^5$	$2\theta(\text{obs})$	$2\theta(\text{calc})$	d(obs)	d(calc)
001	5	0.00686	0.00686	9.50	9.50	9.300	9.300
002	5	0.02750	0.02744	19.09	19.07	4.645	4.650
310	25	0.07780	0.07774	32.39	32.38	2.762	2.763
$\bar{1}12$	50*	0.08028	0.08024	32.92	32.91	2.719	2.719
311	15	0.08553	0.08558	34.01	34.02	2.634	2.633
$\bar{3}12$	100	0.10327	0.10322	37.49	37.48	2.397	2.397
312	60	0.10729	0.10713	38.24	38.21	2.352	2.353
600 } 004 }	80*	0.10968	0.10918	38.68	38.59	2.326	2.331
			0.10973	38.68	38.69		2.325
$\bar{6}01$	15	0.11413	0.11408	39.49	39.48	2.280	2.281
204	5	0.12443	0.12448	41.31	41.32	2.184	2.183
510	5	0.12622	0.12627	41.62	41.63	2.168	2.168
$\bar{5}11$	5	0.13142	0.13148	42.51	42.52	2.125	2.124
$\bar{6}02$	5	0.13278	0.13272	42.74	42.73	2.114	2.114
$\bar{3}13$	50	0.13647	0.13653	43.36	43.37	2.085	2.085
$\bar{4}04$	50*	0.15355	0.15305	46.14	46.06	1.966	1.969
603	5	0.17654	0.17674	49.69	49.72	1.833	1.832
$\bar{3}14$	5	0.18385	0.18358	50.78	50.74	1.796	1.798
$\bar{8}01$	60*	0.19826	0.19840	52.88	52.90	1.730	1.729
020	50	0.20161	0.20175	53.36	53.38	1.715	1.715
$\bar{6}04$	10	0.21050	0.21114	54.62	54.71	1.679	1.676
$\bar{8}02$	10	0.21622	0.21637	55.42	55.44	1.656	1.656

Table 10. Guinier X-ray data for Ta_2S , orthorhombic, $a = 7.381$, $b = 5.574$, $c = 15.195 \text{ \AA}$

hkl	I/I_0	$\sin^2\theta(\text{obs})$ $\times 10^5$	$\sin^2\theta(\text{calc})$ $\times 10^5$	$2\theta(\text{obs})$	$2\theta(\text{calc})$	$d(\text{obs})$	$d(\text{calc})$
002	50	1032	1028	11.66	11.64	7.583	7.596
100	50	1085	1089	11.96	11.98	7.393	7.381
102	10	2124	2116	16.76	16.73	5.285	5.295
004	10	4116	4112	23.41	23.40	3.797	3.798
211	15	6521	6521	29.59	29.59	3.016	3.016
114	10	7106	7110	30.92	30.93	2.890	2.889
212	18	7295	7295	31.34	31.34	2.852	2.852
021	80	7887	7887	32.62	32.64	2.743	2.741
213	80	8573	8577	34.05	34.02	2.631	2.630
121	35	8789	8784	34.89	34.88	2.569	2.570
006	25	9244	9249	35.40	35.41	2.533	2.533
115	80	9416	9421	35.74	35.74	2.510	2.510
300	25	9792	9802	36.47	36.49	2.462	2.460
023	40	9943	9953	36.76	36.78	2.443	2.442
106	50	10354	10338	37.54	37.51	2.394	2.396
302	50	10826	10832	38.42	38.43	2.341	2.340
123	100	11033	11038	38.80	38.81	2.319	2.318
310	40	11726	11709	40.01	40.02	2.249	2.251
221	100	12242	12253	40.96	40.98	2.202	2.200
116			12247		40.97		2.201
215	5	12680	12691	41.72	41.74	2.163	2.162
206	40	13593	13605	43.27	43.28	2.089	2.088
313	20	14027	14021	43.99	43.98	2.057	2.057
223	20	14307	14307	44.45	44.45	2.036	2.036

Table 10: continued

hkl	I/I ₀	$\sin^2\theta$ (obs) x 10 ⁵	$\sin^2\theta$ (calc) x 10 ⁵	2 θ (obs)	2 θ (calc)	d(obs)	d(calc)
125	5	15148	15154	45.81	45.81	1.979	1.979
216	35	15532	15519	46.42	46.40	1.954	1.955
314	25	15817	15824	46.87	46.88	1.937	1.936
008	10	16440	16446	47.84	47.85	1.900	1.899
225	15	18419	18419	50.83	50.83	1.795	1.795
132	5	19286	19800	52.10	52.12	1.754	1.753
230	18	21565	21543	55.34	55.31	1.659	1.660
134	15	22389	22389	56.48	56.48	1.628	1.628
232	15	22593	22571	56.76	56.73	1.621	1.621
213	10	22732	22710	56.95	56.92	1.616	1.616

Table 11. Guinier X-ray data for Ta_6S , monoclinic, $a = 14.158$, $b = 5.284$, $c = 14.789 \text{ \AA}$, $\beta = 118.01^\circ$

hkl	I/I ₀	$\sin^2 \theta (\text{obs})$ $\times 10^5$	$\sin^2 \theta (\text{calc})$ $\times 10^5$	$2\theta (\text{obs})$	$2\theta (\text{calc})$	d(obs)	d(calc)
002	10	1388	1392	13.53	13.55	6.549	6.530
200	5	1524	1519	14.18	14.16	6.241	6.249
$\bar{3}11$	1	4871	4867	25.50	25.54	3.490	3.485
$\bar{3}12$			4886		25.49		3.492
004	1	5561	5569	27.28	27.30	3.266	3.264
311	1	6923	6914	30.51	30.49	2.928	2.929
$\bar{0}20$	25	8480	8499	33.86	33.90	2.645	2.642
021	60	8863	8848	34.64	34.61	2.587	2.590
312	25	8992	8982	34.90	34.88	2.567	2.570
$\bar{3}15$	70	9118	9123	35.15	35.16	2.551	2.550
$\bar{1}15$	20	9508	9498	35.92	35.90	2.498	2.499
$\bar{5}13$	25	9621	9631	36.14	36.16	2.483	2.482
204	20	9818	9818	36.52	36.52	2.458	2.458
022	20	9885	9896	36.65	36.67	2.450	2.449
$\bar{5}11$	100	10263	10258	37.37	37.36	2.404	2.405
$\bar{5}14$	80	10375	10359	37.58	37.55	2.391	2.393
$\bar{6}02$	55	10951	10968	37.65	37.68	2.387	2.385
$\bar{2}23$	85	11110	11104	38.94	38.93	2.370	2.370
023	90	11631	11636	39.88	39.89	2.257	2.258
313	60	11743	11748	40.08	40.09	2.248	2.247
006	1	12523	12529	41.45	41.46	2.177	2.176
$\bar{2}24$	1	12854	12854	42.02	42.02	2.148	2.148
115	50	12919	12913	42.13	42.12	2.144	2.144

Table 11: continued

hkl	I/I ₀	$\sin^2 \theta (\text{obs})$ $\times 10^5$	$\sin^2 \theta (\text{calc})$ $\times 10^5$	$2\theta (\text{obs})$	$2\theta (\text{calc})$	d(obs)	d(calc)
423	70	13617	13611	43.31	43.30	2.087	2.088
605	5	13912	13906	43.80	43.79	2.065	2.066
024	1	14082	14069	44.08	44.06	2.053	2.054