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Leiteite,  $\text{ZnAs}_2\text{O}_4$ : A novel type of tetrahedral layer structure with arsenite chains

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For deposit: Table 4

American Mineralogist, 72, 5-6, 629-632.

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For deposit

Leiteite,  $ZnAs_2O_4$ : A Novel type of  
Tetrahedral Layer Structure with Arsenite Chains<sup>1</sup>

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<sup>1</sup> Structural chemistry of copper and zinc minerals, Part VII.

Table A. Leiteite,  $ZnAs_2O_4$ : Observed and  
calculated structure factors.

### Abstract

Leiteite,  $\text{ZnAs}_2\text{O}_4$  from Tsumeb, Namibia is monoclinic,  $a = 4.542(1)$ ,  $b = 5.022(1)$ ,  $c = 17.597(5)\text{\AA}$ ,  $\beta = 90.81(3)^\circ$ , space group  $P2_1/c$ ,  $Z = 2$ . The crystal structure has been determined by direct methods and refined by the method of least squares to a R factor of 0.048 based on 713 independent reflections measured on an automatic single crystal x-ray diffractometer. The crystal structure consists of open zinc tetrahedral sheets flanked by single arsenite chains on either side. The composite layers are cross-linked through weak (2.8-3.3\AA) As-O bonds. Leiteite represents a new structure type. The average tetrahedral Zn-O distance is 1.99\AA and the average As-O distances and O-As-O angles in the two distinct trigonal pyramidal arsenite groups are 1.79\AA,  $95.5^\circ$  for As(1) and 1.78\AA,  $95.8^\circ$  for As(2).

## OBSERVED AND CALCULATED STRUCTURE FACTORS FOR LEITITE

PAGE 1

H	K	L	10FO	10FC	H	K	L	10FO	10FC	H	K	L	10FO	10FC	H	K	L	10FO	10FC	H	K	L	10FO	10FC
0	0	2	303	-350	1	2	5	172	-179	0	3	5	971	961	3	1	6	867	-806	2	3	7	392	403
0	1	1	718	725	-1	1	8	1450	-1475	-3	0	2	125	-115	-2	3	4	91	-74	0	4	5	164	-157
1	0	0	55	-10	1	1	8	1619	-1663	3	0	2	87	10	3	2	1	645	588	3	2	6	107	8
0	1	2	42	18	0	1	9	164	174	-1	3	4	626	-620	1	2	11	226	256	-1	3	10	437	438
-1	0	2	84	-52	-2	0	6	774	-767	1	3	4	955	-980	2	3	4	124	-56	1	1	14	891	888
0	1	3	85	-97	-2	1	5	487	-462	0	0	12	1814	1826	-1	3	8	1400	1456	-3	1	9	497	-507
1	1	0	287	242	2	0	6	649	-646	-2	2	6	1985	1961	3	2	2	71	-120	1	3	10	679	695
-1	1	1	1088	1040	2	1	5	238	-221	-1	2	9	338	-343	-2	1	11	303	310	-3	2	7	283	-279
0	1	4	68	-51	0	0	10	1159	1166	1	2	9	241	-251	1	3	8	1063	1081	-1	2	13	254	248
1	1	1	979	-1021	-2	1	6	77	-87	-1	1	11	538	-599	0	3	9	454	-439	0	3	11	705	-717
-1	1	2	1804	1800	-1	1	9	732	737	2	2	6	1751	1776	-3	2	3	667	646	3	1	9	547	540
1	0	4	72	-74	1	1	9	664	-746	3	1	0	525	462	0	2	12	249	-270	0	4	6	1103	-1097
1	1	2	2251	2311	2	2	0	2723	-2672	-3	1	1	659	-711	-3	1	7	607	605	1	2	13	402	404
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1	1	3	916	950	2	2	1	284	166	1	1	11	564	627	-2	3	5	799	781	-1	4	5	234	-229
0	1	5	696	-706	0	3	1	953	-948	-1	3	5	752	652	3	2	3	631	604	0	1	15	132	-157
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1	2	3	352	377	-1	2	8	88	-133	-2	2	8	224	-228	-1	0	14	111	-138	-2	2	12	1312	-1278
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-1	2	5	266	263	2	2	5	112	95	3	2	0	114	-35	1	4	3	909	-888	2	4	1	85	78

## OBSERVED AND CALCULATED STRUCTURE FACTORS FOR LEITITE

PAGE 2

H	K	L	10FO	10FC	H	K	L	10FO	10FC	H	K	L	10FO	10FC	H	K	L	10FO	10FC	H	K	L	10FO	10FC
4	0	4	414	-428	1	4	9	616	630	-1	5	2	534	537	2	4	10	1232	1198	0	4	14	608	-593
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-4	1	3	85	-91	4	2	2	628	-595	-4	1	9	139	125	4	3	3	246	224	2	5	5	734	-756
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