

The crystal structure of althausite,  $Mg_4(PO_4)_2(OH,O)(F,\square)$ 

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## Abstract

The crystal structure of althausite was solved by direct methods and refined to a final  $R$  value of 0.022 for 1164 high-angle reflections ( $\sin \theta/\lambda > 0.45 \text{ \AA}^{-1}$ ) with  $I > 2.5\sigma$ . The position of the hydrogen atom was found from a difference Fourier synthesis. The structure is orthorhombic  $Pnma$  with  $a = 8.258(2)$ ,  $b = 6.054(2)$ ,  $c = 14.383(5) \text{ \AA}$ . Magnesium atoms occur in both five- and six-fold coordination, and the coordination polyhedra are highly distorted. The Mg octahedra form chains along  $b$  by edge-sharing. Hydroxyl and fluorine occur in a largely ordered distribution among two different structural sites and occupy alternating positions along 'channels' parallel to  $b$ . Partial vacancy in the (OH,F) sites is confirmed, the population factor for the F site being 81 percent. The crystal-chemical formula of althausite is therefore  $Mg_4(PO_4)_2(OH,O)(F,\square)$  with  $Z = 4$ .

The cleavages in althausite, {001} perfect and {101} distinct, occur along planes crossing relatively few bonds and leave the chains of Mg octahedra unbroken. Bond-strength calculations for althausite and wagnerite are presented and the OH content in wagnerite is discussed.

Preliminary results of hydrothermal syntheses indicate the existence of a series from F-wagnerite to OH,F-wagnerite and from OH-althausite to OH,F-althausite. Infrared spectra of fluorine-free althausite show a splitting of the O-H stretching frequency, proving that two distinct hydroxyl positions are present.

## Introduction

The new magnesium-phosphate mineral althausite was described from serpentine-magnesite deposits in Modum, south Norway, by Raade and Tysseand (1975). Based on a wet-chemical analysis, the empirical formula was given as  $Mg_2PO_4(OH_{0.37}F_{0.25}O_{0.19}\square_{0.19})$ , with vacancy in the (OH,F) sites because of a presumed substitution of the type  $2(OH,F)^- \rightleftharpoons O^{2-}\square$ . Althausite is orthorhombic with  $a = 8.258(2)$ ,  $b = 14.383(5)$ ,  $c = 6.054(2) \text{ \AA}$ ,  $V = 719.0(7) \text{ \AA}^3$ ,  $Z = 8$ . The space group was given as  $Pna2_1$ , but from the extinctions, another possible space group is  $Pnam$  which was omitted. Furthermore, the cleavage was stated to be perfect along {001} and distinct along {101}. New investigations show that the correct cleavages are {010} (perfect, pinacoidal) and {110} (distinct, prismatic). A set of rough measurements of the angle between the face normals of the perfect and the distinct cleavage planes gave 60-63°, in good

agreement with the calculated value,  $(010) \wedge (110) = 60.14^\circ$ . The optical orientation must be changed accordingly to  $X = c$ ,  $Y = b$ ,  $Z = a$ , OAP (010), and the hardness on {010} is  $3\frac{1}{2}$  in the  $c$  direction and 4 in the  $a$  direction.

The type locality for althausite is the Tingelstadjern quarry, Modum, and the original description was based on material from this occurrence. The mineral has also been found in a similar deposit farther to the north, the Overntjern quarry. Here the althausite has a reddish-brown color and occurs in a somewhat different mineral association (talc, magnesite, brown apatite, partly enstatite). However, a more complete account of the mineral parageneses and the distribution of phosphate minerals among the deposits is reserved for a separate paper.

A microprobe analysis of the Overntjern althausite using Tingelstadjern althausite as standard gave the following result (data calculated as direct ratios after background correction; values for the Tingelstadjern



3	312	312	38	2	76	73	21	4	216	214	26	7	57	62	36	1	60	62	21
5	307	306	39	3	225	224	28	5	129	129	21	4	128	130	29	2	61	63	24
6	208	207	33	4	60	3	24	6	635	640	66	5	45	56	47	3	194	199	26
7	184	181	32	5	704	691	73	7	99	94	24	6	333	330	42	4	339	341	28
8	117	117	32	6	98	97	25	8	110	107	25	8	70	71	37	5	96	92	24
L=	3,K=	8	32	7	83	86	27	10	38	36	42	L=	5,K=	8	37	6	106	106	26
2	90	90	31	8	450	442	50	11	141	141	30	1	82	80	31	7	106	81	26
3	389	390	46	9	486	496	54	12	220	224	34	2	117	101	29	8	607	595	65
5	123	128	31	L=	4,K=	92	33	L=	5,K=	289	34	4	91	92	32	9	46	83	30
6	136	131	31	11	4,K=	5	33	1	300	289	34	2	117	101	29	10	108	110	31
L=	3,K=	86	37	1	560	563	58	2	553	543	57	6	375	378	46	11	108	110	46
0	31	30	58	3	26	16	44	3	450	463	58	L=	5,K=	52	48	L=	6,K=	5	45
1	283	289	38	4	100	106	44	4	567	575	57	0	46	52	48	1	409	413	45
L=	35	34	38	5	107	174	26	5	120	119	21	1	87	85	32	2	133	130	24
2	4	57	57	6	35	40	45	6	261	258	31	2	228	234	35	3	35	37	39
L=	4,K=	0	57	7	144	40	27	7	367	363	41	L=	32	19	60	4	707	719	73
0	1908	1940	418	8	61	64	33	8	92	80	25	L=	6,K=	0	18	5	79	81	27
1	225	204	24	9	260	261	35	10	256	255	35	0	38	85	16	7	102	100	29
1	182	174	21	10	157	157	31	11	120	123	30	1	31	36	16	8	199	196	32
3	258	265	28	L=	4,K=	6	31	12	52	40	39	2	302	292	22	9	258	259	36
4	408	385	43	0	284	254	34	L=	5,K=	3	39	3	302	292	33	10	91	85	32
5	652	956	96	1	359	345	40	0	29	19	32	3	281	282	31	L=	6,K=	6	67
6	60	51	21	2	74	73	27	0	288	285	32	4	129	139	21	0	640	641	67
7	110	113	23	3	146	149	26	2	483	480	50	5	97	88	22	1	54	54	30
8	684	680	71	4	418	417	47	3	133	134	21	7	85	89	24	3	160	158	27
8	627	629	66	5	88	74	26	4	201	201	26	8	837	832	86	4	880	897	90
10	81	82	28	6	224	225	33	5	121	121	32	9	118	114	27	5	100	96	28
11	99	98	28	7	116	106	31	6	37	33	38	10	86	92	29	6	52	52	39
L=	4,K=	1	30	8	83	87	34	7	113	109	26	11	128	130	30	7	70	75	34
1	879	889	133	9	60	69	38	10	72	68	30	L=	478	478	54	8	79	63	33
3	136	140	18	L=	4,K=	7	34	11	88	91	32	12	307	315	40	9	95	95	32
4	272	264	30	1	130	134	29	12	220	224	35	1	309	407	41	L=	6,K=	7	49
5	49	10	23	4	130	129	29	L=	5,K=	4	35	2	128	120	18	1	31	31	31
6	208	213	27	5	111	110	31	1	197	196	25	3	71	71	18	3	193	191	30
7	98	99	23	6	111	110	31	2	248	205	30	4	1176	1182	178	4	497	503	35
8	348	350	40	7	64	65	37	4	138	136	42	5	284	283	32	5	341	338	42
9	101	99	26	8	206	209	34	5	370	366	42	6	59	60	24	6	103	97	40
10	30	16	43	L=	4,K=	8	38	7	33	25	41	7	60	59	28	7	48	45	41
L=	4,K=	2	31	0	307	301	36	8	268	260	35	8	304	300	37	L=	6,K=	8	40
0	427	342	44	1	60	60	36	9	103	108	30	9	89	90	29	0	41	40	44
1	600	605	61	2	335	338	44	10	175	178	32	12	307	315	40	1	65	66	44
2	80	80	16	3	338	344	43	L=	5,K=	5	31	L=	1927	1942	362	2	44	47	42
3	298	302	33	4	105	105	33	0	73	67	23	0	64	50	17	3	113	111	42
4	1073	1088	108	5	105	105	33	1	168	163	25	1	252	250	29	4	325	327	41
5	155	132	23	6	119	118	35	L=	402	408	44	3	1768	1828	266	5	35	37	57
6	127	130	23	1	119	118	35	3	35	36	38	5	148	142	23	L=	100	97	34
7	327	325	38	L=	5,K=	0	29	4	98	101	25	6	40	39	31	6	100	97	34
8	104	85	25	5	269	278	29	5	469	468	51	7	100	104	24	L=	6,K=	9	33
9	125	117	26	2	1105	1043	18	8	80	79	28	8	107	104	24	1	190	191	33
10	27	3	53	4	64	72	18	9	91	89	28	9	122	117	27	2	69	73	16
11	59	58	34	5	199	203	18	10	48	46	40	10	182	190	30	L=	460	419	42
L=	242	239	35	6	250	230	20	L=	5,K=	46	40	11	101	102	31	3	460	447	48
1	512	520	53	7	45	41	31	L=	119	116	25	12	48	20	44	4	55	62	21
4	216	223	27	8	389	387	31	1	516	517	55	L=	6,K=	3	27	5	422	428	45
5	165	158	24	9	300	306	29	2	295	301	36	3	286	286	32	6	503	499	61
6	181	184	24	10	300	306	29	3	202	203	30	4	950	968	32	7	583	580	53
7	107	111	25	4	112	112	29	4	205	203	31	5	494	498	31	5	277	277	54
8	113	111	25	5	112	112	29	5	201	208	32	6	40	43	38	8	142	139	28
L=	4,K=	4	32	6	78	78	15	6	38	27	54	7	249	250	33	9	142	119	28
0	989	958	100	L=	5,K=	1	29	8	33	23	54	10	55	58	36	10	122	119	35
1	183	179	24	1	462	484	48	L=	132	129	40	L=	29	37	36	L=	127	136	18
				2	58	67	18	2	338	340	27	0	6	4	0	L=	127	120	120



0	388	384	42	10	310	307	40	4	73	74	53	3	34	45	57	5	113	117	32	4	151	152	28
1	256	265	31	L=	13,K=	1	23	5	196	202	34	4	70	63	32	=	15,K=	7	7	5	89	87	27
2	57	62	26	0	75	77	22	L=	983	993	100	5	142	140	30	0	74	73	34	6	250	252	35
3	266	266	32	1	110	92	22	1	114	117	23	L=	79	77	33	1	114	110	31	7	350	361	44
4	99	89	24	2	200	200	40	0	183	185	27	L=	70	66	35	2	185	187	33	8	69	99	32
5	47	44	32	3	361	362	24	2	285	288	35	3	62	57	39	0	167	171	27	L=	17,K=	1	31
6	131	134	26	4	123	124	24	3	285	289	41	L=	57	57	41	0	145	142	27	0	44	42	31
7	197	195	30	5	209	210	26	4	108	107	25	L=	60	61	39	3	197	198	33	1	224	224	31
8	272	269	36	6	80	81	26	5	60	61	25	L=	57	57	41	2	197	198	32	2	51	56	40
9	46	42	41	7	136	136	28	6	35	37	45	L=	606	608	39	4	239	239	32	3	37	33	33
10	74	66	33	8	125	120	26	7	223	225	45	L=	105	108	45	5	394	394	45	4	58	60	32
L=	12,K=	3	25	9	170	165	31	8	87	88	33	4	77	78	26	6	47	46	58	5	203	201	31
1	68	66	25	L=	13,K=	2	41	9	177	178	33	L=	15,K=	1	27	7	262	259	37	6	44	45	40
2	82	80	24	1	373	385	41	10	147	148	33	5	122	122	27	8	304	302	40	7	150	152	31
3	280	281	34	2	555	561	59	6	26	22	51	L=	26	22	27	9	304	302	40	8	179	174	32
4	331	332	39	3	287	292	34	7	47	48	31	L=	73	73	31	0	73	73	31	9	179	174	32
5	462	465	51	4	94	93	24	8	34	41	25	L=	190	188	33	1	73	77	25	1	59	58	30
6	161	166	28	5	196	193	29	9	133	139	25	L=	63	62	33	2	73	77	26	2	263	269	34
7	32	40	49	6	519	527	56	10	152	158	26	L=	156	155	27	3	340	340	26	3	478	482	53
8	343	349	42	7	195	199	30	1	157	157	27	L=	56	55	27	4	370	378	40	4	193	194	30
9	247	246	35	8	54	58	36	2	130	133	28	L=	31	25	34	5	123	124	43	5	182	185	30
L=	12,K=	4	90	L=	13,K=	3	32	3	496	497	55	4	51	48	41	6	148	146	29	6	125	122	29
0	864	893	35	10	164	158	29	4	210	205	33	5	57	54	30	7	148	146	29	7	147	147	31
1	238	292	28	L=	13,K=	70	25	5	44	43	0	L=	442	448	50	8	154	152	36	L=	17,K=	3	3
2	129	129	28	1	40	37	27	6	30	27	53	6	30	27	50	0	154	152	26	1	95	101	27
3	186	184	28	2	176	177	27	7	831	829	44	7	95	92	30	1	144	146	26	2	53	55	35
4	412	413	46	3	462	466	26	8	398	403	85	L=	95	92	30	2	143	140	26	3	100	101	29
5	99	95	27	4	116	119	35	9	79	76	24	L=	100	83	25	3	427	433	33	4	90	90	30
6	48	47	39	5	270	273	35	10	96	93	24	L=	147	145	26	4	499	506	54	5	245	248	35
7	191	193	31	6	90	88	27	1	78	77	25	L=	405	406	45	6	48	42	35	L=	17,K=	4	28
8	78	78	31	7	109	110	29	2	194	196	29	2	127	126	45	7	52	42	35	1	128	126	28
9	381	390	43	8	95	98	31	3	169	170	28	L=	188	187	29	8	52	60	38	2	132	138	29
L=	12,K=	5	29	9	93	89	32	4	125	122	43	3	34	32	46	9	56	57	40	3	216	217	32
0	68	72	29	10	145	140	26	5	138	142	29	L=	222	221	51	10	207	206	30	4	122	122	29
1	250	252	28	L=	13,K=	4	48	6	89	84	32	L=	15,K=	3	25	1	312	313	30	5	59	66	37
2	84	84	33	1	149	145	26	7	135	142	43	L=	98	93	30	11	317	318	39	L=	17,K=	5	33
3	33	35	30	2	307	305	48	8	64	65	40	L=	269	268	28	12	498	505	35	0	63	61	33
4	105	104	30	3	430	434	48	9	35	40	40	L=	60	53	31	13	153	157	30	1	237	242	35
5	289	288	39	4	28	12	52	10	74	78	31	L=	87	86	29	14	170	172	34	2	34	35	31
6	207	208	31	5	46	39	47	1	111	114	29	L=	396	398	46	15	121	124	27	3	110	109	31
7	179	184	30	6	121	116	27	2	116	117	26	L=	63	58	35	16	121	124	27	4	116	118	32
8	60	51	33	7	36	32	47	3	111	114	29	L=	105	107	32	17	170	172	29	5	146	144	46
9	173	175	30	L=	13,K=	5	28	4	436	435	30	L=	63	58	35	18	167	167	30	L=	17,K=	6	46
0	207	208	31	0	67	65	28	5	184	179	30	L=	105	107	32	19	167	167	30	1	146	144	46
1	179	184	30	1	170	167	28	6	83	85	27	L=	325	324	32	20	167	167	30	2	351	346	44
2	60	51	33	2	157	157	28	7	672	670	70	L=	67	66	45	21	325	324	32	3	178	178	29
3	173	175	30	3	173	172	28	8	83	85	27	L=	67	66	45	22	325	324	32	4	148	149	28
4	196	195	33	4	109	93	28	9	140	138	27	L=	82	84	30	23	324	324	32	5	103	102	28
5	147	151	33	5	59	57	35	10	247	252	27	L=	87	81	30	24	324	324	32	6	115	115	28
6	351	351	43	6	91	93	33	11	102	99	27	L=	87	81	30	25	324	324	32	7	149	147	29
L=	12,K=	8	57	7	97	99	32	12	101	99	28	L=	152	152	31	26	324	324	32	8	171	170	31
0	507	510	57	L=	13,K=	6	33	13	46	44	43	L=	152	152	31	27	324	324	32	9	171	170	31
1	164	167	35	1	229	229	33	14	124	124	31	L=	58	62	35	28	324	324	32	L=	18,K=	1	35
2	78	75	35	2	217	218	32	15	102	102	29	L=	226	227	33	29	324	324	32	1	273	274	35
3	13,K=	0	24	3	214	215	30	16	104	104	29	L=	68	71	33	30	324	324	32	2	76	79	29
4	154	155	24	4	84	80	32	17	109	113	30	L=	350	349	35	31	324	324	32	3	109	105	28
5	516	547	55	5	95	100	32	18	109	113	30	L=	81	78	35	32	324	324	32	4	210	206	33
6	545	547	57	6	261	261	37	19	101	102	31	L=	81	78	35	33	324	324	32	5	40	36	44
7	31	32	36	7	148	152	32	20	112	114	32	L=	67	74	36	34	324	324	32	6	40	36	44
8	235	237	43	L=	13,K=	7	36	21	711	703	36	L=	175	175	36	35	324	324	32	7	405	408	46
9	80	78	46	0	118	110	41	2	291	291	38	L=	254	256	36	36	324	324	32	8	42	39	37
L=	12,K=	6	32	1	322	318	41	3	72	73	32	L=	65	68	34	37	324	324	32	9	63	66	31

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3	216	217	5	32	3	54	57	40	1	50	33	34	0	39	39	45	4	384	373	46	
5	249	251		35	4	78	82	35	2	196	189	31	1	136	138	31	L=	20,K=	3	47	
6	200	197		33	L=	19,K=	0	27	3	46	47	40	L=	212	212	34	1	75	34	47	
7	79	77		33	2	135	130	27	4	45	45	43	L=	27	0	52	3	214	225	35	
L=	18,K=	3		30	3	532	526	29	5	93	96	32	0	99	24	52	4	293	289	39	
1	168	173		48	4	106	108	33	L=	323	326	42	1	34	98	49	L=	20,K=	4	31	
3	36	38		32	5	66	64	35	0	97	98	29	2	59	51	49	1	43	93	42	
4	82	88		37	6	34	37	51	L=	19,K=	3	31	3	34	56	34	2	97	32	31	
5	271	268		37	7	240	233	35	1	184	186	35	4	413	416	48	3	60	57	35	
L=	18,K=	4		31	L=	19,K=	154	32	2	244	245	37	5	172	168	32	L=	21,K=	0	35	
0	171	170		29	0	76	78	30	5	92	91	32	L=	50	1	39	1	281	278	37	
1	138	137		30	1	192	190	30	6	242	240	36	1	177	55	39	2	35	37	37	
2	116	119		30	2	261	264	35	L=	19,K=	4	35	3	304	173	39	3	56	54	35	
3	108	108		31	4	78	79	30	1	93	92	31	4	33	299	45	L=	21,K=	1	32	
4	164	162		31	5	109	109	29	2	373	366	45	5	33	9	37	0	191	191	32	
5	131	130		31	6	261	259	29	3	93	82	31	L=	57	2	37	1	154	153	31	
L=	18,K=	5		37	7	33	34	37	4	62	66	39	0	49	60	37	2	254	207	37	
1	255	260		32	L=	19,K=	2	56	L=	19,K=	5	39	1	75	82	34	1	49	41	39	
2	95	96											2								