

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

CHRISTIAN RØMMING

*Kjemisk Institutt, Universitetet i Oslo, Blindern, Oslo 3, Norway*

AND GUNNAR RAADE

*Institutt for Geologi, Universitetet i Oslo, Blindern, Oslo 3, Norway*

## 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  $60-63^\circ$ , 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







0 388 384 42 10 310 307 40 4 73 74 53 3 34 45 57 5 113 117 32 4 151 152 24  
1 256 265 31 0 75 1 23 196 202 34 4 70 63 32 1 15 7 73 34 5 89 87 27  
2 57 62 26 0 110 92 22 0 983 993 100 23 142 140 30 1 74 73 34 6 250 252 35  
3 266 266 32 1 200 200 27 1 114 117 27 27 77 77 33 1 114 110 31 7 350 361 44  
4 99 89 24 2 361 362 40 2 183 185 27 27 66 66 35 2 195 187 33 8 99 99 32  
5 47 44 32 3 423 124 24 3 285 288 35 35 57 57 39 39 0 167 171 27 0 44 42 34  
6 131 134 26 4 123 124 24 4 108 107 41 41 66 66 41 41 2 45 42 27 1 21 21 31  
7 197 195 30 5 209 210 29 5 60 61 30 30 345 339 39 39 3 197 195 29 2 21 21 33  
8 272 269 36 6 80 81 26 6 136 136 45 45 605 608 44 44 4 239 239 45 3 51 51 40  
9 46 42 41 8 125 120 28 7 7 35 37 25 25 105 108 41 41 5 393 394 44 4 58 58 40  
10 74 66 33 9 136 136 31 9 108 107 25 25 67 67 57 57 6 41 40 45 5 203 201 41  
L= 12,K= 3 10 170 165 32 3 223 225 33 33 77 76 26 26 7 47 46 36 6 44 45 40  
1 68 66 25 1 373 385 41 10 177 178 33 33 122 122 27 27 8 262 259 37 8 44 40 37  
2 82 80 24 2 555 561 59 1 47 48 31 31 22 22 51 51 9 304 302 40 9 179 174 32  
3 280 281 34 3 287 292 34 1 147 148 38 38 26 26 7 7 5 5 263 269 34  
4 331 332 30 4 94 93 24 2 34 41 35 35 8 8 198 200 29 2 478 482 53  
5 462 465 51 5 196 193 29 3 133 139 25 25 156 156 4 4 340 340 40 4 193 194 30  
6 161 166 49 6 519 527 56 4 152 158 26 26 136 136 1 1 370 378 43 4 182 185 30  
7 32 40 49 7 195 199 30 5 157 157 27 27 280 281 34 34 5 123 124 22 5 125 122 29  
8 343 349 42 8 54 58 36 6 110 113 28 28 31 31 2 2 148 146 29 7 147 146 31  
9 247 246 35 10 164 158 32 10 496 497 55 55 4 4 51 54 41 41 7 7 148 146 29  
L= 12,K= 4 10 164 158 32 8 496 497 55 55 4 4 51 54 41 41 7 7 148 146 29  
0 884 893 90 0 69 70 25 9 210 209 33 33 5 5 57 54 30 9 235 224 36 9 177,K= 3  
1 288 292 35 1 40 37 35 10 44 43 0 0 442 448 50 50 154 152 2 2 95 101 27  
2 129 129 25 2 176 177 27 2 831 829 85 85 7 7 30 27 30 0 144 146 26 2 53 55 35  
3 186 184 28 3 462 466 50 1 398 403 44 44 8 8 95 92 30 1 144 146 26 3 100 101 29  
4 412 413 46 4 116 119 26 2 79 76 25 25 147 145 26 26 43 40 40 4 90 90 30  
5 99 95 27 5 270 273 35 2 96 93 24 24 100 100 2 2 427 433 48 4 245 248 35  
6 48 47 39 6 90 88 27 3 78 77 25 25 405 406 45 45 5 5 48 42 35 5 226 217 32  
7 191 193 31 7 109 110 29 5 194 196 29 29 127 126 26 26 6 6 52 60 38 4 132 138 29  
8 78 78 31 8 95 98 31 6 169 170 28 28 188 187 29 29 8 8 52 60 38 4 132 138 29  
L= 12,K= 5 9 93 89 31 5 169 170 28 28 188 187 29 29 8 8 52 60 38 4 132 138 29  
1 381 380 43 10 145 140 32 10 125 122 43 43 6 6 394 396 46 46 8 8 52 60 38 4 132 138 29  
2 280 252 28 1 149 145 26 9 138 142 29 29 34 34 222 221 33 33 1 207 206 30  
3 84 84 35 2 307 305 48 4 430 434 48 48 89 84 32 32 0 98 93 25 4 498 505 35  
4 280 252 28 3 307 305 48 4 430 434 48 48 89 84 32 32 0 98 93 25 4 498 505 35  
5 84 84 35 4 307 305 48 4 430 434 48 48 89 84 32 32 0 98 93 25 4 498 505 35  
6 33 35 52 2 307 305 48 4 430 434 48 48 89 84 32 32 0 98 93 25 4 498 505 35  
7 105 104 30 3 307 305 48 4 430 434 48 48 89 84 32 32 0 98 93 25 4 498 505 35  
8 289 288 39 4 28 12 47 47 40 28 189 185 28 28 2 269 268 34 6 153 157 54  
L= 12,K= 6 5 46 39 33 2 64 65 40 28 189 185 28 28 2 269 268 34 6 153 157 54  
0 207 208 31 6 121 116 52 4 116 117 26 26 58 58 30 30 0 121 124 27 1 170 172 29  
1 179 184 30 8 36 32 47 7 74 76 31 31 5 5 396 398 29 29 0 121 124 27 1 170 172 29  
2 60 60 33 9 46 53 47 7 111 114 29 29 6 6 396 398 29 29 0 121 124 27 1 170 172 29  
3 173 175 30 0 67 65 28 8 436 435 30 30 7 7 105 107 32 32 2 2 38 39 42 1 46 44 46  
4 90 88 30 0 170 167 28 8 436 435 30 30 7 7 105 107 32 32 2 2 38 39 42 1 46 44 46  
5 173 175 30 1 170 167 28 8 436 435 30 30 7 7 105 107 32 32 2 2 38 39 42 1 46 44 46  
6 87 86 33 2 157 157 28 8 436 435 30 30 7 7 105 107 32 32 2 2 38 39 42 1 46 44 46  
7 149 156 32 2 157 157 28 8 436 435 30 30 7 7 105 107 32 32 2 2 38 39 42 1 46 44 46  
L= 12,K= 7 2 157 157 28 8 436 435 30 30 7 7 105 107 32 32 2 2 38 39 42 1 46 44 46  
1 74 72 33 4 3 173 172 29 0 672 670 70 70 1 253 254 34 4 227 228 41 4 227 228 41  
2 213 211 33 5 5 109 111 28 2 140 138 27 27 67 66 30 30 1 81 81 31 1 81 81 31  
3 196 195 33 6 59 57 35 3 247 252 33 33 83 84 30 30 2 2 94 93 30 2 2 94 93 30  
4 147 151 43 7 91 93 33 4 102 97 27 27 87 81 30 30 3 53 61 38 3 53 61 38  
5 147 151 43 8 97 99 33 5 101 99 28 28 87 81 30 30 3 53 61 38 3 53 61 38  
L= 12,K= 8 8 97 99 33 5 101 99 28 28 87 81 30 30 3 53 61 38 3 53 61 38  
0 507 510 57 1 229 229 33 1 124 124 31 31 152 152 43 43 4 253 255 36 4 253 255 36  
1 164 167 32 1 229 229 33 1 124 124 31 31 152 152 43 43 4 253 255 36 4 253 255 36  
2 78 75 35 2 217 218 32 2 214 215 29 29 100 102 29 29 2 226 227 33 1 164 167 32  
L= 13,K= 0 3 3 214 215 29 29 100 102 29 29 2 226 227 33 1 164 167 32  
1 154 155 24 4 84 80 30 4 107 104 29 29 6 6 350 349 43 3 3 350 349 43  
2 516 515 55 5 95 80 32 5 109 113 30 30 5 5 109 113 30 30 5 5 109 113 30 30  
3 545 547 57 6 261 261 37 6 101 102 31 31 7 7 81 78 35 3 3 301 303 39 1 113 104 42  
4 34 37 36 7 148 152 32 7 112 114 32 7 112 114 32 7 112 114 32 7 112 114 32 7 112 114 32  
5 31 32 43 7 112 114 32 7 112 114 32 7 112 114 32 7 112 114 32 7 112 114 32 7 112 114 32  
6 235 237 32 0 65 60 36 0 711 703 36 0 711 703 36 0 711 703 36 0 711 703 36 0 711 703 36  
7 26 24 46 0 118 110 31 1 291 291 38 1 291 291 38 1 291 291 38 1 291 291 38 1 291 291 38  
8 80 78 32 3 322 318 41 2 72 73 32 2 72 73 32 2 72 73 32 2 72 73 32 2 72 73 32 2 72 73 32

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3	216	217	32	3	54	57	40	1	50	33	34	0	39	39	45	4	384	378	46	2	158	155	31
5	249	251	35	4	78	82	35	2	196	189	31	1	136	138	31	L= 20, K=	75	34	47	3	216	211	33
6	200	197	33	L= 19, K=	130	0	27	3	46	47	40	2	212	212	34	1	75	34	47	L= 21, K=	121	120	31
7	79	77	33	1	135	130	27	4	45	45	43	0	27	24	52	3	234	225	35	0	60	60	35
L= 18, K=	3	3	33	2	532	526	29	5	93	96	32	1	99	98	29	L= 20, K=	293	285	39	2	245	250	35
1	168	173	30	3	106	108	33	6	323	326	42	1	34	31	49	L= 20, K=	4	4	31	3	41	86	34
3	36	38	48	4	66	64	33	L= 19, K=	98	98	29	2	34	31	34	1	97	93	42	1	97	93	34
4	82	86	32	5	34	37	35	0	97	91	31	2	59	56	49	2	43	32	31	3	41	86	34
5	271	268	37	6	240	233	32	1	184	186	29	3	413	416	46	3	60	57	35	L= 22, K=	216	219	34
L= 18, K=	4	4	37	7	163	154	32	2	244	245	35	4	172	166	32	L= 21, K=	278	278	35	0	282	286	33
0	171	170	31	L= 19, K=	1	78	30	4	59	52	37	L= 20, K=	1	1	46	1	281	275	37	1	137	141	33
1	138	137	29	0	76	78	30	5	92	91	32	1	50	55	39	2	35	37	37	3	114	115	31
2	116	119	30	1	192	190	30	6	242	240	36	3	177	173	39	3	55	54	35	L= 22, K=	372	372	45
3	168	162	30	2	261	264	35	L= 19, K=	93	92	31	4	304	299	39	0	191	191	32	0	261	258	37
4	164	130	31	4	78	79	29	1	373	366	45	5	33	3	45	1	154	153	37	1	36	32	54
5	131	130	31	5	109	109	29	2	93	82	31	L= 20, K=	2	2	37	2	264	257	37	2	114	117	31
L= 18, K=	5	5	37	6	261	259	29	3	62	66	39	0	49	60	37	L= 21, K=	49	41	39	1	114	117	31
1	255	260	37	7	33	34	56	4	62	66	39	1	75	82	34	1	49	41	39	1	114	117	31
2	95	96	32	L= 19, K=	2	2	56	L= 19, K=	5	5	39	2	75	82	34	1	49	41	39	1	114	117	31