

Status Primary QM: Star (S) Pressure/Temperature: Ambient Chemical Formula: Ca ( S O<sub>4</sub> )  
 Empirical Formula: Ca O<sub>4</sub> S Weight %: Ca29.44 O47.01 S23.55 Atomic %: Ca16.67 O66.67 S16.67  
 ANX: ABX4 Compound Name: Calcium Sulfate Mineral Name: anhydrite Common Name:  $\beta$ -Ca ( S O<sub>4</sub> )

Radiation: CuK $\alpha$ 1  $\lambda$ : 1.5406Å d-Spacing: Calculated Intensity: Calculated I/Ic: 1.73

SYS: Orthorhombic SPGR: Bmmb (63)

Author's Cell [ AuthCell a: 6.9920(10)Å AuthCell b: 6.9990(10)Å AuthCell c: 6.2400(10)Å

AuthCell Vol: 305.37Å<sup>3</sup> AuthCell Z: 4.00 AuthCell MolVol: 76.34 ]

Author's Cell Axial Ratio [ c/a: 0.892 a/b: 0.999 c/b: 0.892 ] Dcalc: 2.961g/cm<sup>3</sup> Dstruc: 2.96g/cm<sup>3</sup>

SS/FOM: F(30) = 96.7(0.0076, 41) R-factor: 0.021

Space Group: Bmmb (63) Molecular Weight: 136.14

Crystal Data [ XtlCell a: 6.992Å XtlCell b: 6.999Å XtlCell c: 6.240Å XtlCell  $\alpha$ : 90.00° XtlCell  $\beta$ : 90.00°

XtlCell  $\gamma$ : 90.00° XtlCell Vol: 305.37Å<sup>3</sup> XtlCell Z: 4.00 ]

Crystal Data Axial Ratio [ c/a: 0.892 a/b: 0.999 c/b: 0.892 ]

Reduced Cell [ RedCell a: 4.686Å RedCell b: 4.686Å RedCell c: 6.999Å RedCell  $\alpha$ : 90.00°

RedCell  $\beta$ : 90.00° RedCell  $\gamma$ : 96.51° RedCell Vol: 152.68Å<sup>3</sup> ]

TDP Type: B Crystal (Symmetry Allowed): Centrosymmetric

SG Symmetry Operators:

Seq	Operator	Seq	Operator	Seq	Operator	Seq	Operator
1	x,y,z	3	x,-y,-z	5	x,-y+1/2,z	7	x,y+1/2,-z
2	-x,-y,-z	4	-x,y,z	6	-x,y+1/2,-z	8	-x,-y+1/2,z

Atomic Coordinates:

Atom	Num	Wyckoff	Symmetry	x	y	z	SOF	IDP	AET
Ca	1	4c	mm2	0.0	0.25	0.3478	1.0	0.77611	8-d
S	2	4c	mm2	0.0	0.75	0.1556	1.0	0.69139	4-a
O	3	8g	.m.	0.17	0.75	0.0157	1.0	1.13528	1#a
O	4	8f	m..	0.0	0.5814	0.2972	1.0	1.102	1#a

Anisotropic Thermal Displacement Parameters:

Atom	Num	ADP11	ADP22	ADP33	ADP12	ADP13	ADP23
Ca	1	0.879986	0.646616	0.801765	0.0	0.0	0.0
S	2	0.703988	0.685804	0.684433	0.0	0.0	0.0
O	3	0.703988	1.64593	1.05598	0.0	0.191972	0.0
O	4	1.54486	0.627021	1.1342	0.0	0.0	0.174695

CAS: 7778-18-9 Pearson: oC24.00 LPF Prototype Structure: Ca [ S O<sub>4</sub> ],oS24,63

LPF Prototype Structure (Alpha Order): Ca O<sub>4</sub> S

Subfile(s): LPF Pattern, Common Phase, Inorganic, Pharmaceutical (Excipient), Primary Pattern, Cement and Hydration Product, Ceramic (Bioceramic), Forensic, Mineral Related (Mineral , Natural)

Entry Date: 01/05/2005 Last Modification Date: 01/13/2011 Former PDF's #: 01-070-0909

00-003-0162 (Deleted), 00-003-0163 (Deleted), 00-003-0368 (Alternate), 00-003-0377 (Deleted),  
 00-006-0226 (Deleted), 00-037-1496 (Primary), 01-071-4906 (Alternate), 01-072-0916 (Alternate),  
 Cross-Ref PDF #'s: 01-074-2421 (Alternate), 01-075-5972 (Deleted), 01-086-2270 (Alternate), ✓ 04-007-4744 (Alternate), ✓  
 04-007-9727 (Alternate), ✓ 04-008-0191 (Alternate), ✓ 04-008-2186 (Alternate), ✓ 04-013-4615  
 (Alternate), ✓ 04-013-4616 (Alternate), ✓ 04-013-4617 (Alternate)

#### References:

Type	Reference
Primary Reference	Calculated from LPF using POWD-12++.
Structure	"Anhydrite: a Refinement". Morikawa H., Minato I., Tomita T., Iwaj S. Acta Crystallogr., Sec. B: Struct. Crystallogr. Cryst. Chem. 31, 2164 (1975).

Database Comments: ANX: ABX4. LPF Collection Code: 1404662. Sample Source or Locality: Berchtesgaden, Germany.  
 Temperature Factor: Reported Anisotropic temperature factors (in Beta) were converted to B. Unit Cell  
 Data Source: Single Crystal.

#### d-Spacings (163) - 04-007-6682 (Fixed Slit Intensity) - Cu K $\alpha$ 1 1.54056Å

2 $\theta$	d(Å)	I	h	k	l	*	2 $\theta$	d(Å)	I	h	k	l	*	2 $\theta$	d(Å)	I	h	k	l	*
19.0470	4.655600	1	1	0	1		41.3172	2.183340	66	3	0	1		55.7376	1.647840	140	2	3	2	
22.9234	3.876350	50	1	1	1		43.3452	2.085770	66m	1	3	1		56.1060	1.637890	3	1	4	1	
25.4312	3.499500	999m	0	2	0		43.3452	2.085770	m	3	1	1		57.7885	1.594140	23	3	3	1	
25.4312	3.499500	m	2	0	0		45.4572	1.993650	47	1	0	3		59.0204	1.563770	33m	2	4	0	
28.5865	3.120000	23	0	0	2		46.8348	1.938170	33	2	2	2		59.0204	1.563770	m	4	2	0	
31.3647	2.849680	338	0	1	2		47.3735	1.917380	4	1	1	3		59.5184	1.551870	1	3	0	3	
31.9670	2.797350	32	1	2	1		48.6944	1.868410	144	0	3	2		60.6775	1.524970	27m	0	4	2	
36.2921	2.473280	80	2	2	0		49.1432	1.852390	32	3	2	1		60.6775	1.524970	m	4	0	2	
38.6474	2.327800	194m	0	2	2		52.2925	1.748000	72m	4	0	0		61.1162	1.515070	10m	1	3	3	
38.6474	2.327800	m	2	0	2		52.2925	1.748000	m	0	4	0		61.1162	1.515070	m	3	1	3	
40.8190	2.208830	217	2	1	2		52.8038	1.732270	3	1	2	3		62.2570	1.490020	50	4	1	2	

## 04-007-6682

Feb 4, 2013 10:19 AM (Doebelinn)

2 $\theta$	d(Å)	I	h	k	l	*
65.4625	1.424600	28m	0	2	4	
65.4625	1.424600	m	2	0	4	
65.7727	1.418630	9	3	2	3	
66.8333	1.398670	15m	2	4	2	
66.8333	1.398670	m	4	2	2	
66.9790	1.395980	21	2	1	4	
68.6861	1.365390	6m	5	0	1	
68.6861	1.365390	m	3	4	1	
70.1450	1.340520	1m	1	5	1	
70.1450	1.340520	m	5	1	1	
71.4343	1.319460	44	2	2	4	
71.7083	1.315090	2	1	4	3	
72.8806	1.296800	15	0	3	4	
73.1874	1.292120	1	3	3	3	
74.2341	1.276470	54m	0	5	2	
74.2341	1.276470	m	4	3	2	
74.5858	1.271320	2	5	2	1	
77.0537	1.236640	9	4	4	0	
77.6535	1.228580	1	1	0	5	
78.6224	1.215850	34	2	3	4	
79.0705	1.210080	1	1	1	5	
79.8985	1.199610	19	2	5	2	
81.6817	1.177870	3m	3	5	1	
81.6817	1.177870	m	5	3	1	
82.6508	1.166500	20	0	6	0	
82.7520	1.165330	21m	0	4	4	
82.7520	1.165330	m	6	0	0	
82.8760	1.163900	13	4	0	4	
83.1719	1.160510	6m	3	4	3	
83.1719	1.160510	m	5	0	3	
83.2851	1.159220	4	1	2	5	
84.1379	1.149630	4	4	4	2	
84.2731	1.148130	9	4	1	4	
84.5013	1.145610	1m	1	5	3	
84.5013	1.145610	m	5	1	3	
85.8042	1.131520	1	1	6	1	
88.2334	1.106530	20	2	6	0	
88.4459	1.104420	38m	2	4	4	
88.4459	1.104420	m	4	2	4	
88.8744	1.100200	3	3	0	5	
89.6555	1.092630	2m	0	6	2	
89.6555	1.092630	m	6	0	2	
90.2406	1.087060	1m	1	3	5	
90.2406	1.087060	m	3	1	5	

2 $\theta$	d(Å)	I	h	k	l	*
91.1436	1.078630	16	6	1	2	
91.4264	1.076030	1	5	4	1	
94.4312	1.049550	1	3	2	5	
95.2260	1.042880	11	2	6	2	
95.3937	1.041490	18m	4	3	4	
95.3937	1.041490	m	0	5	4	
95.5743	1.040000	8m	0	0	6	
95.5743	1.040000	m	3	5	3	
96.6542	1.031230	12	4	5	2	
96.9512	1.028860	4m	3	6	1	
96.9512	1.028860	m	0	1	6	
99.8251	1.006820	3	1	6	3	
100.0067	1.005480	2	1	4	5	
100.9715	0.998462	6	2	5	4	
101.1884	0.996908	15m	0	2	6	
101.1884	0.996908	m	2	0	6	
102.3424	0.988777	19	6	3	2	
102.6182	0.986868	8m	2	1	6	
102.6182	0.986868	m	7	0	1	
104.0586	0.977109	1m	5	5	1	
104.0586	0.977109	m	7	1	1	
105.0968	0.970288	16m	4	6	0	
105.0968	0.970288	m	6	4	0	
105.2824	0.969087	13	4	4	4	
106.9255	0.958692	8	2	2	6	
107.9933	0.952159	5	0	7	2	
108.4667	0.949317	1m	0	3	6	
108.4667	0.949317	m	7	2	1	
111.0817	0.934205	2	0	6	4	
111.1891	0.933605	1	6	0	4	
111.5893	0.931383	1m	3	4	5	
111.5893	0.931383	m	5	0	5	
112.4796	0.926518	6m	4	6	2	
112.4796	0.926518	m	6	4	2	
112.6853	0.925409	3	6	1	4	
113.1383	0.922987	1m	1	5	5	
113.1383	0.922987	m	5	1	5	
113.9536	0.918695	8	2	7	2	
114.3463	0.916659	1	2	3	6	
115.9684	0.908454	1m	3	7	1	
115.9684	0.908454	m	7	3	1	
117.1802	0.902537	8m	2	6	4	
117.1802	0.902537	m	6	2	4	
117.6239	0.900415	1	7	0	3	

2 $\theta$	d(Å)	I	h	k	l	*
117.7506	0.899813	1	5	2	5	
118.7899	0.894949	5	4	5	4	
118.9948	0.894005	11m	0	4	6	
118.9948	0.894005	m	4	0	6	
120.6458	0.886572	5m	5	6	1	
120.6458	0.886572	m	4	1	6	
121.1712	0.884271	1	1	0	7	
122.8077	0.877297	1	1	1	7	
123.3924	0.874875	3	0	8	0	
123.6058	0.874000	3	8	0	0	
124.0947	0.872013	1	7	2	3	
125.4130	0.866779	9	6	3	4	
125.6198	0.865974	14m	2	4	6	
125.6198	0.865974	m	4	2	6	
126.9664	0.860837	9	6	5	2	
127.9154	0.857324	1	1	2	7	
130.3506	0.848703	3	2	8	0	
130.5699	0.847954	3	8	2	0	
131.1669	0.845937	1	1	6	5	
132.4835	0.841603	4m	0	7	4	
132.4835	0.841603	m	8	0	2	
132.8235	0.840509	1m	7	3	3	
132.8235	0.840509	m	3	7	3	
134.2089	0.836156	9	4	7	2	
134.3953	0.835583	9	8	1	2	
134.6481	0.834811	3m	0	5	6	
134.6481	0.834811	m	4	3	6	
135.3800	0.832606	1	3	0	7	
138.2377	0.824427	12	6	6	0	
138.4233	0.823919	10m	4	6	4	
138.4233	0.823919	m	6	4	4	
138.8676	0.822714	2	5	6	3	
139.1409	0.821981	1	5	4	5	
140.5078	0.818403	6m	2	7	4	
140.5078	0.818403	m	8	2	2	
143.1150	0.811982	6m	3	8	1	
143.1150	0.811982	m	2	5	6	
143.9671	0.809996	2	3	2	7	
145.6362	0.806262	1m	5	7	1	
145.6362	0.806262	m	7	5	1	
148.4782	0.800371	2m	3	6	5	
148.4782	0.800371	m	7	4	3	