Entry # 96-155-0389

Phase classification

Name	Potassium aluminium silicate
Formula	$AlKO_4Si$
I/Ic	1.090000
Sample Name	1550388
Quality	C (calculated)

References

Publication

Bibliography	Gregorkiewitz M, "Synthese und charakterisierung por\"oser silicate", PhD Thesis, TU Darmstadt 1-792 (1980).

Origin of data

Source of entry	COD (Crystallography Open Database)
Link to orig. entry	1550388

Crystal structure

Crystallographic data

Space group	P n 21 m (31)
Crystal system	orthorhombic
Cell parameters	a= 15.67000 Å b= 9.07000 Å c= 8.56000 Å
Z	12

Atom coordinates

Element	Oxid.	*x*	*y*	*z*	Bi	Focc
K		-0.294	0.023	0.000	1.437000	1.000000
K		-0.210	-0.039	0.500	1.437000	1.000000
K		0.062	-0.008	0.500	1.973000	1.000000
K		0.109	0.006	0.000	1.973000	1.000000
K		0.397	-0.024	0.500	1.058000	1.000000
K		0.452	-0.019	0.000	1.058000	1.000000
Al		-0.276	0.334	0.311	0.363000	1.000000
Al		-0.114	0.158	0.192	0.363000	1.000000
Al		0.054	0.325	0.307	0.363000	1.000000
Al		0.231	0.168	0.310	0.363000	1.000000
Al		0.401	0.314	0.189	0.363000	1.000000
Al		0.564	0.144	0.309	0.363000	1.000000
O		-0.204	0.197	0.288	1.018000	1.000000
O		-0.038	0.284	0.219	1.018000	1.000000
O		0.128	0.198	0.250	1.018000	1.000000
O		0.297	0.274	0.207	1.018000	1.000000
O		0.460	0.186	0.278	1.018000	1.000000
O		0.630	0.273	0.239	1.018000	1.000000
O		-0.082	-0.009	0.256	1.042000	1.000000
O		0.248	-0.015	0.286	1.042000	1.000000
O		0.581	-0.023	0.227	1.042000	1.000000
O		-0.284	0.381	0.500	1.318000	1.000000
O		-0.136	0.154	0.000	1.318000	1.000000
O		0.037	0.327	0.500	1.318000	1.000000
O		0.245	0.208	0.500	1.318000	1.000000
O		0.430	0.311	0.000	1.318000	1.000000
O		0.582	0.132	0.500	1.318000	1.000000

Diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
15.6700	17.5	1	0	0	2
7.8499	0.5	1	1	0	4
7.8350	4.2	2	0	0	2
7.5122	0.0	1	0	1	4
6.2253	33.8	0	1	1	4
5.9291	0.7	2	1	0	4
5.7855	21.6	1	1	1	8
5.7795	98.9	2	0	1	4
5.2233	0.4	3	0	0	2
4.8741	10.7	2	1	1	8
4.5350	15.0	0	2	0	2
4.5264	51.8	3	1	0	4
4.4588	0.2	3	0	1	4
4.3562	0.9	1	2	0	4
4.2800	200.6	0	0	2	2
4.1288	1.1	1	0	2	4

4.0014	4.2	3	1	1	8
3.9249	7.0	2	2	0	4
3.9175	0.0	4	0	0	2
3.8824	144.3	1	2	1	8
3.7577	0.0	1	1	2	8
3.7561	0.0	2	0	2	4
3.5964	8.5	4	1	0	4
3.5678	226.8	2	2	1	8
3.5622	187.1	4	0	1	4
3.4703	3.3	2	1	2	8
3.4244	273.3	3	2	0	4
3.3156	129.5	4	1	1	8
3.3106	0.3	3	0	2	4
3.1794	83.5	3	2	1	8
3.1340	0.1	5	0	0	2
3.1127	667.0	0	2	2	4
3.1099	1000.0	3	1	2	8
3.0530	1.9	1	2	2	8
2.9686	20.8	1	3	0	4
2.9646	15.0	4	2	0	4
2.9622	31.6	5	1	0	4
2.9430	0.0	5	0	1	4
2.8927	0.9	2	2	2	8
2.8898	0.0	4	0	2	4
2.8507	4.5	0	3	1	4
2.8206	18.4	2	3	0	4
2.8072	0.3	1	0	3	4
2.8047	163.5	1	3	1	8
2.8013	29.3	4	2	1	8
2.7993	278.0	5	1	1	8
2.7534	0.1	4	1	2	8
2.7218	18.4	0	1	3	4
2.6817	30.7	1	1	3	8
2.6811	95.2	2	0	3	4
2.6789	18.4	2	3	1	8
2.6739	127.8	3	2	2	8
2.6166	344.8	3	3	0	4
2.6117	228.4	6	0	0	2
2.5782	8.5	5	2	0	4
2.5711	11.7	2	1	3	8
2.5286	0.4	5	0	2	4
2.5097	14.2	6	1	0	4
2.5041	3.7	3	0	3	4
2.5023	14.4	3	3	1	8
2.4980	29.4	6	0	1	4
2.4687	0.7	5	2	1	8
2.4393	4.6	1	3	2	8
2.4370	7.0	4	2	2	8
2.4357	9.7	5	1	2	8
2.4138	25.6	3	1	3	8
2.4083	23.3	6	1	1	8
2.3934	7.2	4	3	0	4
2.3869	25.3	1	2	3	8
2.3552	15.2	2	3	2	8
2.3079	2.8	2	2	3	8
2.3064	6.8	4	0	3	4
2.3050	0.8	4	3	1	8
2.2675	33.0	0	4	0	2
2.2632	11.0	6	2	0	4
2.2441	0.8	1	4	0	4
2.2386	9.1	7	0	0	2
2.2353	58.6	4	1	3	8
2.2325	129.7	3	3	2	8
2.2294	13.9	6	0	2	4
2.2085	3.1	5	2	2	8
2.1921	19.2	3	2	3	8
2.1880	22.2	6	2	1	8
2.1781	6.5	2	4	0	4
2.1759	6.9	5	3	0	4
2.1734	6.2	7	1	0	4
2.1708	5.8	1	4	1	8
2.1657	0.3	7	0	1	4
2.1649	9.5	6	1	2	8
2.1400	233.9	0	0	4	2
2.1203	0.0	1	0	4	4

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2.1065	50.0	7	1	1	8
2.0890	1.4	4	3	2	8
2.0800	108.5	3	4	0	4
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2.0644	1.9	2	0	4	4
2.0571	23.0	1	3	3	8
2.0558	49.7	4	2	3	8
2.0550	16.0	5	1	3	8
2.0212	2.3	3	4	1	8
2.0129	2.8	2	1	4	8
2.0073	2.2	7	2	0	4
2.0059	2.9	2	3	3	8
2.0037	15.4	0	4	2	4
2.0007	2.2	6	2	2	8
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1.9836	0.1	7	0	2	4
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1.9764	35.2	6	3	0	4
1.9625	0.9	4	4	0	4
1.9588	2.7	8	0	0	2
1.9543	8.0	7	2	1	8
1.9412	1.9	2	4	2	8
1.9396	8.3	5	3	2	8
1.9378	4.3	7	1	2	8
1.9353	16.6	0	2	4	4
1.9347	15.2	3	1	4	8
1.9285	4.3	3	3	3	8
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1.9257	1.2	6	3	1	8
1.9207	0.1	1	2	4	8
1.9146	2.0	8	1	0	4
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1.8174	0.5	7	2	2	8
1.8148	7.7	3	2	4	8
1.8020	2.3	1	5	0	4
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1.7633	0.5	1	5	1	8
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1.6725	17.8	2	0	5	4
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1.6553	19.0	6	0	4	4
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1.6461	2.1	4	5	0	4
1.6448	2.2	2	1	5	8
1.6439	5.2	8	3	0	4
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1.6013	1.2	3	1	5	8
1.5969	12.5	9	2	1	8
1.5953	1.1	4	3	4	8
1.5934	23.0	1	2	5	8
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1.5908	49.4	3	5	2	8
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1.5441	5.4	10	1	0	4
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1.5313	18.2	3	2	5	8
1.5308	3.0	0	5	3	4
1.5265	0.8	2	4	4	8
1.5257	2.2	5	3	4	8
1.5249	1.6	7	1	4	8
1.5236	5.0	1	5	3	8
1.5218	8.4	7	3	3	8
1.5213	1.7	8	2	3	8
1.5196	6.4	10	1	1	8
1.5195	48.8	9	2	2	8
1.5117	73.4	0	6	0	2
1.5088	2.3	9	3	0	4
1.5047	3.9	1	6	0	4
1.5024	0.4	5	0	5	4
1.5024	0.8	2	5	3	8
1.4930	1.7	7	4	2	8
1.4915	13.1	3	4	4	8
1.4899	22.9	6	5	0	4

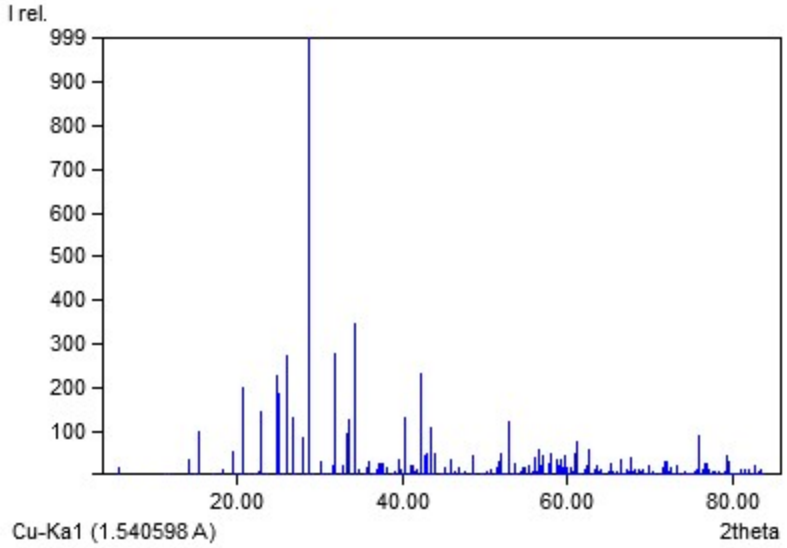
1.4897	1.1	0	3	5	4
1.4863	7.4	9	0	3	4
1.4859	17.9	9	3	1	8
1.4843	8.4	2	6	0	4
1.4830	55.7	1	3	5	8
1.4825	0.1	4	2	5	8
1.4823	2.7	8	4	0	4
1.4822	43.0	5	1	5	8
1.4820	2.9	1	6	1	8
1.4811	2.3	10	2	0	4
1.4739	0.7	5	5	2	8
1.4715	1.7	10	0	2	4
1.4690	1.3	3	5	3	8
1.4682	10.2	6	4	3	8
1.4678	4.5	6	5	1	8
1.4667	12.7	9	1	3	8
1.4641	1.2	7	2	4	8
1.4635	3.8	2	3	5	8
1.4625	4.9	2	6	1	8
1.4605	18.7	8	4	1	8
1.4594	5.6	10	2	1	8
1.4525	0.4	10	1	2	8
1.4521	1.9	3	6	0	4
1.4519	10.9	6	3	4	8
1.4464	0.7	4	4	4	8
1.4449	1.2	8	0	4	4
1.4326	6.2	3	3	5	8
1.4318	8.7	6	0	5	4
1.4316	1.1	3	6	1	8
1.4269	0.7	8	1	4	8
1.4267	24.1	0	0	6	2
1.4262	1.1	5	2	5	8
1.4258	17.1	4	5	3	8
1.4254	5.5	0	6	2	4
1.4245	2.1	11	0	0	2
1.4244	1.7	8	3	3	8
1.4230	6.0	9	3	2	8
1.4208	0.3	1	0	6	4
1.4195	0.1	1	6	2	8
1.4143	7.1	6	1	5	8
1.4123	0.9	9	2	3	8
1.4103	1.9	4	6	0	4
1.4094	1.7	7	5	0	4
1.4073	0.9	11	1	0	4
1.4071	32.7	6	5	2	8
1.4052	0.2	11	0	1	4
1.4037	0.0	1	1	6	8
1.4036	0.3	2	0	6	4
1.4024	1.7	2	6	2	8
1.4007	1.8	8	4	2	8
1.3996	4.0	10	2	2	8
1.3939	1.4	5	4	4	8
1.3925	0.4	4	3	5	8
1.3916	10.1	4	6	1	8
1.3912	3.0	10	3	0	4
1.3909	9.1	7	4	3	8
1.3906	3.7	7	5	1	8
1.3887	8.3	11	1	1	8
1.3871	0.5	2	1	6	8
1.3810	37.8	9	4	0	4
1.3784	0.5	1	5	4	8
1.3771	0.3	7	3	4	8
1.3767	4.6	8	2	4	8
1.3763	0.0	3	0	6	4
1.3755	0.4	5	5	3	8
1.3751	12.2	3	6	2	8
1.3735	7.5	10	0	3	4
1.3732	0.8	10	3	1	8
1.3654	9.4	6	2	5	8
1.3633	2.9	9	4	1	8
1.3627	2.6	2	5	4	8
1.3616	7.2	5	6	0	4
1.3611	7.2	1	4	5	8
1.3609	1.7	0	2	6	4
1.3607	2.8	3	1	6	8

1.3599	0.2	7	0	5	4
1.3591	1.6	11	2	0	4
1.3580	11.9	10	1	3	8
1.3558	0.1	1	2	6	8
1.3516	0.2	11	0	2	4
1.3506	0.1	9	0	4	4
1.3460	20.1	2	4	5	8
1.3455	10.8	5	3	5	8
1.3449	10.3	7	1	5	8
1.3447	2.2	5	6	1	8
1.3423	2.7	11	2	1	8
1.3408	0.2	2	2	6	8
1.3405	0.6	4	0	6	4
1.3395	1.8	4	6	2	8
1.3387	1.5	7	5	2	8
1.3376	8.2	3	5	4	8
1.3369	6.5	6	4	4	8
1.3369	1.1	11	1	2	8
1.3358	7.2	9	1	4	8
1.3338	0.5	9	3	3	8
1.3310	0.9	1	6	3	8
1.3309	2.4	8	5	0	4
1.3261	0.4	4	1	6	8
1.3231	1.7	10	3	2	8
1.3218	0.2	3	4	5	8
1.3207	1.1	6	5	3	8
1.3169	1.8	3	2	6	8
1.3168	16.2	2	6	3	8
1.3154	1.3	8	4	3	8
1.3151	2.0	8	5	1	8
1.3145	0.7	10	2	3	8
1.3142	30.4	9	4	2	8
1.3083	29.3	6	6	0	4
1.3058	6.6	12	0	0	2
1.3047	1.2	4	5	4	8
1.3037	1.5	8	3	4	8
1.3026	15.5	7	2	5	8
1.2985	0.0	5	0	6	4
1.2975	2.4	5	6	2	8
1.2953	0.5	11	2	2	8
1.2944	1.3	9	2	4	8
1.2941	3.8	3	6	3	8
1.2940	0.5	6	3	5	8
1.2933	4.3	6	6	1	8
1.2925	20.5	12	1	0	4
1.2913	0.4	1	7	0	4
1.2909	7.6	12	0	1	4
1.2901	1.2	4	4	5	8
1.2891	1.1	10	4	0	4
1.2890	0.1	8	0	5	4
1.2887	0.3	11	3	0	4
1.2859	2.4	1	3	6	8
1.2856	1.2	4	2	6	8
1.2854	2.3	5	1	6	8
1.2811	2.2	0	7	1	4
1.2784	0.2	2	7	0	4
1.2780	3.9	12	1	1	8
1.2779	0.9	7	4	4	8
1.2769	0.5	1	7	1	8
1.2762	5.3	8	1	5	8
1.2747	2.6	10	4	1	8
1.2745	0.0	11	0	3	4
1.2743	1.8	11	3	1	8
1.2731	4.1	2	3	6	8
1.2709	3.2	8	5	2	8
1.2659	0.6	5	5	4	8
1.2643	1.4	2	7	1	8
1.2643	0.2	4	6	3	8
1.2643	0.1	10	0	4	4
1.2636	0.9	7	5	3	8
1.2621	2.5	11	1	3	8
1.2576	8.4	3	7	0	4
1.2561	12.8	9	5	0	4
1.2548	2.2	12	2	0	4
1.2528	0.8	7	6	0	4

1.2526	89.6	3	3	6	8
1.2525	3.8	5	4	5	8
1.2522	1.4	10	1	4	8
1.2520	8.7	6	0	6	4
1.2512	8.8	6	6	2	8
1.2505	1.9	10	3	3	8
1.2490	0.0	12	0	2	4
1.2483	0.2	5	2	6	8
1.2451	11.9	0	5	5	4
1.2442	0.3	3	7	1	8
1.2430	1.4	9	4	3	8
1.2428	3.2	9	5	1	8
1.2416	2.9	12	2	1	8
1.2412	1.5	1	5	5	8
1.2403	22.9	6	1	6	8
1.2402	7.7	7	3	5	8
1.2399	20.2	8	2	5	8
1.2396	0.8	7	6	1	8
1.2373	24.9	12	1	2	8
1.2363	0.4	1	7	2	8
1.2347	12.3	0	6	4	4
1.2343	0.1	10	4	2	8
1.2339	0.9	11	3	2	8
1.2331	0.1	9	3	4	8
1.2309	1.1	1	6	4	8
1.2302	1.1	4	7	0	4
1.2296	5.0	2	5	5	8
1.2288	0.7	5	6	3	8
1.2270	6.9	11	2	3	8
1.2255	0.7	4	3	6	8
1.2249	4.3	2	7	2	8
1.2227	0.2	6	5	4	8
1.2207	6.7	9	0	5	4
1.2196	3.8	2	6	4	8
1.2192	0.0	1	0	7	4
1.2185	0.6	8	4	4	8
1.2179	3.0	10	2	4	8
1.2177	3.0	4	7	1	8
1.2119	0.5	0	1	7	4
1.2111	2.6	3	5	5	8
1.2106	4.8	6	4	5	8
1.2098	0.0	9	1	5	8
1.2083	0.8	1	1	7	8
1.2082	1.8	2	0	7	4
1.2075	0.3	0	4	6	4
1.2069	1.5	6	2	6	8
1.2066	44.2	3	7	2	8
1.2062	0.0	11	4	0	4
1.2062	2.9	8	5	3	8
1.2054	0.4	13	0	0	2
1.2053	11.9	9	5	2	8
1.2042	31.8	12	2	2	8
1.2040	0.0	1	4	6	8
1.2031	1.4	7	0	6	4
1.2023	1.7	7	6	2	8
1.2016	0.7	3	6	4	8
1.1988	0.3	12	3	0	4
1.1977	0.4	2	1	7	8
1.1974	1.5	5	7	0	4
1.1967	1.2	8	6	0	4
1.1949	2.0	13	1	0	4
1.1944	1.1	11	4	1	8
1.1936	0.2	13	0	1	4
1.1934	0.6	2	4	6	8
1.1931	1.2	5	3	6	8
1.1927	1.2	7	1	6	8
1.1907	0.6	3	0	7	4
1.1893	0.3	6	6	3	8
1.1874	0.1	12	0	3	4
1.1872	0.5	12	3	1	8
1.1866	12.3	4	5	5	8
1.1859	3.0	5	7	1	8
1.1858	0.2	11	0	4	4
1.1858	0.7	10	5	0	4
1.1858	2.6	8	3	5	8

1.1852	0.9	8	6	1	8
1.1834	0.7	13	1	1	8
1.1823	0.3	4	7	2	8
1.1805	2.0	3	1	7	8
1.1798	6.4	0	7	3	4
1.1788	9.7	9	2	5	8
1.1776	0.5	4	6	4	8
1.1773	0.9	1	2	7	8
1.1773	0.4	12	1	3	8
1.1770	1.1	7	5	4	8
1.1765	1.9	3	4	6	8
1.1764	1.9	1	7	3	8
1.1758	0.2	11	1	4	8
1.1748	0.6	10	4	3	8
1.1746	0.6	10	5	1	8
1.1744	11.7	11	3	3	8
1.1675	0.0	2	2	7	8
1.1673	0.7	4	0	7	4
1.1666	5.0	2	7	3	8
1.1664	0.2	10	3	4	8
1.1662	22.3	7	4	5	8
1.1649	1.0	13	2	0	4
1.1629	0.1	7	2	6	8
1.1610	0.2	11	4	2	8
1.1607	8.1	6	7	0	4
1.1603	2.2	9	4	4	8
1.1602	0.8	13	0	2	4
1.1578	2.5	4	1	7	8
1.1571	9.8	5	5	5	8
1.1568	0.1	6	3	6	8
1.1559	0.3	10	0	5	4
1.1544	0.1	12	3	2	8
1.1543	0.2	13	2	1	8
1.1540	0.1	4	4	6	8

Diffraction pattern graphics



Experimental

Physical Properties

Meas. density	2.57200 g/cm³
Calc. density	2.59100 g/cm³

Remarks

Remarks

Comments	- synthetic - Diffraction pattern calculated by Match!. - I/Ic calculated by Match!. - Space group has been derived from given symmetry operations.

Entry # 96-154-0706

Phase classification

Name	Ca3 (Si O4) O
Mineral Name	Alite
Formula	Ca_3O_5Si
I/Ic	0.730000
Sample Name	1540705
Quality	C (calculated)

References

Publication

Bibliography	de la Torre A.G., Bruque S., Campo J., Aranda M.A.G., "The superstructure of C3S from synchrotron and neutron powder diffractionand its role in quantitative phase analyses", Cement and Concrete Research **32**, 1347-1356 (2002).

Origin of data

Source of entry	COD (Crystallography Open Database)
Link to orig. entry	1540705

Crystal structure

Crystallographic data

Space group	C 1 m 1 (8)
Crystal system	monoclinic
Cell parameters	a= 33.10780 Å b= 7.03550 Å c= 18.52110 Å β= 94.137 º
Z	36

Atom coordinates

Element	Oxid.	*x*	*y*	*z*	Bi	Focc
O		0.698	0.000	0.298	1.000000	1.000000
O		0.031	0.000	0.602	1.000000	1.000000
O		0.130	0.188	0.669	1.000000	0.590000
Ca		0.724	0.000	0.402	1.000000	1.000000
O		0.130	0.875	0.213	1.000000	0.500000
O		0.428	0.179	0.204	1.000000	1.000000
O		0.138	0.030	0.088	1.000000	0.500000
O		0.513	0.000	0.423	1.000000	1.000000
O		0.562	0.000	0.153	1.000000	0.410000
Ca		-0.012	0.000	0.494	1.000000	1.000000
Si		0.567	0.000	0.243	1.000000	1.000000
O		0.434	0.190	0.793	1.000000	1.000000
O		0.331	0.000	0.084	1.000000	1.000000
O		0.539	0.187	0.255	1.000000	0.590000
Si		-0.098	0.000	0.077	1.000000	1.000000
Ca		0.402	0.000	0.078	1.000000	1.000000
Si		0.825	0.000	0.334	1.000000	1.000000
Ca		0.667	0.232	0.015	1.000000	0.500000
Ca		0.585	0.281	0.092	1.000000	0.500000
O		0.447	0.000	0.328	1.000000	1.000000
Ca		0.155	0.271	0.821	1.000000	0.500000
Ca		0.661	0.229	0.520	1.000000	0.500000
O		0.094	0.186	0.474	1.000000	1.000000
O		0.586	0.000	0.166	1.000000	0.590000
O		0.219	0.179	0.876	1.000000	1.000000
O		0.793	0.844	0.363	1.000000	0.500000
Ca		0.259	0.000	0.101	1.000000	1.000000
O		0.200	0.864	0.154	1.000000	0.500000
Ca		0.483	0.277	0.657	1.000000	0.500000
Si		0.895	0.000	0.574	1.000000	1.000000
O		0.283	0.000	0.222	1.000000	1.000000
Ca		-0.002	0.218	0.847	1.000000	0.500000
Ca		0.666	0.241	0.019	1.000000	0.500000
O		0.366	0.000	-0.067	1.000000	1.000000
O		0.769	0.000	0.506	1.000000	1.000000
Ca		0.241	0.257	0.258	1.000000	0.500000
Ca		0.331	0.240	0.681	1.000000	0.500000
O		0.781	0.187	0.083	1.000000	1.000000
O		0.034	0.000	0.122	1.000000	1.000000
Ca		0.813	0.260	0.493	1.000000	0.500000
Ca		0.249	0.000	0.606	1.000000	1.000000

Ca	0.156	0.272	0.821	1.000000	0.500000
Si	0.233	0.000	-0.073	1.000000	1.000000
Ca	0.827	0.264	-0.009	1.000000	0.500000
O	0.372	0.000	0.739	1.000000	1.000000
O	0.219	0.193	0.376	1.000000	0.590000
O	0.538	0.000	0.832	1.000000	1.000000
Ca	-0.082	0.000	0.765	1.000000	1.000000
Ca	0.339	0.222	0.182	1.000000	0.500000
Ca	-0.097	0.265	0.413	1.000000	0.500000
O	0.804	0.000	-0.080	1.000000	1.000000
Ca	0.335	0.235	0.172	1.000000	0.500000
O	0.110	0.000	0.648	1.000000	0.410000
O	0.940	0.000	0.387	1.000000	1.000000
O	0.876	0.000	0.149	1.000000	1.000000
O	0.479	0.000	0.076	1.000000	1.000000
Si	0.418	0.000	0.255	1.000000	1.000000
O	0.436	0.000	0.471	1.000000	1.000000
O	0.883	0.189	0.527	1.000000	1.000000
O	0.765	0.184	0.633	1.000000	1.000000
Ca	0.244	0.241	0.762	1.000000	0.500000
O	-0.050	0.000	0.107	1.000000	1.000000
O	0.893	0.190	0.030	1.000000	1.000000
O	0.603	0.000	0.305	1.000000	0.590000
Ca	0.311	0.000	0.334	1.000000	1.000000
Ca	0.580	0.277	0.084	1.000000	0.500000
O	0.286	0.000	0.723	1.000000	1.000000
O	0.615	0.000	0.550	1.000000	1.000000
O	0.113	0.000	0.833	1.000000	1.000000
O	0.370	0.000	0.268	1.000000	1.000000
Si	0.159	0.000	0.662	1.000000	1.000000
O	0.105	0.000	0.352	1.000000	1.000000
Si	0.560	0.000	0.758	1.000000	1.000000
O	0.210	0.000	0.001	1.000000	1.000000
Si	0.421	0.000	0.747	1.000000	1.000000
O	0.173	0.191	0.211	1.000000	0.500000
O	0.442	0.000	0.671	1.000000	1.000000
Ca	0.588	0.000	-0.074	1.000000	1.000000
Ca	0.151	0.254	0.329	1.000000	0.500000
O	0.240	0.000	0.342	1.000000	0.410000
O	0.662	0.000	-0.084	1.000000	1.000000
Ca	0.240	0.250	0.258	1.000000	0.500000
Ca	-0.083	0.275	-0.085	1.000000	0.500000
Ca	0.062	0.000	0.736	1.000000	1.000000
Ca	-0.082	0.000	0.262	1.000000	1.000000
O	0.864	0.867	0.315	1.000000	0.500000
O	0.701	0.000	0.770	1.000000	1.000000
O	0.956	0.000	0.903	1.000000	1.000000
Ca	0.331	0.236	0.677	1.000000	0.500000
O	-0.010	0.000	0.749	1.000000	1.000000
Si	0.224	0.000	0.424	1.000000	1.000000
O	0.809	0.191	0.799	1.000000	1.000000
Ca	0.490	0.260	0.159	1.000000	0.500000
O	0.992	0.000	0.252	1.000000	1.000000
O	0.702	0.000	0.579	1.000000	1.000000
Ca	0.576	0.250	0.597	1.000000	0.500000
Ca	0.653	0.000	0.665	1.000000	1.000000
O	0.548	0.193	0.272	1.000000	0.410000
O	0.352	0.000	0.444	1.000000	1.000000
O	0.609	0.000	0.770	1.000000	1.000000
O	0.178	0.000	0.583	1.000000	0.590000
Ca	0.585	0.000	0.426	1.000000	1.000000
O	0.200	0.192	0.430	1.000000	0.410000
O	0.873	0.000	0.859	1.000000	1.000000
Ca	0.065	0.000	0.242	1.000000	1.000000
Ca	0.814	0.261	0.500	1.000000	0.500000
O	0.195	0.000	0.726	1.000000	0.590000
O	0.471	0.000	-0.070	1.000000	1.000000
Si	0.824	0.000	0.842	1.000000	1.000000
O	0.533	0.184	0.003	1.000000	1.000000
O	0.264	0.000	0.478	1.000000	0.590000
O	-0.057	0.000	0.592	1.000000	1.000000
O	0.494	0.193	0.536	1.000000	1.000000
O	0.264	0.000	0.481	1.000000	0.410000
O	0.872	0.000	0.649	1.000000	1.000000
Ca	0.150	0.254	0.329	1.000000	0.500000

O	0.176	0.185	0.705	1.000000	0.410000
O	0.617	0.000	0.041	1.000000	1.000000
Ca	0.659	0.000	0.161	1.000000	1.000000
O	0.844	0.123	0.400	1.000000	0.500000
Ca	0.565	0.223	0.572	1.000000	0.500000
O	0.654	0.000	0.425	1.000000	1.000000
Si	0.751	0.000	0.584	1.000000	1.000000
O	0.714	0.000	0.032	1.000000	1.000000
Ca	-0.005	0.235	0.346	1.000000	0.500000
Ca	-0.084	0.275	-0.085	1.000000	0.500000
O	0.033	0.000	0.410	1.000000	1.000000
Si	0.092	0.000	-0.089	1.000000	1.000000
O	0.281	0.000	-0.053	1.000000	1.000000
Si	0.484	0.000	0.491	1.000000	1.000000
O	0.616	0.000	0.260	1.000000	0.410000
Si	0.082	0.000	0.425	1.000000	1.000000
Ca	-0.094	0.293	0.410	1.000000	0.500000
Si	0.753	0.000	0.091	1.000000	1.000000
Ca	-0.002	0.000	0.010	1.000000	1.000000
Ca	0.732	0.000	-0.092	1.000000	1.000000
Ca	-0.000	0.232	0.842	1.000000	0.500000
O	0.735	0.000	0.171	1.000000	1.000000
Ca	-0.005	0.238	0.344	1.000000	0.500000
O	0.107	0.187	-0.046	1.000000	1.000000
O	0.043	0.000	0.897	1.000000	1.000000
Ca	0.657	0.218	0.522	1.000000	0.500000
Ca	0.826	0.270	-0.011	1.000000	0.500000
O	0.803	0.092	0.262	1.000000	0.500000
O	0.180	0.000	0.584	1.000000	0.410000
Ca	0.390	0.000	0.573	1.000000	1.000000
Ca	0.491	0.257	0.160	1.000000	0.500000
Ca	0.482	0.266	0.656	1.000000	0.500000
Si	0.502	0.000	0.000	1.000000	1.000000
Ca	0.244	0.250	0.752	1.000000	0.500000
O	0.187	0.000	0.480	1.000000	0.590000
Ca	0.319	0.000	0.841	1.000000	1.000000
O	0.325	0.000	0.593	1.000000	1.000000
O	0.546	0.182	0.709	1.000000	1.000000
Si	0.162	0.000	0.168	1.000000	1.000000

Diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
18.4728	1.5	0	0	1	2
16.5108	5.0	2	0	0	2
12.7768	0.1	2	0	-1	2
11.8915	1.5	2	0	1	2
9.2364	1.3	0	0	2	2
8.3206	2.0	2	0	-2	2
8.2554	0.5	4	0	0	2
7.8239	0.4	2	0	2	2
7.7481	3.7	4	0	-1	2
7.3423	0.5	4	0	1	2
6.8811	3.2	1	1	0	4
6.4802	0.0	1	1	-1	4
6.4167	0.4	1	1	1	4
6.3884	3.0	4	0	-2	2
6.1576	1.0	0	0	3	2
5.9457	36.7	4	0	2	2
5.9280	77.0	3	1	0	4
5.9107	0.6	-2	0	3	2
5.7094	0.8	3	1	-1	4
5.6378	1.5	2	0	3	2
5.5818	3.0	3	1	1	4
5.5583	1.4	-1	1	2	4
5.5036	9.8	6	0	0	2
5.4788	24.1	1	1	2	4
5.3818	1.8	6	0	-1	2
5.1733	3.3	6	0	1	2
5.1159	0.4	4	0	-3	2
5.0794	1.4	3	1	-2	4
4.9031	1.4	3	1	2	4
4.8854	1.1	6	0	-2	2
4.8152	1.3	5	1	0	4

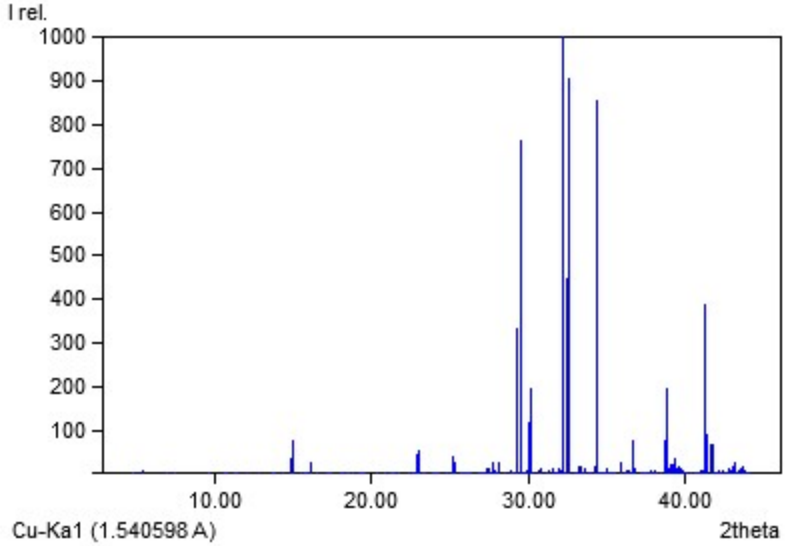
4.7735	0.2	4	0	3	2
4.7205	2.9	5	1	-1	4
4.6233	1.5	-1	1	3	4
4.6182	0.6	0	0	4	2
4.6008	3.6	5	1	1	4
4.5847	1.2	6	0	2	2
4.5547	1.2	1	1	3	4
4.5332	2.2	-2	0	4	2
4.3665	1.6	2	0	4	2
4.3649	4.2	5	1	-2	4
4.3560	0.0	3	1	-3	4
4.2589	0.7	6	0	-3	2
4.1900	0.2	3	1	3	4
4.1806	3.8	5	1	2	4
4.1603	4.3	4	0	-4	2
4.1277	0.8	8	0	0	2
4.0917	2.5	8	0	-1	2
3.9679	1.6	8	0	1	2
3.9638	1.3	6	0	3	2
3.9181	3.7	7	1	0	4
3.9120	2.0	4	0	4	2
3.8938	1.0	5	1	-3	4
3.8803	3.2	7	1	-1	4
3.8740	43.7	8	0	-2	2
3.8616	50.8	-1	1	4	4
3.8082	3.5	1	1	4	4
3.7871	0.1	7	1	1	4
3.7138	2.7	-3	1	4	4
3.6999	1.4	5	1	3	4
3.6946	0.2	0	0	5	2
3.6873	1.1	7	1	-2	4
3.6711	0.8	8	0	2	2
3.6705	3.1	6	0	-4	2
3.6621	0.0	-2	0	5	2
3.5764	2.3	3	1	4	4
3.5512	1.4	2	0	5	2
3.5491	2.3	8	0	-3	2
3.5317	40.0	7	1	2	4
3.5178	27.0	0	2	0	2
3.4668	4.1	-4	0	5	2
3.4557	1.1	0	2	1	4
3.4405	0.0	2	2	0	4
3.4242	1.4	5	1	-4	4
3.4184	4.0	6	0	4	2
3.3992	0.2	7	1	-3	4
3.3916	0.7	2	2	-1	4
3.3732	0.3	2	2	1	4
3.3196	0.5	8	0	3	2
3.3022	4.1	10	0	0	2
3.2920	1.5	10	0	-1	2
3.2874	2.0	0	2	2	4
3.2851	2.2	4	0	5	2
3.2756	3.9	-1	1	5	4
3.2532	9.3	9	1	0	4
3.2488	13.6	5	1	4	4
3.2401	11.4	2	2	-2	4
3.2395	6.8	9	1	-1	4
3.2362	1.1	4	2	0	4
3.2349	1.4	1	1	5	4
3.2194	1.3	7	1	3	4
3.2108	24.4	10	0	1	2
3.2084	3.5	2	2	2	4
3.2031	1.5	4	2	-1	4
3.1942	5.5	8	0	-4	2
3.1916	1.9	-3	1	5	4
3.1831	2.8	10	0	-2	2
3.1753	25.4	6	0	-5	2
3.1724	11.0	4	2	1	4
3.1695	0.5	9	1	1	4
3.1319	0.1	9	1	-2	4
3.0822	7.1	3	1	5	4
3.0815	4.4	4	2	-2	4
3.0802	0.1	7	1	-4	4
3.0788	1.4	0	0	6	2
3.0668	1.2	-2	0	6	2

3.0545	0.4	0	2	3	4
3.0407	333.4	10	0	2	2
3.0276	761.8	4	2	2	4
3.0229	19.0	-2	2	3	4
3.0088	0.1	9	1	2	4
3.0086	3.4	5	1	-5	4
3.0017	1.5	10	0	-3	2
2.9880	1.7	2	0	6	2
2.9844	7.1	2	2	3	4
2.9729	115.0	8	0	4	2
2.9699	14.5	6	0	5	2
2.9640	192.8	6	2	0	4
2.9556	2.8	9	1	-3	4
2.9554	7.1	-4	0	6	2
2.9445	2.1	6	2	-1	4
2.9090	7.2	6	2	1	4
2.9031	0.8	7	1	4	4
2.8986	10.0	4	2	-3	4
2.8594	3.0	5	1	5	4
2.8572	0.4	8	0	-5	2
2.8547	6.1	6	2	-2	4
2.8319	2.9	4	2	3	4
2.8264	10.3	10	0	3	2
2.8262	1.3	-1	1	6	4
2.8189	2.2	4	0	6	2
2.8034	0.2	9	1	3	4
2.7984	11.2	0	2	4	4
2.7947	1.6	1	1	6	4
2.7909	0.7	6	2	2	4
2.7828	6.3	10	0	-4	2
2.7791	1.6	-2	2	4	4
2.7768	3.0	-3	1	6	4
2.7735	1000.0	6	0	-6	2
2.7722	0.0	7	1	-5	4
2.7611	1.2	11	1	0	4
2.7577	0.7	11	1	-1	4
2.7518	449.1	12	0	0	2
2.7508	5.9	12	0	-1	2
2.7435	1.5	9	1	-4	4
2.7394	904.3	2	2	4	4
2.7122	2.5	6	2	-3	4
2.7047	0.3	11	1	1	4
2.6950	15.5	11	1	-2	4
2.6936	11.5	12	0	1	2
2.6909	1.4	12	0	-2	2
2.6899	17.9	3	1	6	4
2.6862	16.7	4	2	-4	4
2.6774	1.6	8	2	0	4
2.6675	9.0	8	2	-1	4
2.6592	1.4	8	0	5	2
2.6581	9.2	-5	1	6	4
2.6390	1.4	0	0	7	2
2.6357	4.4	-2	0	7	2
2.6322	3.4	8	2	1	4
2.6311	0.3	6	2	3	4
2.6157	15.9	4	2	4	4
2.6111	1.0	7	1	5	4
2.6080	475.7	6	0	6	2
2.6043	856.0	8	2	-2	4
2.5989	4.5	10	0	4	2
2.5985	0.2	11	1	2	4
2.5867	3.5	12	0	2	2
2.5843	0.8	11	1	-3	4
2.5830	0.6	9	1	4	4
2.5827	0.9	12	0	-3	2
2.5771	0.9	2	0	7	2
2.5680	2.2	-4	0	7	2
2.5579	9.8	8	0	-6	2
2.5554	5.2	10	0	-5	2
2.5476	4.4	0	2	5	4
2.5399	0.2	8	2	2	4
2.5397	0.3	6	2	-4	4
2.5369	1.0	-2	2	5	4
2.5341	2.0	5	1	6	4
2.5229	4.0	9	1	-5	4

2.4992	27.1	2	2	5	4
2.4984	0.3	8	2	-3	4
2.4945	12.4	7	1	-6	4
2.4765	0.1	-1	1	7	4
2.4692	6.5	-4	2	5	4
2.4627	6.9	4	0	7	2
2.4592	0.5	11	1	3	4
2.4517	0.4	1	1	7	4
2.4515	1.4	6	2	4	4
2.4495	77.5	-6	0	7	2
2.4474	4.9	12	0	3	2
2.4465	9.8	-3	1	7	4
2.4427	4.6	12	0	-4	2
2.4423	11.5	11	1	-4	4
2.4143	0.6	8	2	3	4
2.4076	0.8	10	2	0	4
2.4037	1.0	10	2	-1	4
2.4009	0.3	4	2	5	4
2.3902	1.3	13	1	-1	4
2.3892	2.7	13	1	0	4
2.3868	0.3	8	0	6	2
2.3783	5.0	10	0	5	2
2.3768	1.6	3	1	7	4
2.3715	2.4	10	2	1	4
2.3676	4.4	9	1	5	4
2.3673	2.3	-5	1	7	4
2.3648	0.8	8	2	-4	4
2.3612	5.3	14	0	-1	2
2.3602	7.5	10	2	-2	4
2.3587	1.3	14	0	0	2
2.3571	1.2	6	2	-5	4
2.3533	2.1	7	1	6	4
2.3521	4.0	13	1	-2	4
2.3492	1.9	13	1	1	4
2.3393	0.1	1	3	0	4
2.3375	1.4	10	0	-6	2
2.3259	77.8	14	0	-2	2
2.3222	2.2	1	3	-1	4
2.3193	3.3	1	3	1	4
2.3188	4.0	14	0	1	2
2.3168	196.3	0	2	6	4
2.3153	37.9	6	0	7	2
2.3116	3.9	-2	2	6	4
2.3112	11.6	9	1	-6	4
2.3098	0.4	-2	0	8	2
2.3091	3.3	0	0	8	2
2.3035	19.6	11	1	4	4
2.3004	8.4	10	2	2	4
2.3000	3.0	8	0	-7	2
2.2937	20.7	3	3	0	4
2.2924	3.1	12	0	4	2
2.2874	1.4	12	0	-5	2
2.2856	2.8	11	1	-5	4
2.2834	35.6	10	2	-3	4
2.2804	4.3	3	3	-1	4
2.2802	4.8	13	1	-3	4
2.2774	6.5	2	2	6	4
2.2759	11.5	13	1	2	4
2.2720	0.0	3	3	1	4
2.2706	15.3	8	2	4	4
2.2704	0.3	-1	3	2	4
2.2693	10.6	6	2	5	4
2.2666	3.4	-4	0	8	2
2.2649	4.6	1	3	2	4
2.2646	0.0	5	1	7	4
2.2645	0.2	2	0	8	2
2.2628	10.7	-4	2	6	4
2.2577	7.3	14	0	-3	2
2.2522	0.5	7	1	-7	4
2.2468	2.0	14	0	2	2
2.2339	0.7	3	3	-2	4
2.2183	0.3	3	3	2	4
2.2178	3.3	8	2	-5	4
2.2100	2.4	5	3	0	4
2.2033	0.2	10	2	3	4

2.2006	0.3	5	3	-1	4
2.1998	1.9	4	2	6	4
2.1991	4.6	-1	1	8	4
2.1905	8.0	-1	3	3	4
2.1881	0.1	5	3	1	4
2.1863	1.6	-6	0	8	2
2.1833	75.9	13	1	-4	4
2.1833	140.2	4	0	8	2
2.1831	1.0	1	3	3	4
2.1825	387.6	10	2	-4	4
2.1805	2.4	-3	1	8	4
2.1793	89.4	1	1	8	4
2.1781	3.4	13	1	3	4
2.1780	59.7	6	2	-6	4
2.1750	1.4	10	0	6	2
2.1680	66.1	9	1	6	4
2.1674	67.4	12	2	0	4
2.1670	31.3	12	2	-1	4
2.1648	0.5	14	0	-4	2
2.1611	65.0	5	3	-2	4
2.1601	0.5	3	3	-3	4
2.1540	0.9	8	0	7	2
2.1514	0.2	14	0	3	2
2.1445	1.8	11	1	5	4
2.1389	2.9	3	3	3	4
2.1386	7.6	12	2	1	4
2.1381	0.8	10	0	-7	2
2.1377	3.2	5	3	2	4
2.1373	0.1	12	2	-2	4
2.1344	2.4	12	0	5	2
2.1305	4.9	7	1	7	4
2.1295	0.6	12	0	-6	2
2.1269	0.5	11	1	-6	4
2.1261	0.9	-5	1	8	4
2.1239	1.6	3	1	8	4
2.1213	0.2	8	2	5	4
2.1168	1.8	9	1	-7	4
2.1110	10.5	0	2	7	4
2.1093	0.1	-2	2	7	4
2.1039	6.9	15	1	-1	4
2.1010	5.9	15	1	0	4
2.1000	8.8	7	3	0	4
2.0962	15.3	5	3	-3	4
2.0950	15.5	6	2	6	4
2.0941	0.8	7	3	-1	4
2.0911	23.8	-1	3	4	4
2.0903	0.3	10	2	4	4
2.0839	4.5	12	2	2	4
2.0825	4.7	1	3	4	4
2.0818	0.1	12	2	-3	4
2.0802	2.3	8	0	-8	2
2.0799	0.7	15	1	-2	4
2.0791	1.6	7	3	1	4
2.0789	1.4	2	2	7	4
2.0765	10.5	6	0	8	2
2.0741	0.9	-4	2	7	4
2.0716	7.9	15	1	1	4
2.0713	0.2	13	1	-5	4
2.0688	4.6	8	2	-6	4
2.0676	2.1	16	0	-1	2
2.0675	15.3	10	2	-5	4
2.0667	5.4	-3	3	4	4
2.0656	0.9	13	1	4	4
2.0643	7.5	5	3	3	4
2.0638	3.3	16	0	0	2
2.0621	0.4	7	3	-2	4
2.0565	0.2	14	0	-5	2
2.0551	2.2	-2	0	9	2
2.0525	0.4	0	0	9	2

Diffraction pattern graphics



Experimental

Physical Properties

Calc. density	3.17200 g/cm³

Remarks

Remarks

Comments	- Diffraction pattern calculated by Match!. - I/Ic calculated by Match!. - Space group has been derived from given symmetry operations.

Entry # 96-900-8656

Phase classification

Name	
Formula	HKO
I/Ic	4.400000
Sample Name	9008655
Quality	C (calculated)

References

Publication

Bibliography	Wyckoff R. W. G., "Second edition. Interscience Publishers, New York, New Yorkrocksalt structure", Crystal Structures **1**, 85-237 (1963).

Origin of data

Source of entry	COD (Crystallography Open Database)
Link to orig. entry	9008655

Crystal structure

Crystallographic data

Space group	F m -3 m (225)
Crystal system	cubic
Cell parameters	a= 5.78000 Å
Z	4

Atom coordinates

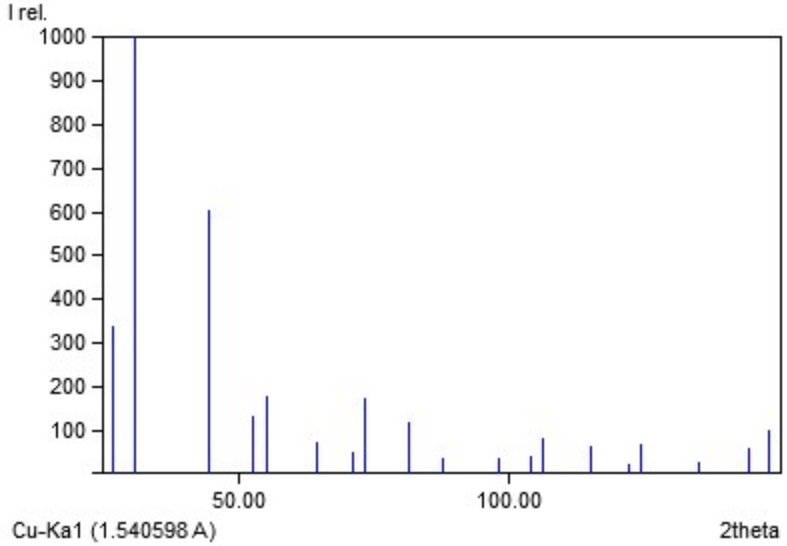
Element	Oxid.	*x*	*y*	*z*	Bi	Focc
K		0.000	0.000	0.000	1.000000	1.000000
O		0.500	0.500	0.500	1.000000	1.000000

Diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
3.3371	335.0	1	1	1	8
2.8900	1000.0	2	0	0	6
2.0435	601.0	2	0	2	12
1.7427	129.1	3	1	1	24
1.6685	175.3	2	2	2	8
1.4450	69.8	4	0	0	6
1.3260	45.9	3	1	3	24
1.2924	170.0	4	0	2	24
1.1798	115.8	4	2	2	24
1.1124	33.8	5	1	1	24
1.0218	35.9	4	0	4	12
0.9770	39.2	5	3	1	48
0.9633	80.3	6	0	0	6
0.9139	62.0	6	0	2	24
0.8814	20.1	5	3	3	24
0.8714	64.4	6	2	2	24
0.8343	24.3	4	4	4	8
0.8094	58.1	7	1	1	24
0.8015	96.8	4	6	0	24

Diffraction pattern graphics



Experimental

Physical Properties

Calc. density	1.93000 g/cm³

Remarks

Remarks

Comments	- Diffraction pattern calculated by Match!. - I/Ic calculated by Match!.

Entry # 96-101-1177

Phase classification

Name	Silicon oxide - $-alpha
Mineral Name	Quartz low
Formula	O_2Si
I/Ic	3.010000
Sample Name	1011176
Quality	C (calculated)

References

Publication

Bibliography	Machatschki F, "Die Kristallstruktur von Tiefquarz Si O2 und Aluminiumorthoarsenat AlAs O4", Zeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik,Kristallchemie (-144,1977) **94**, 222-230 (1936).

Origin of data

Source of entry	COD (Crystallography Open Database)
Link to orig. entry	1011176

Crystal structure

Crystallographic data

Space group	P 32 2 1 S (-1)
Crystal system	trigonal (hexagonal axes)
Cell parameters	a= 4.90000 Å c= 5.40000 Å
Z	3

Atom coordinates

Element	Oxid.	*x*	*y*	*z*	Bi	Focc
Si	4.0	0.469	0.000	0.000	1.000000	1.000000
O	-2.0	0.403	0.253	0.122	1.000000	1.000000

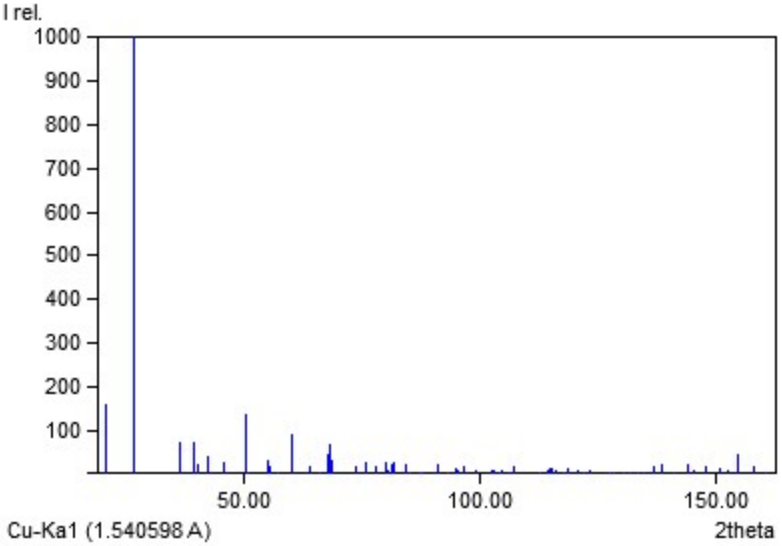
Diffraction data

Diffraction lines

d [Å]	Int.	h	k	l	Mult.
4.2435	159.3	1	0	0	6
3.3366	1000.0	1	0	1	6
2.4500	72.0	1	1	0	6
2.2780	70.3	1	0	2	6
2.2311	22.7	1	1	1	12
2.1218	38.5	2	0	0	6
1.9748	24.8	2	0	1	6
1.8144	137.0	1	1	2	12
1.8000	2.0	0	0	3	2
1.6683	31.6	2	0	2	6
1.6571	15.0	1	0	3	6
1.6039	3.9	2	1	0	12
1.5375	87.7	2	1	1	12
1.4506	15.2	1	1	3	12
1.4145	4.4	3	0	0	6
1.3789	43.6	2	1	2	12
1.3726	66.0	2	0	3	6
1.3683	31.6	3	0	1	6
1.2865	17.4	1	0	4	6
1.2530	26.8	3	0	2	6
1.2250	16.4	2	2	0	6
1.1975	25.1	2	1	3	12
1.1946	8.1	2	2	1	12
1.1824	21.9	1	1	4	12
1.1769	24.0	3	1	0	12
1.1499	18.6	3	1	1	12
1.1390	2.7	2	0	4	6
1.1156	0.3	2	2	2	12
1.1122	2.4	3	0	3	6
1.0789	21.9	3	1	2	12
1.0609	3.9	4	0	0	6
1.0466	13.3	1	0	5	6
1.0410	9.2	4	0	1	6

1.0328	15.0	2	1	4	12
1.0127	8.8	2	2	3	12
0.9882	6.8	1	1	5	12
0.9874	2.7	4	0	2	6
0.9851	5.1	3	1	3	12
0.9766	3.6	3	0	4	6
0.9735	7.5	3	2	0	12
0.9625	0.3	2	0	5	6
0.9581	14.4	3	2	1	12
0.9260	0.7	4	1	0	12
0.9158	4.8	3	2	2	12
0.9140	11.0	4	0	3	6
0.9127	13.4	4	1	1	12
0.9072	5.0	2	2	4	12
0.9000	1.9	0	0	6	2
0.8958	12.2	2	1	5	12
0.8871	8.8	3	1	4	12
0.8804	2.5	1	0	6	6
0.8759	8.0	4	1	2	12
0.8584	2.6	3	0	5	6
0.8563	0.6	3	2	3	12
0.8487	0.2	5	0	0	6
0.8448	2.7	1	1	6	12
0.8384	1.2	5	0	1	6
0.8341	2.0	4	0	4	6
0.8285	17.8	2	0	6	6
0.8234	21.8	4	1	3	12
0.8167	4.4	3	3	0	6
0.8101	11.1	2	2	5	12
0.8096	22.0	5	0	2	6
0.8075	7.9	3	3	1	12
0.8020	15.5	4	2	0	12
0.7957	12.9	3	1	5	12
0.7933	7.6	4	2	1	12
0.7896	41.8	3	2	4	12
0.7849	15.8	2	1	6	12
0.7817	0.4	3	3	2	12

Diffraction pattern graphics



Experimental

Physical Properties

Meas. density	2.66000 g/cm³
Calc. density	2.66500 g/cm³

Remarks

Remarks

Comments	- Diffraction pattern calculated by Match!. - I/Ic calculated by Match!. - Space group has been derived from given symmetry operations.