Quartz

Joseph R. Smyth

Adopt-a-Mineral Project
Example Paper

I. Introduction

Quartz, or α-quartz, is the mineral form of SiO_2 stable at low temperatures and pressures. The English word derives from the Saxon word querkluftertz (cross-vein ore) (Gaines et al., 1997). It occurs in igneous, sedimentary, metamorphic, and hydrothermal mineral environments, particularly in continental regions. It is, however rare in oceanic rocks. As the structure is acentric, it occurs in both left and right-handed varieties and is both piezoelectric and pyroelectric. It is usually nearly pure and accepts only very limited amounts of other elements in substitution. Polymorphs include β-quartz, tridymite, cristobalite, coesite, stishovite, and keatite.

II. Physical Properties

The physical and optical properties of quartz are outlined in Table 1. It is generally colorless, but many colored varieties have been described, including rose quartz (pink), amethyst (purple), citrine (yellow) and smoky quartz (gray). The luster is vitreous, and there is no cleavage so it exhibits conchoidal fracture. The hardness is seven, and the density is 2.67 g/cm^3. Optically, it is uniaxial, positive with a maximal birefringence of 0.0095.

Table 1. General and Physical Properties of Quartz (Deer et al., 1963)
_____

Chemical Formula	SiO_2
Optical Properties	Uniaxial positive
	Nω = 1.5443
	Nε = 1.5538
Cleavage	None
Common crystal forms	Prism {1010}
	Pyramids {1011} and {0111}
Luster	Vitreous
Color, Opacity	Transparent, colorless
	Also gray (smoky quartz), blue, purple (amethyst),
	yellow (citrine), pink (rose quartz)
Hardness	7

_____

III. Chemistry

Quartz is always nearly pure silica with less than 0.2 percent of total impurities. Typical chemical analyses are given in Table 2.

Table 2. Typical chemical analyses of quartz (Deer et al., 1963).

	1	2	3	4
SiO2	99.97	99.98	99.53	99
TiO2	0.048	0.015	0	0
Al2O3	0.042	0	0.02	0
Cr2O3	0	0	0	0
Fe2O3	0.007	0.07	0.05	0
FeO	0	0.04	0.05	0
MnO	0.009	0	0	0.02
MgO	0.008	0.09	0	0
CaO	0.01	0	0	0
Na2O	0	0	0	0
K2O	0	0	0	0
H2O	0	0	0	0
Total	100.094	100.195	99.65	99.02
	3.330549	3.3315	3.314516	3.295559
Oxygens /formula unit	4	4	4	4
Si	1.998208	1.997837	1.999036	1.999829
Ti	0.000722	0.000225	0	0
Al	0.000989	0	0.000473	0
Cr	0	0	0	0
Fe3+	0.000105	0.001053	0.000756	0
Fe2+	0	0.000668	0.00084	0
Mn	0.000152	0	0	0.000342
Mg	0.000238	0.002681	0	0
Ca	0.000214	0	0	0
Na	0	0	0	0
K	0	0	0	0
H	0	0	0	0
	2.000629	2.002464	2.001105	2.000171

IV. Structure

The structure of quartz consists of corner-sharing SiO_4 tetrahedra so that each Si is bonded to four oxygens, and each oxygen is bonded to two silicon atoms. The resulting structure forms an open three-dimensional framework, so that quartz is classified as a tektosilicate or framework silicate. Quartz is the stable form of SiO_2 at atmospheric temperature and pressure. It is denser than tridymite and cristobalite, the high temperature forms, but less dense than the high pressure forms, coesite and stishovite. At 573 ºC, trigonal low quartz transforms reversibly to hexagonal high quartz.

The crystallographic data for quartz are outlined in Table 3. The structure is acentric, so exists in right- and left-handed enantiomorphs. The space groups are $P3_121$ (right handed) or $P3_221$ (left-handed). The structure is illustrated in Fig. 1.

Table 3. Crystallographic Information

_____

Crystal System	Trigonal
Point Group	32
Space Group	$P3_121$ or $P3_221$
Unit Cell Parameters	
a	4.1937Å
c	5.4047Å
Z (No. of Formula Units per Cell)	3
Density (calculated)	2.648 g/cm^3
Density (measured)	2.65 g/cm^3

_____

Table 4. Atom coordinates for quartz at 298K (Kihara et al., 1990)
_____

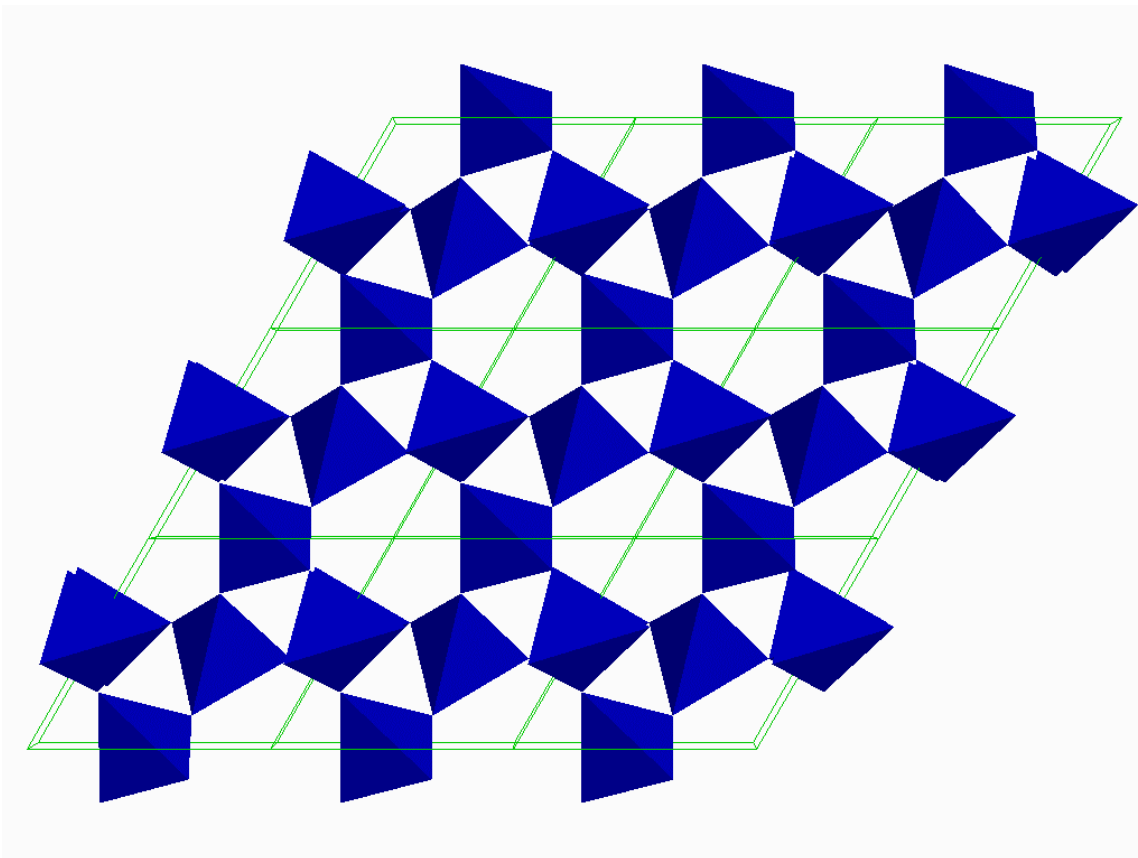| Atom	x/a	y/b	z/c
Si	0.4697	0	0
O	0.4133	0.2672	0.1188

_____

Figure 1. The crystal structure of quartz (*c*-axis projection).

V. X-ray diffraction

An X-ray powder diffraction pattern was obtained for a sample of pure quartz and is shown in Figure 2. The background and alpha-2radiation were subtracted and peaks were located using the program package DSMNT (Scintag Inc, 1998). The processed pattern, derived peaks are shown in Figure 2 compared to the standard pattern number 46-1045 (JCPDS, 2000). A powder pattern was calculated from the structure data of Kihara et al. (1990) and is presented in Figure 4. The observed and calculated diffraction peaks are given in Table 5.
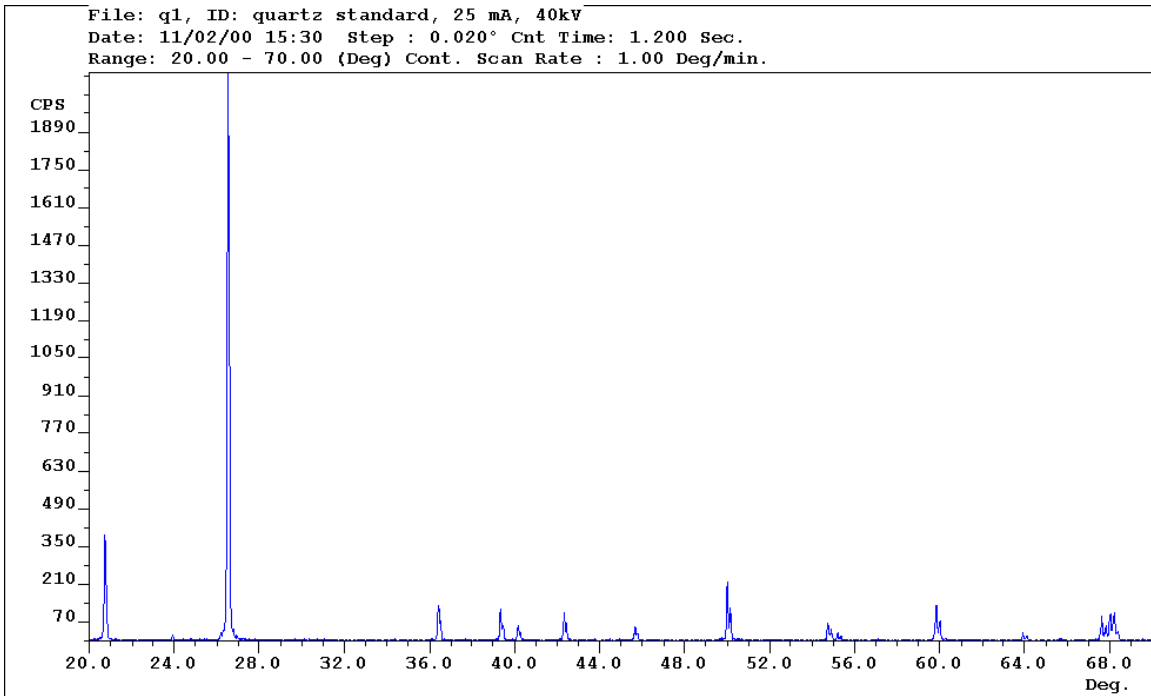
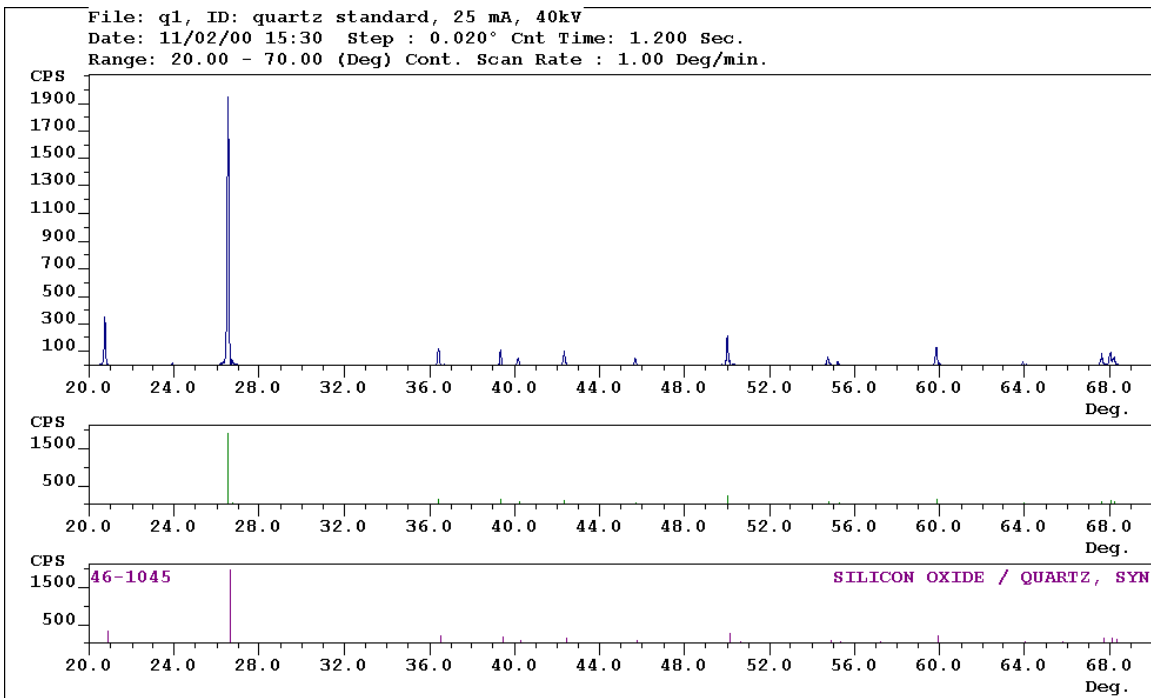Figure 2. X-ray powder diffraction pattern of quartz.

Figure 3. X-ray powder diffraction pattern of quartz showing peaks derived from the pattern compared to the JCPDS standard pattern number 46-1045.
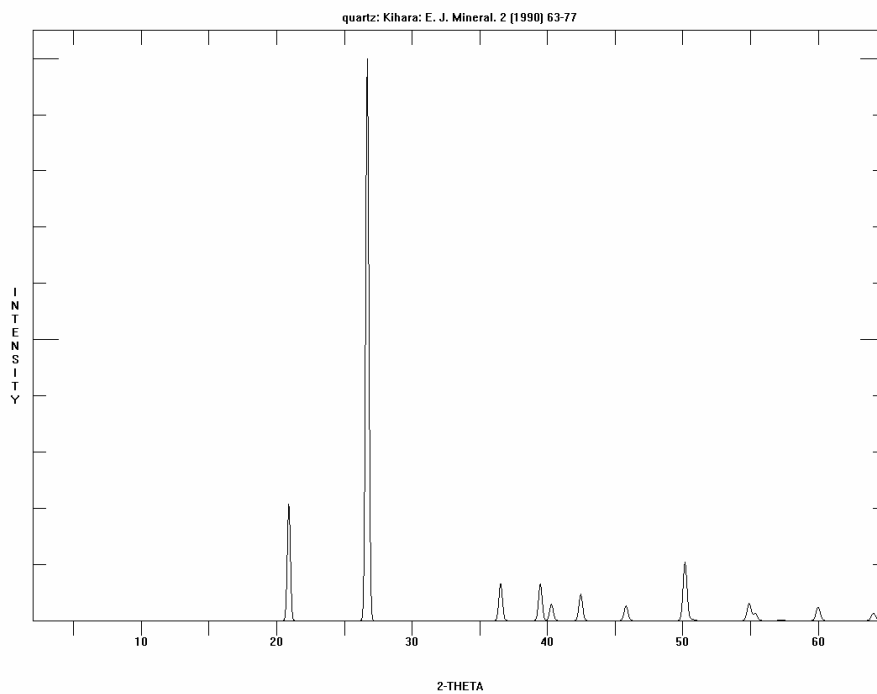
Figure 4. Calculated powder diffraction pattern for quartz using the program XPOW (Downs et al., 1993).

Table 5. Observed and Calculated X-ray Powder Diffraction Peaks (CuKα radiation)

OBSERVED			CALCULATED					
2-θ	d(Å)	REL INT	2-θ	REL INT	d(Å)	*h*	*k*	*l*
20.82	4.263	21.8	20.88	20.65	4.2554	1	0	0
26.62	3.346	100.0	26.66	69.88	3.3434	0	1	1
			26.66	30.12	3.3434	1	0	1
36.52	2.458	10.0	36.57	6.48	2.4569	1	1	0
39.44	2.283	7.9	39.50	0.60	2.2812	0	1	2
			39.50	6.10	2.2812	1	0	2
40.26	2.238	3.3	40.32	2.97	2.2366	1	1	1
42.41	2.130	4.8	42.49	5.29	2.1277	2	0	0
45.75	1.982	3.72	45.83	0.81	1.9798	0	2	1
			45.83	1.41	1.9798	2	0	1
50.10	1.819	13.1	50.18	10.29	1.8179	1	1	2
			50.67	0.40	1.8016	0	0	3
54.83	1.673	4.4	54.92	0.55	1.6717	2	0	2
			54.92	2.17	1.6717	0	2	2
			55.38	1.22	1.6590	0	1	3
			57.28	0.15	1.6084	2	1	0

VI. Occurrences

The occurrences of quartz have been reviewed recently by Gaines et al. (1997). Quartz is an abundant mineral in igneous, metamorphic, hydrothermal, and sedimentary environments. In plutonic igneous rocks, it is abundant in silicic rocks ranging composition from quartz diorite to granite but absent in more mafic compositions. In volcanic rocks, it is common in quartz latites to rhyolites, but uncommon in vitric silicic tuffs. It is common to abundant in welded silicic tuffs. In metamorphic rocks, it is abundant in schists and gneisses of pelitic to granitic compositions. In hydrothermal rocks, it is an abundant as the principal gangue mineral; in low to high temperature vein deposits. Because of its resistance to chemical weathering, it is the principal mineral phase in sandstones and abundant in other non-marine sedimentary rocks. It is also abundant as cryptocrystalline chert in marine limestones and dolomites.

Numerous varieties have been described, and defined mainly on color. Quartz is most commonly colorless and transparent. Rose quartz is pink and contains minor Mn impurities, recently identified as dumortrierite. Citrine is yellow, and amethyst is purple.

VII. References

Deer, W.A., R. A. Howie, and J. Zussman (1963) *Rock-Forming Minerals* Vol 4. Longmans, London, 435pp.

Downs, R.T., K.L. Bartelmehs, G. V. Gibbs, and M. B. Boysen, Jr. (1993) Interactive software for calculating and displaying X-ray or neutron powder diffractometer patterns of crystalline materials. *American Mineralogist* 78, 1104-1107.

Gaines, R.V., H.C.W. Skinner, E.E. Foord, B. Mason, A. Rosenzweig, V.T. King and E. Dowty (1997*) Dana's New Mineralogy*, Eighth Edition, New York, John Wiley & Sons, 1819 pp.

Kihara, K. (1990) An X-ray study of the temperature dependence of the quartz structure. *European Journal of Mineralogy* 2, 63-77.

LePage, Y., L. D. Calvert, and E. J. Gabe (1980) Parameter variation in low quartz between 94 and 298K. *Journal of Physical Chemistry of Solids*, 41, 721-725.