



**MATERIALS SCIENCE
& ENGINEERING**
TEXAS A&M UNIVERSITY

Introduction to Materials Science & Engineering

Crystallographic Points

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Structure and elastic properties of quartz at pressure

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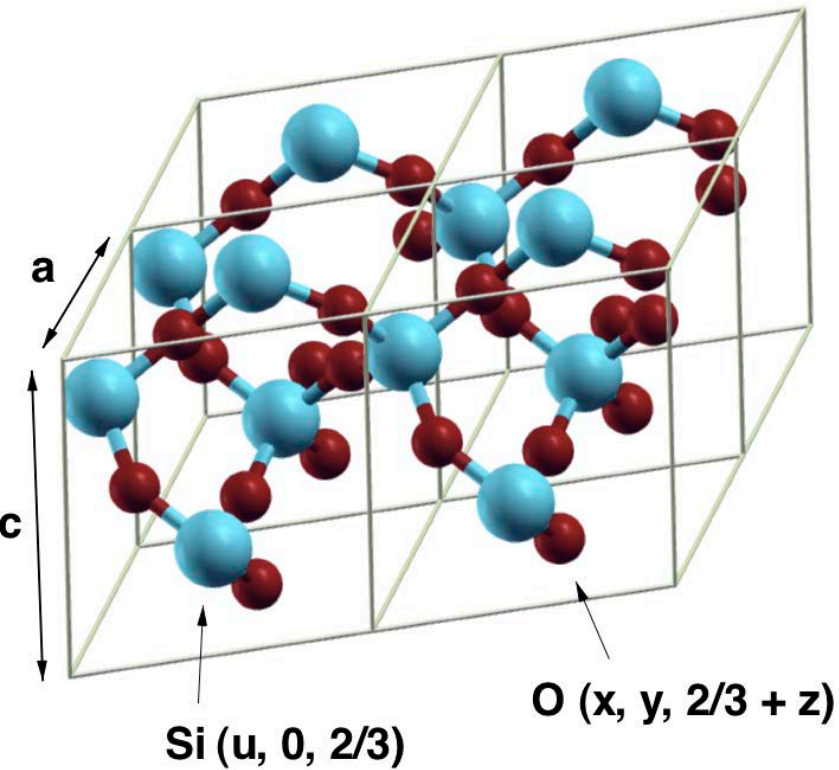
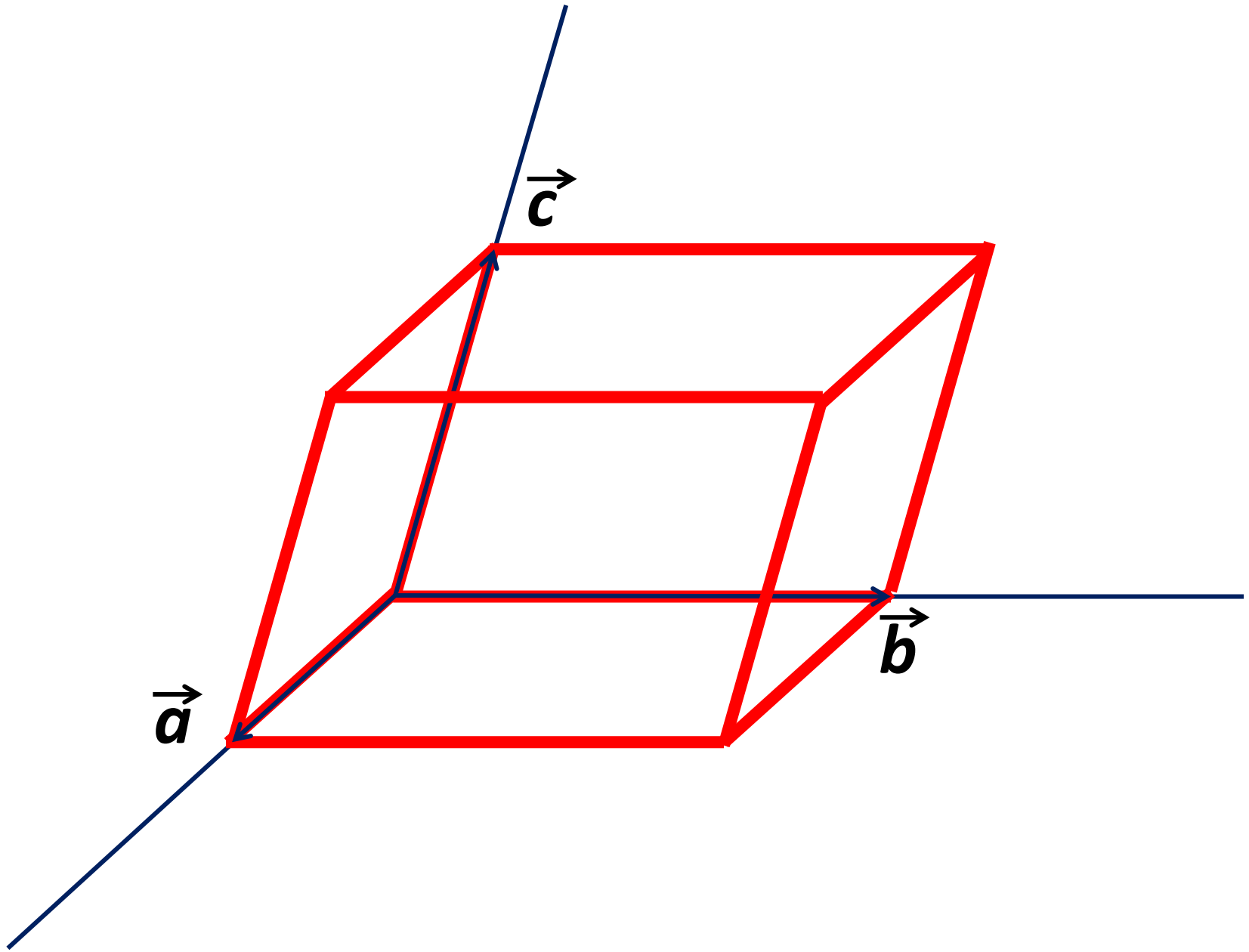


Table 3. Positional and thermal parameters

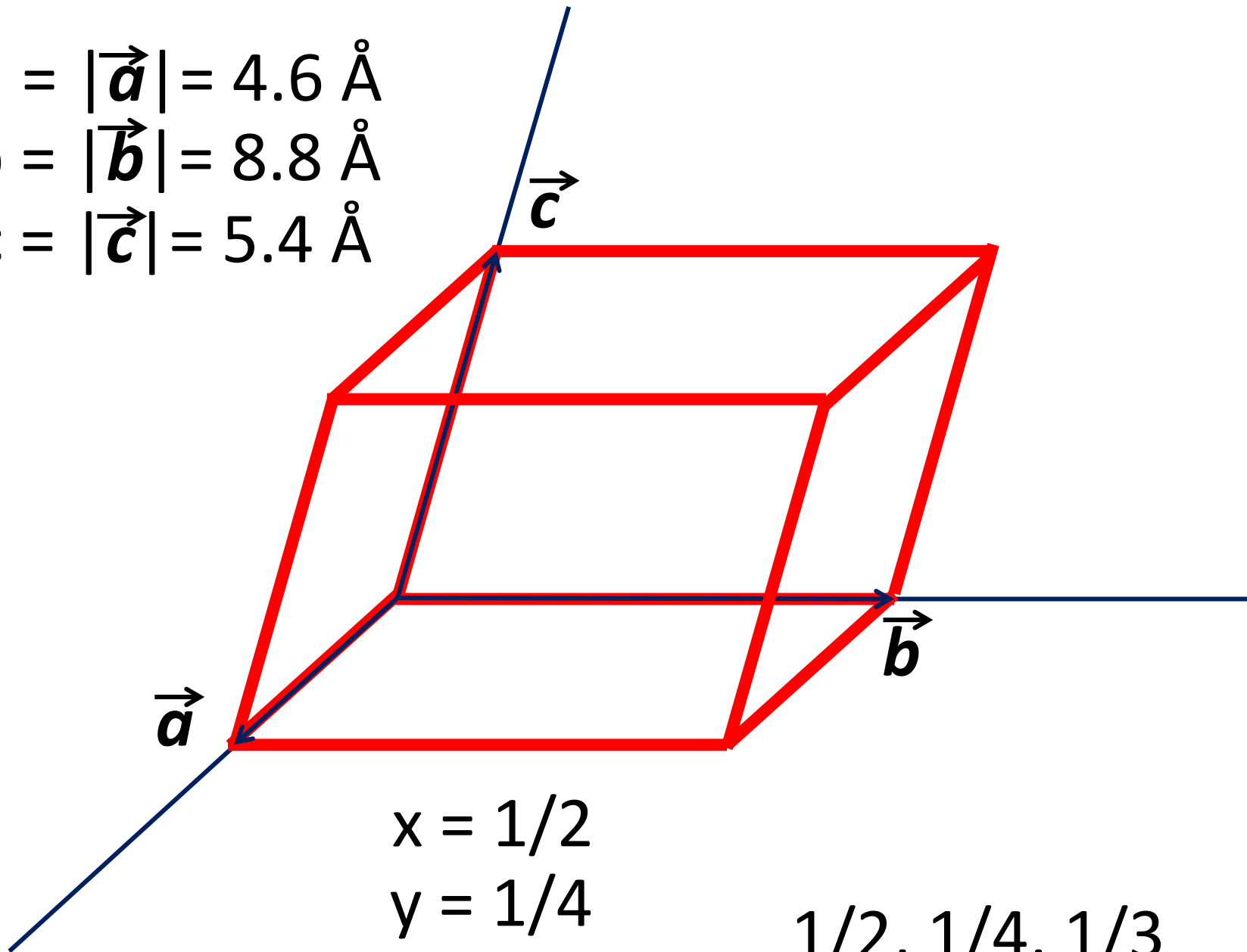
	1 atm	20.7*	37.6
$x(\text{Si})$	0.4697(1)**	0.4630(2)	0.4581(2)
$x(\text{O})$	0.4135(3)	0.4111(6)	0.4079(6)
$y(\text{O})$	0.2669(2)	0.2795(4)	0.2867(5)
$z(\text{O})$	0.1191(2)	0.1095(2)	0.1039(3)
$B(\text{Si})$	0.62(2)	0.44(2)	0.47(2)
$B(\text{O})$	1.05(2)	0.86(3)	0.88(3)
$\beta_{11}(\text{Si})^\dagger$	0.93(2)	0.70(4)	0.79(4)
$\beta_{22}(\text{Si})$	0.78(2)	0.57(5)	0.68(5)
$\beta_{33}(\text{Si})$	0.49(2)	0.35(2)	0.35(2)
$\beta_{13}(\text{Si})$	-0.001(7)	0.02(1)	-0.05(1)
$\beta_{11}(\text{O})$	1.90(6)	1.48(9)	1.55(10)
$\beta_{22}(\text{O})$	1.44(5)	1.08(8)	1.23(9)
$\beta_{33}(\text{O})$	0.83(3)	0.76(3)	0.69(3)
$\beta_{12}(\text{O})$	1.06(5)	0.75(8)	0.75(10)
$\beta_{13}(\text{O})$	-0.25(3)	-0.34(6)	-0.40(6)
$\beta_{23}(\text{O})$	-0.35(3)	-0.29(4)	-0.32(4)



$$a = |\vec{a}| = 4.6 \text{ \AA}$$

$$b = |\vec{b}| = 8.8 \text{ \AA}$$

$$c = |\vec{c}| = 5.4 \text{ \AA}$$



$$x = 1/2$$

$$y = 1/4$$

$$z = 1/3$$

$$1/2, 1/4, 1/3$$

