

XTALDRAW

You can download and run XTALDRAW on a PC, or use the machines in BESC385.

Create a text file with the following script and save it:

Quartz

```
4.9137 4.9137 5.4047 90 90 120 *P3_221
0 0 .6666666666666667
Si
.4697 0 0 4 2
ANIONS
O
.4133 .2672 .1188
END
```

Open the file with XTALDRAW

Save the image by using PrtScn

Open Photoshop or any image editor.

New Image file (ctrl N); paste (ctrl V); and crop image.

In XTALDRAW, click on 'edit' and 'geometry file'

There are two Si-O distances listed

What are the Si – O _____ and _____

What is the volume of the Si tetrahedron? _____ Å³.

2. Create a text file for forsterite (olivine) with the following text

Forsterite

```
4.7503 10.187 5.9771 90 90 90 Pbnm
Si
.4266 .09413 .25 4 2
Mg1
0 0 0 2 3
Mg2
-.0084 .2775 .25 2 3
anions
O1
.7664 .0914 .25
O2
.2215 .4472 .25
O3
.2778 .1631 .0332
end
```

What is the coordination number of Si? _____

What is the Si – O1 distance? _____

What is the Si – O2 distance? _____

What is the Si – O3 distance? _____

What is the coordination number of Mg1? _____

What is the coordination number of Mg2? _____

Which Mg site has the larger volume? _____