Assignment 1

BME 282

October 22nd, 2022

Group 21

ABSTRACT

Crystalline modeling software aid with the visualization of crystal structures and provide information on its unit cell properties. Among the broad selection of crystalline modeling tools, this study discusses VESTA, CrystalMaker, Avogadro, Atomsk, Professor Kwan's Crystal Viewer and WebCSD. To understand the functions offered by these crystalline modeling tools, α-cristobalite and graphite were modeled in each software. These software were evaluated by comparing their ability to model the unit cells, as well as the information they provide of α-cristobalite and graphite. The comparative analysis revealed that VESTA and CrystalMaker are equipped with the most suitable functions for users to construct and manipulate complex crystal unit cell structures. Avogadro, Atomsk, and Professor Kwan's Crystal Viewer performed poorly out of the six softwares due to their limitations in available functions, databases, and user-interface. The ability for these software to build such unit cells and provide information are valuable for research purposes in the manufacturing industry.

I. INTRODUCTION

Cristobalite is a polymorph type of SiO2 [1]. There are two types of cristobalite – alpha and beta, also referred to as low and high cristobalite, respectively. The unit cell structure of beta cristobalite is in the cubic system, space group Fd3m origin 2 [2]. Beta cristobalite is stable near its melting point of 1900K and stays metastable down to 500K; below this temperature, the unit cell structure transforms to the tetragonal alpha cristobalite [3]. Alpha cristobalite has two space groups that occur randomly [3]. In this assignment, we have chosen to model the $P4_12_12$ form of alpha cristobalite [4].

Similarly, there are types of graphite as well. The common type of graphite takes on a hexagonal structure with the space group $P6_3/mmc$; also called alpha graphite [5]. Other types of graphite include beta graphite, with graphene stacked with an ABC sequence instead of the ABA sequence that occurs in alpha graphite [6].

The objective of this study was to determine the suitability of six softwares for modeling the structure of cristobalite and graphite, including Vesta [7], CrystalMaker [8], Avogadro [9], Atomsk [10], Professor Charles Kwan's Activities [11], and WebCSD [12]. The study was focused on developing investigative and collaborative techniques in exploring new engineering tools, while also establishing spatial knowledge of crystal composition arrangements. This was accomplished by recording the process of modeling the two materials, then analyzing the benefits and flaws of each software based on the accuracy of the models' atomic composition and dimensions, as well as the level of flexibility that the software offers in the sculpting of unit cells.

II. RESULTS AND DISCUSSION

A. Tool 1: VESTA [7]

VESTA is a 3D visualization tool developed by JP-Minerals, used for crystal structural modelling and many other functions [7]. VESTA allows the user to select the crystal system and the space group of crystals, which upon selection highlights the lattice parameter inputs required (Appendix I). After the unit cell skeleton is made, atoms can be added to the corresponding

coordinates via the structure parameters menu (Appendix II). Using the distance tool, the distance between the atoms could be measured (Appendix III) which then was used to determine the maximum length parameters when creating the bonds between the atoms (Appendix IV). The produced unit cell (Fig. 1) could be viewed in many different styles (Appendix V).

The manual has a figure that suggests that if volumetric data is entered into the program, it is possible to make a cut-out model of the unit cell [13]. Unfortunately, we could not find the volumetric data for alpha cristobalite that would allow us to explore this option.

B. Tool 2: CrystalMaker 2017 [8]

CrystalMaker is another 3D visualization tool, published by CrystalMaker Software Ltd. [8]. We explored the 2017 Legacy version. The software is not free; however, users can still try out the trial program which offers almost all features bar saving.

The functionality for modelling unit cells were almost the exact same as VESTA; other than the interface differences, it felt like the same program (Appendices VI-VIII). One problem that the users may run into is the fact that the default atomic radii for the atoms do not update to the covalent radii once the bonds were added. The problem can be solved by manually updating the atomic radii of the atoms in the unit cell by utilizing the element editor menu (Appendix IX).

We could not find a way to make a cut-out model of the unit cell with the functions of the program.

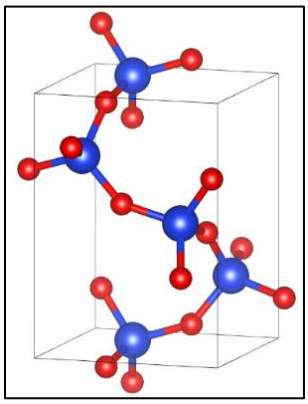

Fig. 1

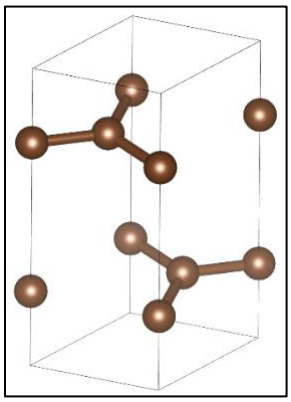

Fig. 2

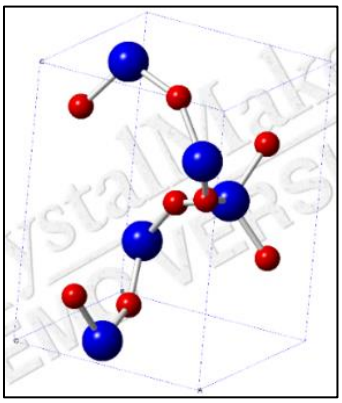

Fig. 3

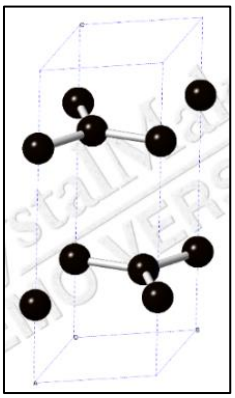

Fig. 4

C. Tool 3: Avogadro [9]

In Avogadro, users are able to create unit cells from scratch however, it is limited in that it can not have more than 1 element and has low flexibility on the way atoms are placed. For this reason, cristobalite and graphite unit cells cannot be made from scratch. Instead, α-cristobalite and graphite unit cells are made using Avogadro's large selection of ready-made crystal unit cells. The unit cell of α-cristobalite (Fig. 5) has the proper number of silicon and oxygen atoms, and good placement. It displays accurate relative atomic size as well as angle and distance (Appendix X). The unit cell of graphite (Fig. 6) has the incorrect number of carbon atoms but the

incorrect placement. Both unit cells have the shape, space group, and other useful information is displayed in the top left corner.

D. Tool 4: Atomsk [10] and OVITO [14]

Atomsk must be run on Windows PowerShell. Knowledge of the command lines is required to make unit cells. It will create the unit cell as a .cfg file to open in a visualizer, OVITO or in a .xsf file to open in a text editor and see its information. It has limited capabilities in customizing unit cells. For this reason, Atomsk is not able to create cristobalite from scratch. The .cif file of α-cristobalite from [4] is opened in OVITO (Fig. 7). This displays 1 less silicon and oxygen atom. Atomsk is able to create the graphite unit cell using the command in Appendix XI. Inputting the cfg file to OVITO displays the unit cell of graphite (Fig. 8). OVITO displays the position, distance, and angles of the atoms (Appendix XII).

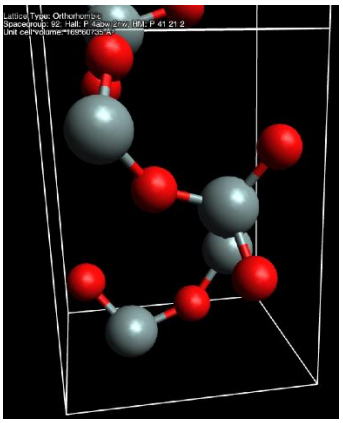

Fig. 5

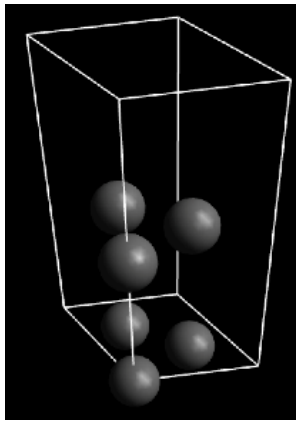

Fig. 6

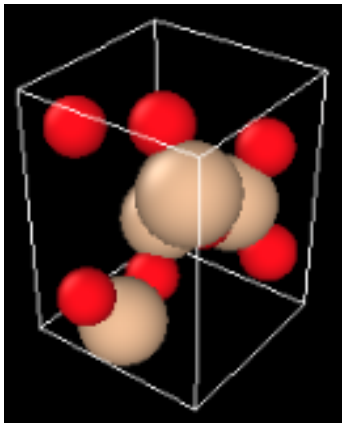

Fig. 7

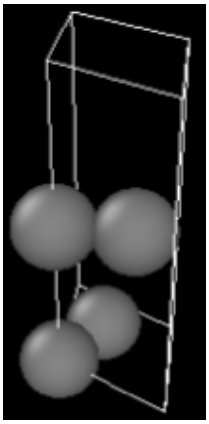

Fig. 8

E. Tool 5: Professor Charles Kwan's Activities [11]

The Crystal Structure Viewer developed by Dr. Charles Kwan is an applet that showcases three-dimensional unit cell structures commonly observed in metals and ceramics. Although the software was equipped with tools to visualize elementary Bravais lattices and a pre-established selection of materials, it was not suitable for examining complete cristobalite and graphite structures as it only displayed the general architecture of a tetragonal site (Fig. 9). In addition, the larger depiction of O^{-2} ions shown in Appendix XIII contradict against the atomic radius trend, which gradually decreases from left to right of the periodic table due to the stronger electrostatic force induced by the addition of protons. The measurements of distance and angles between the ions were inaccessible. The software could be used to visualize the general structure of the hexagonal close-packed unit cell of graphite shown in Fig. 10, but the model did not encompass the specific attributes of atomic networks within graphite, including the types of atoms involved, measurement of space between atoms, and relative ionic sizes.

F. Tool 6: WebCSD [12]

WebCSD, also referred to as Access Structures, provides public access to material structure databases. For cristobalite, only the alpha-cristobalite structure was available in the platform's database. The software rendered a tetragonal unit cell belonging to the $P4_12_12$ space

group as shown in Fig. 11. The unit cell with dimensions a=4.908Å, b=4.908Å, and c=6.784 Å contained five Si^{+4} ions, but incorrectly rendered only seven out of the eight O^{-2} ions in a typical α-cristobalite unit cell. The software could be used to measure the distance and angle between the ions, which resulted to be 1.63Å and 134.6 degrees as displayed in Appendix XIV. The relative atomic sizes depicted in Appendix XV were in alignment with the conventional trends in the periodic table regarding atomic radii mentioned above.

Furthermore, for graphite, the WebCSD software showed two stacked layers of hexagonal carbon networks characterized by 1.43 Å spacing between the carbon ions shown in Appendix XVI, close to the value of 1.44 Å provided in [15]. As shown in Fig. 12, the outer carbons of the structure were bonded by a double bond to the carbons of the hexagonal ring. The software did not support the function of building customized lattice structures, nor cut-out images.

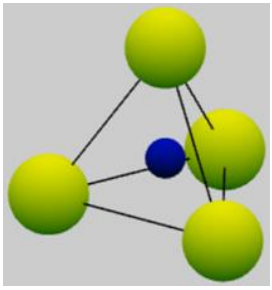

Fig. 9

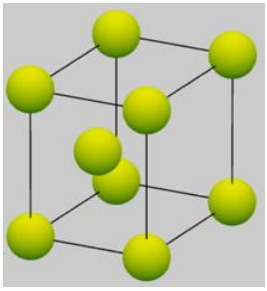

Fig. 10

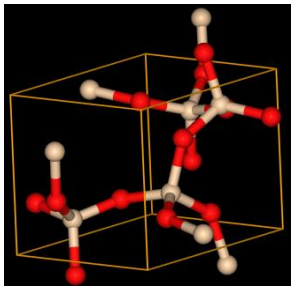

Fig. 11

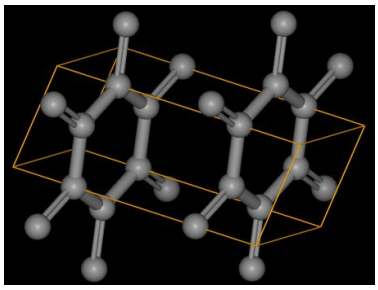

Fig. 12

G. Cut-Out Image

As none of the software methods explored were able to produce a cut-out image of the unit cells, we used a CAD program, Onshape, to manually construct the cut-out images for both alpha cristobalite (Fig. 13) and alpha graphite (Fig. 14) unit cells.

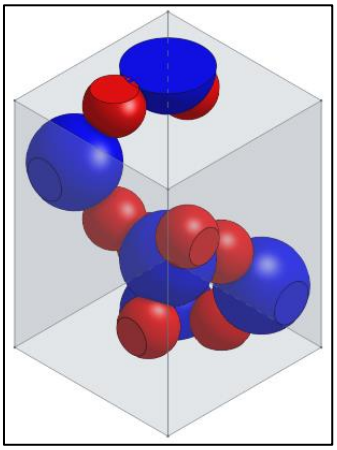

Fig. 13

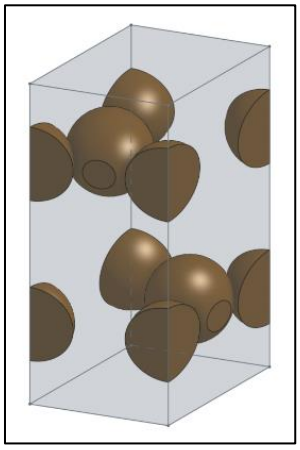

Fig. 14

III. CONCLUSIONS

Overall, after conducting a comparative analysis (Appendix XVII) it was revealed that VESTA was the most suitable software for modeling α-cristobalite and graphite with its functions to facilitate the assembly of unit cells, examination of the structure's composition, and reading of Crystallographic Information Files (.cif). VESTA and CrystalViewer would in particular be the most suitable for cases where the software is being used for inquiry purposes, where the user would benefit from the ability to manually build and alter the crystal structure for research. However, the relatively complex interface coupled with the limited database of pre-made crystal structures requires the user to expend time on developing technical knowledge of the software. For users seeking a "quick-search" of materials, the WebCDS is recommended as it extracts relevant information from a large pool of published research on crystalline structure through the least number of steps.

Avogadro, Atomsk, and Professor Kwan's Crystal Viewer are not recommended for making complex unit cell crystal structures. Avogadro is best used for visualizing molecules, rather than unit cells with its "draw and optimize" functions. Atomsk is not user friendly as users will have to learn every command for what they need to do in order to make it. Even then, users would not be able to see the structure unless imported into a visualizing software like OVITO. Another issue with Atomsk was that it was not compatible with Mac OS. Professor Kwan's Crystal Viewer provides visualization for only a restricted selection of materials and frequently seen basis structures. For the tool to be useful, the user would require preliminary knowledge on the basis of the crystal lattice to recognize that the model relates to the material structure being investigated.

To extend, none of the softwares discussed captured vacancy or dislocations of atoms that occur in crystal defects. Hence, it was evident that the scope of the software did not encompass factors such as thermal vibrations, solidification, and plastic deformation within the crystal lattice, ultimately demonstrating insufficient replication of crystal structures existing in nature. Further research is required on resources developed to visualize crystal defects to solidify knowledge on anomalies in lattice structures.

To certain limitations, the software explored in this activity serve as valuable visualization tools in the study of material science as it provides insight on the fundamental factors that influence the physical properties of materials critical to all manufacturing processes.

IV. References

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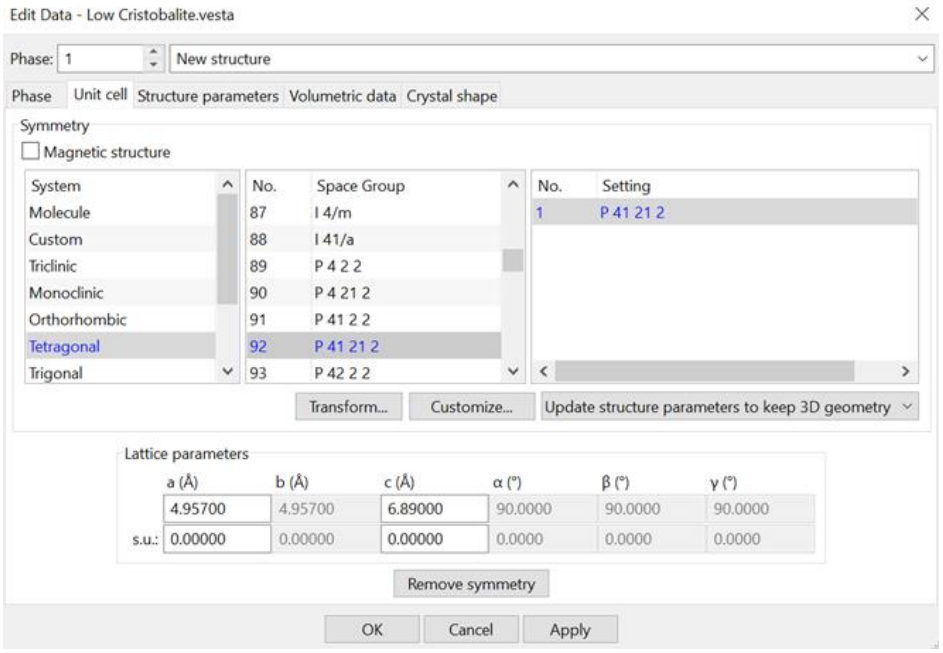
V. APPENDICES

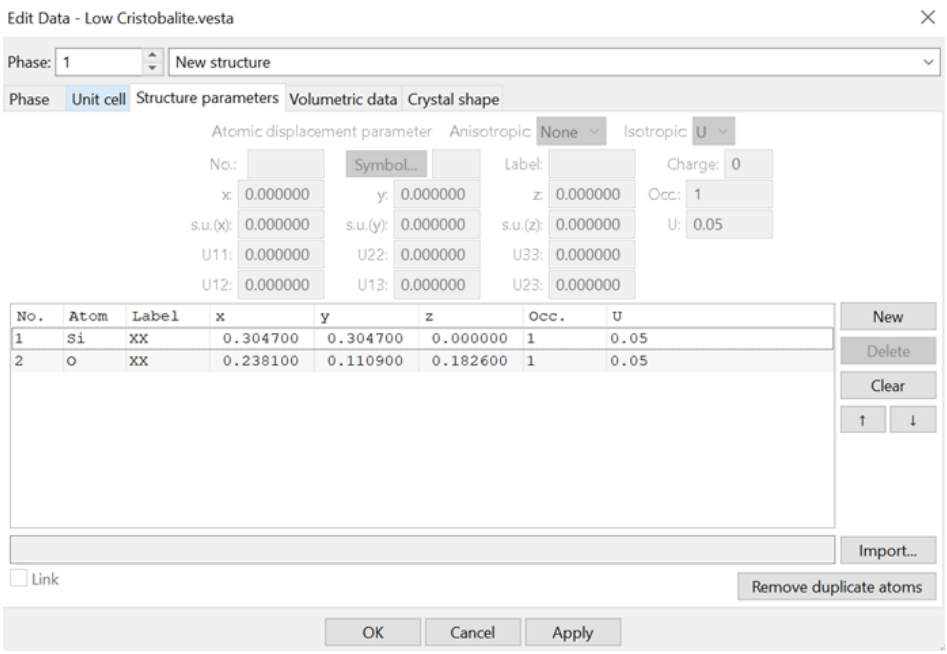
APPENDIX I

VESTA UNIT CELL MENU



APPENDIX II

VESTA STRUCTURE PARAMETERS MENU



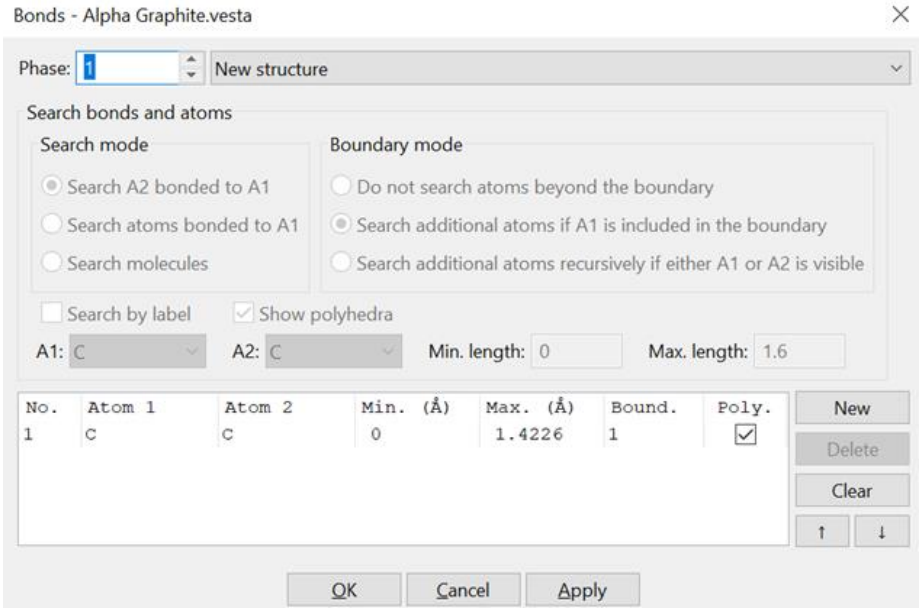
APPENDIX III

VESTA DISTANCE TOOL

```
Bond: 1(XX-XX) =  1.42259(0) Å
   1      XX   C   1.00000   1.00000   0.75000 ( 1,  1,  1)+ -x, -y, -z
   2      XX   C   0.66667   0.33333   0.75000 ( 1,  1,  1)+ -x, -y, -z
```

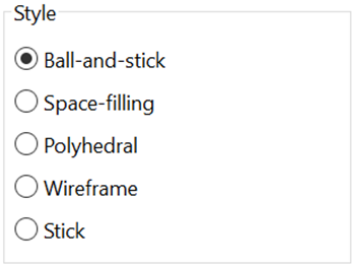
APPENDIX IV

VESTA BONDS MENU



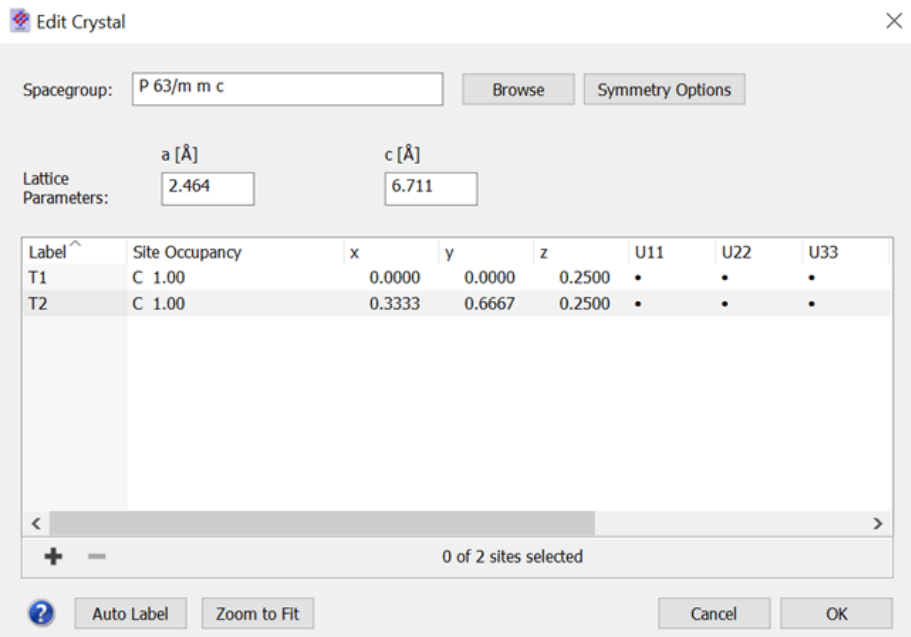
APPENDIX V

VESTA VIEW STYLES



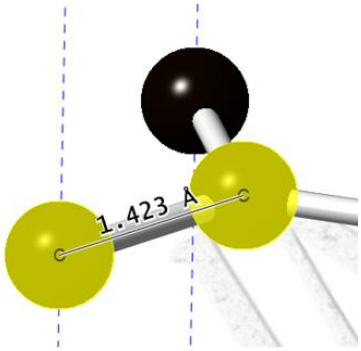
APPENDIX VI

CRYSTALMAKER 2017 EDIT CRYSTAL MENU



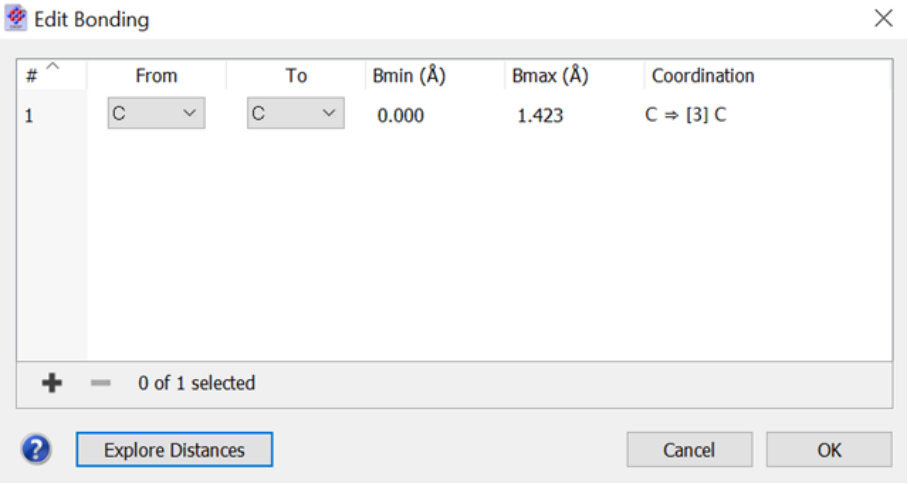
APPENDIX VII

CRYSTALMAKER 2017 DISTANCE TOOL



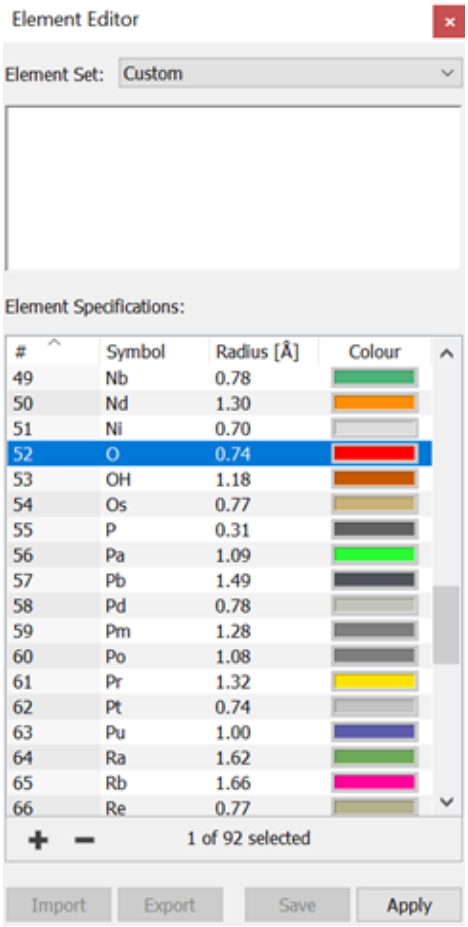
APPENDIX VIII

CRYSTALMAKER 2017 EDIT BONDING MENU



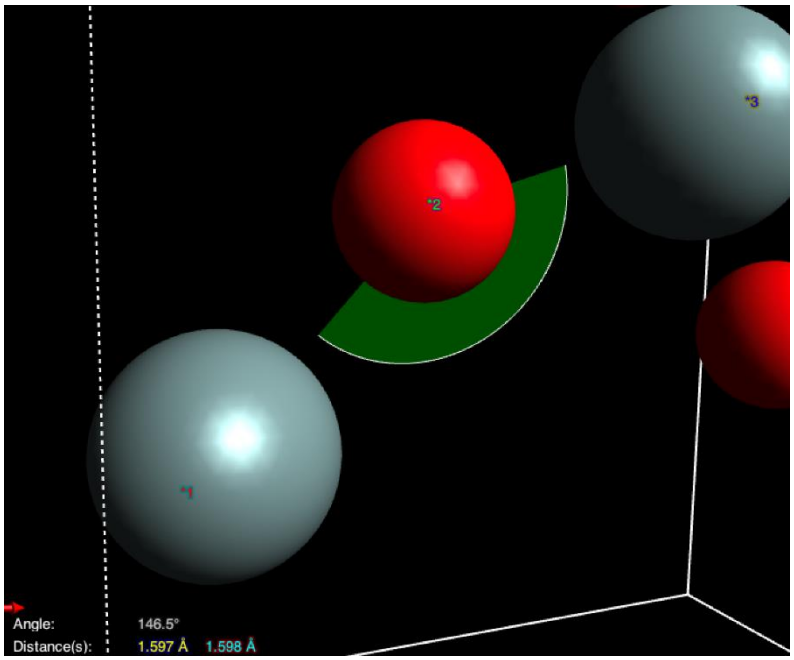
APPENDIX IX

CRYSTALMAKER 2017 ELEMENT EDITOR MENU



APPENDIX X

[AVOGADRO] DISPLAYING DISTANCE, AND ANGLES



APPENDIX XI

[ATOMSK] THE COMMAND TO MAKE GRAPHITE IN ATOMSK

```
PS C:\Users\magdy> atomsk --create graphite 2.464 6.11 C graphite2.cfg
 _____________________________________________
|                 _________                   |
|     o---o      A T O M S K                  |
|    o---o|      Version b0.11.2               |
|    |   |o      (C) 2010 Pierre Hirel        |
|    o---o       https://atomsk.univ-lille.fr |
|_____________________________________________|
 >>> Creating system:
 ..> C with hexagonal graphite structure with box vectors H1=[2-1-10], H2=[-12-10], H3=[0001].
 ..> System was successfully created.
 >>> Writing output file(s) (4 atoms):
 ..> Successfully wrote CFG file: graphite2.cfg
 \o/ Program terminated successfully!
     Total time: 0.012 s.; CPU time: 0.000 s.
```

APPENDIX XII

[OVITO] DISPLAYING POSITION, DISTANCE, ANGLES OF ATOMS

Filter...

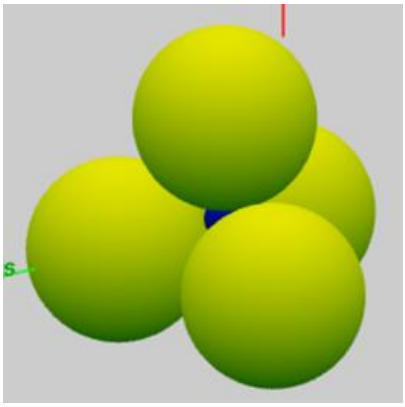
	Position	Particle Type
0	1.5104 1.5104 0	1 (Si)
1	0.968102 3.9889...	1 (Si)
2	3.4466 3.4466 3....	1 (Si)
3	3.9889 0.968102...	1 (Si)
4	1.18026 0.54973...	2 (O)

Pair A-B	Distance	Vector
0 - 1	3.06665	-0.542296 2.4785 1.72257
0 - 2	4.40078	1.9362 1.9362 3.44515
0 - 3	5.75695	2.4785 -0.542296 5.16772
1 - 2	3.06665	2.4785 -0.542296 1.72257
1 - 3	5.48812	3.0208 -3.0208 3.44515

Triplet A-B-C	Angle
1 - 0 - 2	44.1497
0 - 1 - 2	91.7007
0 - 2 - 1	44.1497

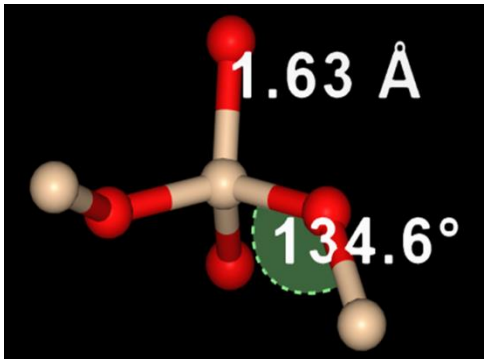
Appendix XIII

[Prof. Kwan's Activity] Misrepresented relative ionic sizes of Si4+ (blue) and O-2 (green) in a silicate tetrahedron



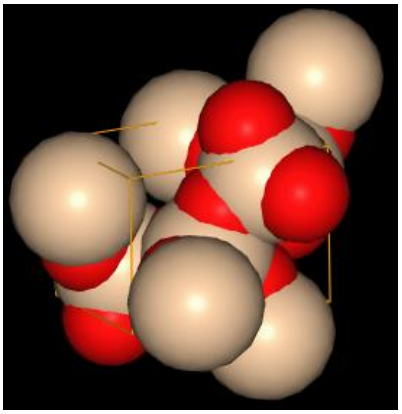
Appendix XIV

[WebCSD] Distance and angle between ions in the α-cristobalite unit cell



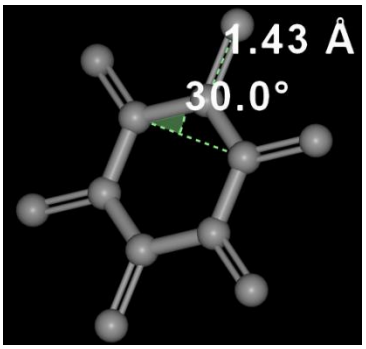
Appendix XV

[WebCSD] Depiction of relative ionic sizes in the α-cristobalite unit cell



APPENDIX XVI

[WEBCSD] DISTANCE AND ANGLE BETWEEN IONS IN THE GRAPHITE UNIT CELL



APPENDIX XVII

SOFTWARE COMPARISON CHART

	Unit Cell (C for Cristobalite, G for Graphite)	Displays proper # of O atoms (8)	Displays proper # of Si atoms (5)	Displays proper # of C atoms (6)	Displays bond linkage (stick)	Displays atomic distance and angles	Displays accurate relative atomic size	Supports CIF File Format	Can produce cross-sectional view	Can Build Unit Cell from Scratch
Vesta	C	Yes	Yes		yes	yes	yes	yes	no	yes
	G			yes	yes	yes	yes	yes	no	yes
CrystalViewer	C	yes	yes		yes	yes	no	yes	no	yes
	G			yes	yes	yes	yes	yes	no	yes
Avogadro	C	yes	yes		yes	yes	yes	no	no	no
	G			no	no	yes	yes	no	no	no
Atomsk/ OVITO	C	yes	no		yes	yes	yes	yes	no	no
	G			no	no	yes	yes	no	no	no
Prof.Charles Kwan's Activity	C	no	no		no	no	no	no	no	no
	G			yes	no	no	no	no	no	no
WebCSD	C	no	yes		yes	yes	yes	no	no	no
	G			yes	yes	yes	yes	no	no	no