

Figure 1 The structure of zirconia.

(b) (3 marks) Of the seven crystal systems shown in Figure 3.13a of Book 3 Part 1, to which does this structure belong?

(c) (3 marks) Use WebLab ViewerLite to measure the shortest Zr—O distance in picometres.

2.2

(d) (3 marks) Use WebLab ViewerLite to measure the shortest Zr—Zr distance in picometres.

(e) (7 marks) From the unit cell, determine the number of Zr atoms and O atoms in the structure. Then determine the empirical formula of the compound, and the number of formula units in the unit cell.

(f) (4 marks) Give the coordination number and describe the geometry (i) around a Zr atom, and (ii) around an O atom. You may find that it helps to view more than one unit cell: in order to do this, go into 'Crystal cell' under the 'Tools' menu, and then into 'preferences'.

(g) (3 marks) Can this structure be described in terms of the occupation of either octahedral or tetrahedral holes in a close-packed structure? Briefly explain why.

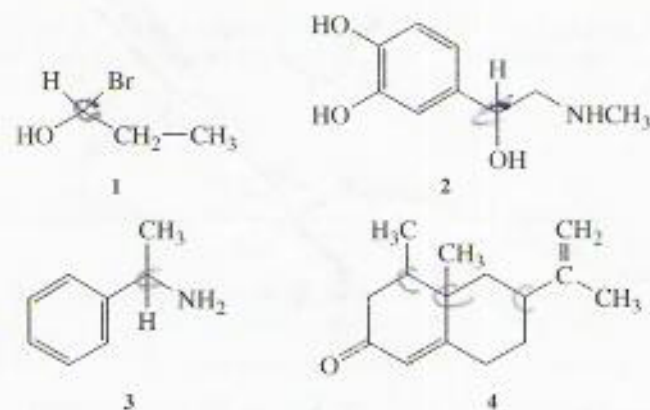
(h) (6 marks) Draw a unit cell projection of the zirconia structure shown in Figure 1.

(i) (8 marks) Compute the density of zirconia, and give your answer in both g cm^{-3} and kg m^{-3} .

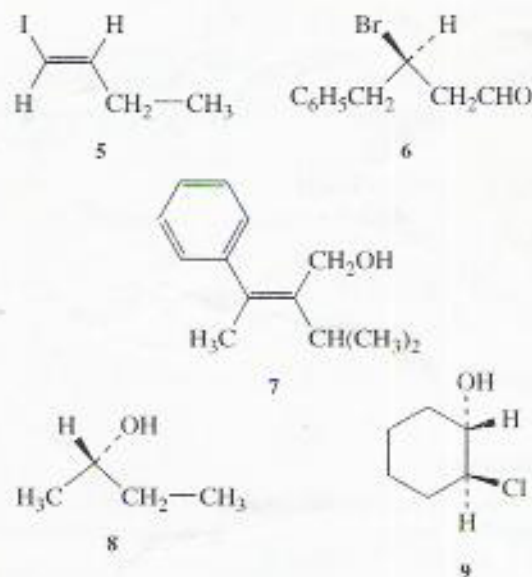
Question 3

This question carries 30 per cent of the marks for this assignment, and tests Learning Outcomes 9–13 and 15 of Book 3, Part 2.

(a) (10 marks) Redraw the structures 1–4 below and identify all the chiral centres in each structure by placing a * next to the appropriate atom(s).



(b) (10 marks) Assign *R/S* or *E/Z* labels to describe the configurations of molecules 5–9 below.



(c) (10 marks) Number the atoms in both the molecules 10 and 11, and designate the configuration (*R/S*) at both of the chiral centres in each molecule. Identify the stereochemical relationship between the two molecules. (Hint Use the algorithm in Figure 9.1 on p. 167 of Book 3 Part 2 to help you. Please bear in mind, however, that the 'YES' and 'NO' labels above the arrows leading from the box 'Are they superimposable on their mirror images?' are the wrong way round. The algorithm should read 'YES' they are diastereomers and 'NO' they are enantiomers.)

