Members of your team \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

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**Corundum**

Since the principal quantum numbers of Al and O are 3 and 2 respectively, why are the oxygen atoms larger than the aluminum atoms?

a) are the oxygen atoms in an A-B-C-A-B-C arrangement or an A-B-A-B arrangement?

b) Is this CCP or HCP?

c) Is the structure a perfect lattice or is it imperfect?

a) what is the coordination environment around the aluminum ions?

b) are the aluminum atoms centered in the polyhedra?

c) what is the average Al-O bond length?

a) In order to maintain charge neutrality, what is the charge on each Cr ion?

b) how many valence electrons are in this Cr ion?

c) draw an appropriate crystal field splitting diagram for the Cr and populate it with the electrons.

d) Given that rubies appear red, calculate the ∆o and report it in cm-1.

**Beryl**

a) what is the coordination environment around the aluminum ions?

b) are the aluminum atoms centered in the polyhedra?

c) what is the average Al-O bond length?

a) In order to maintain charge neutrality, what is the charge on each Cr ion?

b) how many valence electrons are in this Cr ion?

c) draw an appropriate crystal field splitting diagram for the Cr and populate it with the electrons.

d) Given that emeralds appear green, calculate the ∆o and report it in cm-1.

e) given the structures of Beryl and Corundum, explain using a physical model why the two materials have such different harndesses.

**Breakdown of CFT**

Given the background of the theory, that the central metal d orbitals are split due to repulsive electronic interactions with the ligands, predict which metal complex in each pair would have a higher crystal field:

a) Cr surrounded by 6 oxygen ions at 2.0 Å. Cr surrounded by 6 water molecules at 2.0 Å

b) Cr surrounded by 6 oxygen ions at 2.0 Å. Cr surrounded by 6 oxygen ions at 1.9 Å

Go back and record here the average Cr-O distances in emerald \_\_\_\_\_\_\_ and in ruby

\_\_\_\_\_\_\_. Does the color of emerald and ruby match that predicted by the distance argument you just calculated?

a) why is the modeling of ions in a crystal lattice as point charges reasonable?

b) why is the modeling of ions in a crystal lattice as point charges *un*reasonable?

c) looking at the structures of beryl and corundum, which seems more ionic and which seems more covalent. Why?

Questions:

Indicate on the diagram how you can tell that the ∆o for beryl is lower than that for corundum.

Show (circle the transition line) the electronic transitions responsible for the green color in emerald and red color in ruby.

{{Figure 1.4 from “Readings on color; The science of color,” volume 2, by Alex Byrne and David R. Hilbert, MIT Press, 1997” is presented here.}}