In groups of 2-3 students please work through the following problems based on J. Solid State Chem. 2019, 269, 553-557.

1. What is the space group of the title compound (see Table 1)? What does the space group say about the angles between the *a*, *b*, and *c* axes?

1. Please generate the unit cell in Vesta from the data in Table 2. Based on the structure you built in Vesta, calculate both the chemical formula for the entire unit cell and the empirical formula based on that unit cell.

1. The authors of this paper attempted to synthesize this material by mixing together stoichiometric ratios of 1 mol Pr: 2 mol Cu: 3 mol Te. However, the elemental analysis reveals that the formula is non-stoichiometric. What did the authors find?
2. The synthesized material maintains the same crystalline structure as the one you built in Vesta. Which element in the chemical composition; praseodymium, copper, or tellurium; should be most affected by the differences in the observed empirical formula? Using the concept of atomic site occupancy, rationalize how this observed data affects the overall structure.
3. What must the occupancies of each atomic site have to be to match the observed empirical formula?
4. What is the coordination number and coordination geometry around Cu?

1. What is the distance between two Te2 sites along the c axis for Pr-Cu-Te shown in figure 1?
   1. What would you expect to happen to this distance if Pr was replaced with Dy? Explain your reasoning.