Physical Chemistry Density of an Organocobalt Crystal Virginia B. Pett The College of Wooster

A series of organocobalt complexes have been synthesized and crystallized by students at The College of Wooster. These compounds are simplified models for coenzyme B_{12} . For the complex in which the organic ligand R = ethyl and L = water the GMW is 458.79 g mol⁻¹.



A student measured the density of the crystals by finding a solvent mixture in which the crystal neither sank nor rose to the surface. The density of the mixed solvent, and thus of the crystal was found to be 1.49 g cm⁻³. This method of determining the density is called "flotation."

The crystal chosen for diffraction study extinguished polarized light and was $0.3 \ge 0.3 \ge 0.1$ mm in size.

X-ray diffraction photographs gave the size and shape of the unit cell in the crystal. The lattice constants are 21.820, 7.386, 25.652 Å, 90, 101, 90°. The volume of the unit cell is 4055 Å. From systematically absent reflections, it was determined that the crystal system is monoclinc, and the space group is C2/c. This space group has 8 symmetry operations, and in this crystal there are 8 molecules in each unit cell (Z = 8).

Calculate the density of the crystal from the X-ray information in the previous paragraph and compare it to the density measured by flotation.

Hint: recall the definition of density from general chemistry. Calculate the density of one unit cell, given the mass of the 8 molecules and the volume of the unit cell. Take note of units.