DATA REPORT

Powder X-ray diffraction of flucytosine, $C_4H_4FN_3O$

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(Received 30 November 2019; accepted 8 December 2019)

Flucytosine, CAS #2022-85-7, crystallizes in the tetragonal space group *P*41212 (#94) with a = 6.643768(27), c = 23.89009(10) Å, V = 1054.500(7) Å^3, and Z = 8. In this work, the sample was obtained from the United States Pharmacopeial Convention (USP) Lot #R03100 and analyzed as-received. The room temperature (295 K) crystal structure was refined using synchrotron (λ = 0.412826 Å) powder diffraction data and optimized using the density functional theory (DFT). When looking down the *a*-axis, the crystal structure consists of multiple ribbon-like structures stacked into columns. The powder X-ray diffraction pattern of the compound has been submitted to ICDD® for inclusion in the Powder Diffraction File™ (PDF®). The agreement of the Rietveld-refined and DFT-optimized structures is good, with the largest difference in the external amine group with an overall root mean displacement of 0.056 Å. There is also evidence of unit cell expansion at higher temperatures, as the volume of the unit cell at 298 K was 1.6–1.9% greater than the two unit cells obtained at 150 K. A N–H···O hydrogen bond exists in the inter-ribbon region between the flucytosine molecules, resulting in a 3D hydrogen bond network. © *2020 International Centre for Diffraction Data*. [doi:10.1017/S0885715619000903]

Key words: flucytosine, Ancobon, Rietveld refinement, density functional theory

Flucytosine, also called 5-fluorocytosine (commercial name Ancobon), is an antifungal drug used to treat Candida (yeast) and cryptococcosis infections. Flucytosine, CAS #2022-85-7, crystallizes in the tetragonal space group $P4_12_12$ (#94) with a = 6.643768(27), c = 23.89009(10) Å, V = 1054.500(7) Å^3, and Z = 8. A reduced cell search in the Cambridge Structural Database (Groom *et al*., 2016) yielded one previous structure determination (Hulme and Tocher, 2006), using single-crystal X-ray diffraction collected at 150 K. A powder pattern calculated from this crystal structure is included in the Powder Diffraction file as entry 02-090-1047. Powder diffraction patterns calculated from low-temperature, single-crystal data typically have diffraction peaks with 2θ positions that differ from room temperature powder diffraction data. These differences subsequently hinder phase identification at room temperature, thus the need for high-quality, room temperature X-ray diffraction data (Kaduk *et al*., 2014).

In this work, the sample was obtained from the United States Pharmacopeial Convention (USP) Lot #R03100 and analyzed as-received. The diffraction data were collected on beamline 11-BM at the Advanced Photon Source at Argonne National Laboratory. The room temperature (295 K) crystal structure was refined using synchrotron (λ = 0.412826 Å) powder diffraction data and optimized using the density functional theory (DFT). Hydrogen positions were also included as a part of the structure and were re-calculated during the refinement (Figure 1).

The agreement of the Rietveld-refined and DFT-optimized structures is good, with the largest difference in the external amine group with an overall root-mean-squared displacement of 0.056 Å. When looking down the *a*-axis, the crystal structure consists of multiple ribbon-like structures stacked into columns. There is also evidence of unit cell expansion at higher temperatures, as the volume of the unit cell at 295 K was 1.6–1.9% greater than the unit cells obtained at 150 K. We noticed similar hydrogen bonding between the structures at 150 K and 298 K. Specifically, we also found the N1–H2···O1 hydrogen bond that exists in the inter-ribbon region between the flucytosine molecules, resulting in a 3D hydrogen bond network. The powder X-ray diffraction pattern of the compound has been submitted to ICDD® for inclusion in the Powder Diffraction File™ (PDF®; Gates and Blanton, 2019).

ACKNOWLEDGEMENTS

The authors thank the SIR Department at the Illinois Math and Science Academy for offering us this research opportunity.

FUNDING INFORMATION

The use of the Advanced Photon Source at Argonne National Laboratory was supported by the U.S. Department of Energy, Office of Science, and Office of Basic Energy Sciences under Contract No. DE-AC02-06CH11357. This work was supported by the International Centre for Diffraction Data (ICDD).

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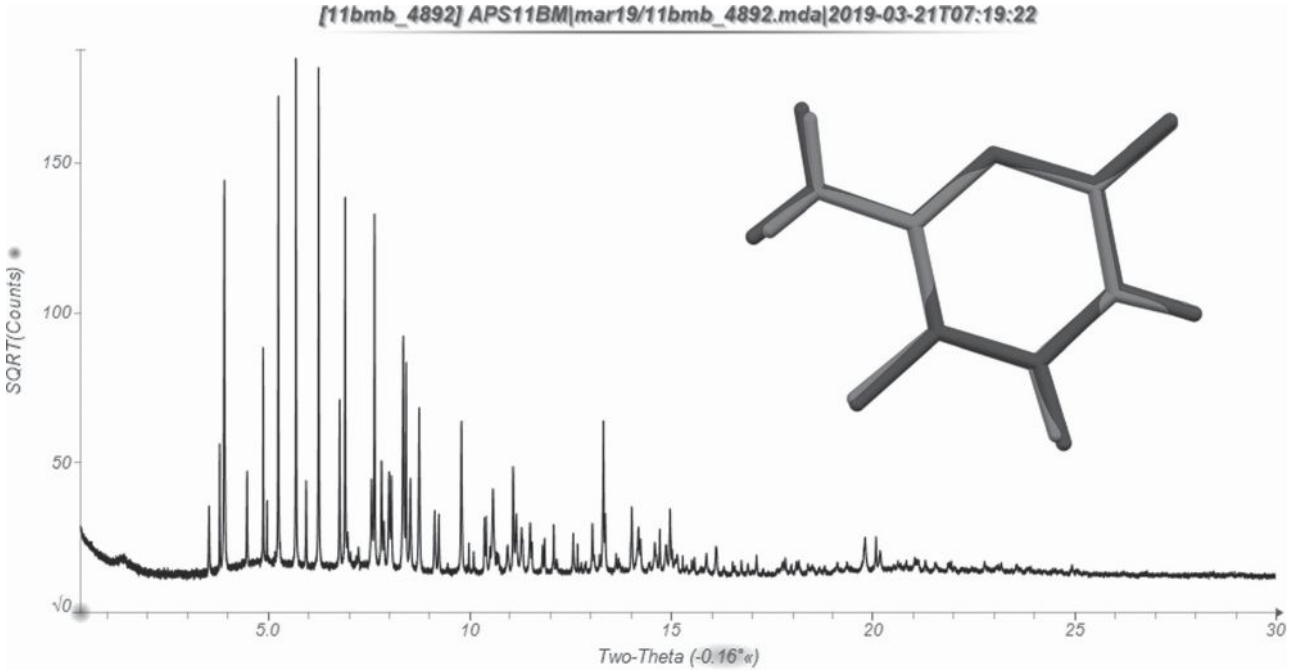

Figure 1. (Colour online) Powder X-ray diffraction pattern of flucytosine. The Rietveld refinement structure is indicated in red, and the DFT-optimized structure is indicated in blue.

DEPOSITED DATA

CIF and/or RAW data files were deposited with ICDD. You may request this data from ICDD at info@icdd.com.

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