Powder X-ray diffraction of escitalopram oxalate oxalic acid hydrate, $(C_{20}H_{21}FN_2O)_2(C_2O_4)(H_2C_2O_4)(H_2O)_{0.16}$

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Commercial escitalopram oxalate crystallizes as a hydrated adduct with oxalic acid, in the space group $P2_1$ with $a = 8.029897(21)$, $b = 25.09397(6)$, $c = 11.138930(31)$ Å, $\beta = 106.7759(2)°$, $V = 2148.992(7)$ Å^3, and $Z = 4$. The agreement of the Rietveld and previous single-crystal structures is excellent; the root-mean-square Cartesian displacements of the non-H atoms of the two independent cations are 0.076 and 0.067 Å, respectively. The water molecule refined to a slightly different position and occupancy. The pattern is included in the Powder Diffraction File™ (PDF®) as entry 00-064-1507. © *The Author(s), 2021. Published by Cambridge University Press on behalf of International Centre for Diffraction Data.* [doi:10.1017/S0885715621000026]

Key words: excitolopram, X-ray diffraction, Powder Diffraction File

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Escitalopram oxalate (Lexapro) is approved by the FDA for the treatment of depression and anxiety disorders. Commercial escitalopram oxalate crystallizes as a hydrated adduct with oxalic acid, in the space group $P2_1$ with $a = 8.029897(21)$, $b = 25.09397(6)$, $c = 11.138930(31)$ Å, $\beta = 106.7759(2)°$, $V = 2148.992(7)$ Å^3, and $Z = 4$. A reduced cell search in the Cambridge Structural Database (Groom *et al.*, 2016) yielded the crystal structure of the $(H_2O)_{0.25}$ hydrate (de Diego *et al.*, 2011; Refcode WASGAA). In this work, the sample was ordered from Sigma-Aldrich (Lot #053M4712V) and analyzed as-received. The crystal structure at room temperature (295 K) was refined using synchrotron ($\lambda = 0.413891$ Å) powder diffraction data and Rietveld refinement techniques.

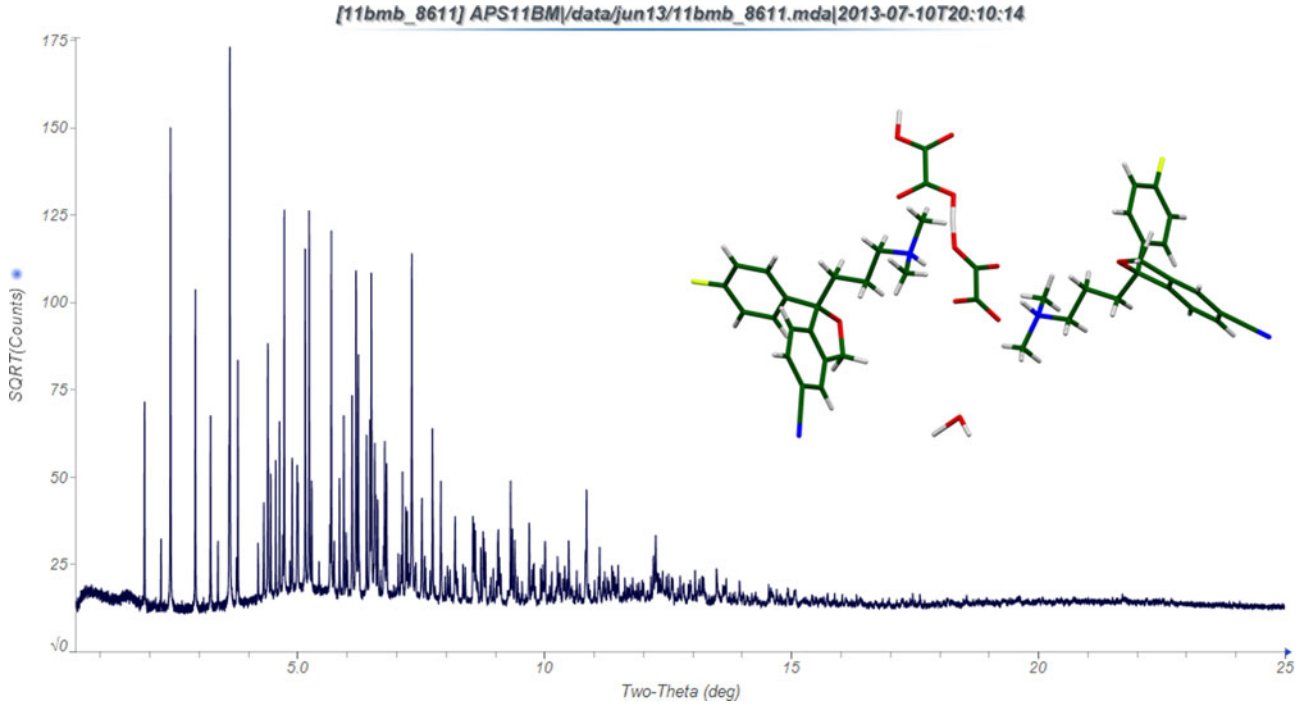

Figure 1. Powder X-ray diffraction pattern of escitalopram oxalate oxalic acid hydrate, with the molecular structure.

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The diffraction data were collected at beamline 11-BM at the Advanced Photon Source, Argonne National Laboratory. Figure 1 shows the powder X-ray diffraction pattern and the molecular structure. The agreement of the Rietveld and single-crystal structures is excellent; the root-mean-square Cartesian displacements of the non-H atoms of the two independent cations are 0.076 and 0.067 Å, respectively. The water molecule refined to a slightly different position and occupancy. The pattern is included in the Powder Diffraction File™ (PDF®) as entry 00-064-1507 (Gates-Rector and Blanton, 2019).

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DEPOSITED DATA

The supplementary material for this article, which includes Crystallographic Information Framework (CIF) files containing the results of the Rietveld refinement (including the raw data) was deposited with the ICDD. The data can be requested at info@icdd.com.

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