Powder X-ray diffraction of levothyroxine sodium pentahydrate, $C_{15}H_{10}I_4NNaO_4(H_2O)_5$

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(Received 6 January 2015; accepted 1 July 2015)

The room-temperature crystal structure of levothyroxine sodium pentahydrate has been refined using synchrotron powder diffraction data. The compound crystallizes in space group P1 (#1) with a = 8.2489(4), b = 9.4868(5), c = 15.8298(6) Å, α = 84.1387(4), β = 83.1560(3), γ = 85.0482(3) deg, V = 1220.071(9) Å^3, and Z = 2. Hydrogen atoms (missing from the previously-reported structure) were included. © *2015 International Centre for Diffraction Data*.
[doi:10.1017/S0885715615000676]

Key words: levothyroxine sodium, Synthroid, density functional theory, Rietveld refinement

Levothyroxine sodium pentahydrate (marketed as Synthroid) is a synthetic form of the thyroid hormone, thyroxine, which is used in the treatment of thyroid hormone deficiency. Commercial levothyroxine sodium pentahydrate crystallizes in the triclinic space group P1 (#1), with a = 8.2489(4) Å, b = 9.4868(5) Å, c = 15.8298(6) Å, α = 84.1387(4)°, β = 83.1560(3)°, γ = 85.0482(3)°, V = 1220.071(9) Å^3, and Z = 2. A reduced cell search in the Cambridge Structural Database yielded a previously reported crystal structure (Allen, 2002), which did not include hydrogens (Katrusiak *et al.*, 2004). In this work, the sample was ordered from United States Pharmacopeia, and analyzed as received. The

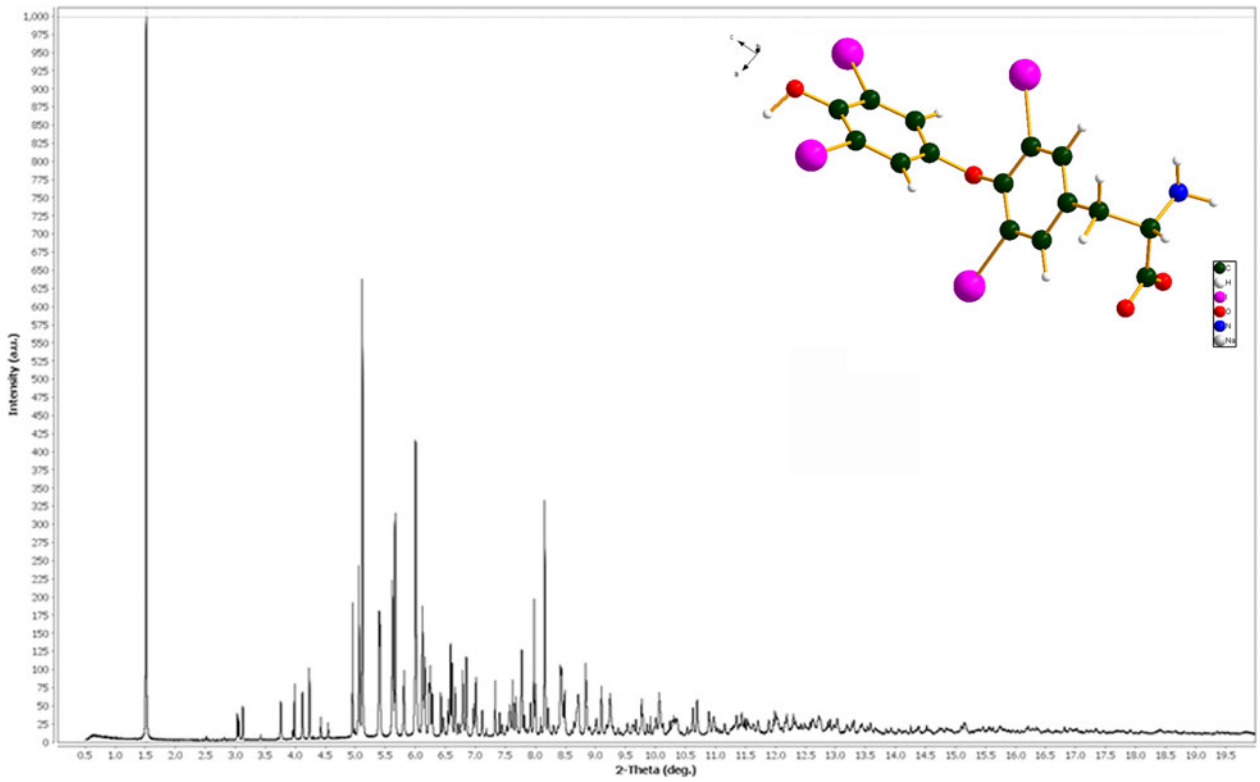

Figure 1. (Color online) Powder X-ray diffraction pattern of levothyroxine sodium pentahydrate.

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room-temperature crystal structure was refined using synchrotron ($\lambda = 0.413\,891$ Å) powder diffraction data, density functional theory, and Rietveld refinement techniques. Hydrogen positions were included as part of the structure, and recalculated during the refinement. The diffraction data were collected on beamline 11-BM at the Advanced Photon Source, Argonne National Laboratory. Figure 1 shows the powder X-ray diffraction pattern of the compound.

SUPPLEMENTARY MATERIALS

For supplementary material for this article, please visit http://dx.doi.org/10.1017/S0885715615000676

ACKNOWLEDGEMENTS

Use of the Advanced Photon Source at Argonne National Laboratory was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357. This work was partially supported by the International Centre for Diffraction Data. The authors thank Lynn Ribaud for his assistance in data collection.

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