Powder X-ray diffraction of albuterol sulfate $(C_{13}H_{22}NO_3)_2SO_4$

J.A. Kaduk,[1] C.E. Crowder,[2] K. Zhong,[2,a)] T.G. Fawcett,[2] and M.R. Suchomel[3]
[1]*Illinois Institute of Technology, 3101 S. Dearborn Street, Chicago, Illinois 60616*
[2]*ICDD, 12 Campus Boulevard, Newtown Square, Pennsylvania 19073-3273*
[3]*Argonne National Laboratory, Advanced Photon Source, 9700 S. Cass Avenue, Argonne, Illinois 60439*

(Received 10 March 2014; accepted 12 March 2014)

Albuterol sulfate (marketed as ProAir HFA or Ventolin HFA) is an important pharmaceutical used for the treatment of asthma. Commercial albuterol sulfate crystallizes in the monoclinic space group *Cc* (9), with $a = 28.0698(1)$ Å, $b = 6.18638(3)$ Å, $c = 16.92605(5)$ Å, $\alpha = 90°$, $\beta = 81.1328(3)°$, $\gamma = 90°$, $V = 2904.097(19)$ Å^3, and $Z = 4$. Previous structure determination did not include hydrogens (Leger et al., 1978). In this work, the sample was ordered from Sigma-Aldrich. The structure was solved and refined using synchrotron ($\lambda = 0.413914$ Å) powder diffraction data, and Rietveld and density functional techniques. Figure 1 shows the Powder X-ray diffraction pattern of the compound.

Leger, J. M., Goursolle, M.. Gadret, M. and Carpy, A. (**1978**). "Structure cristalline du sulfate de salbutamol [tert-butylamino-2 (hydroxy-4 hydroxyméthyl-3 phényl)-1 éthanol.0.5H2SO4]," Acta Cryst. B **34**, 1203–1208. CSD Refcode SALBUT.

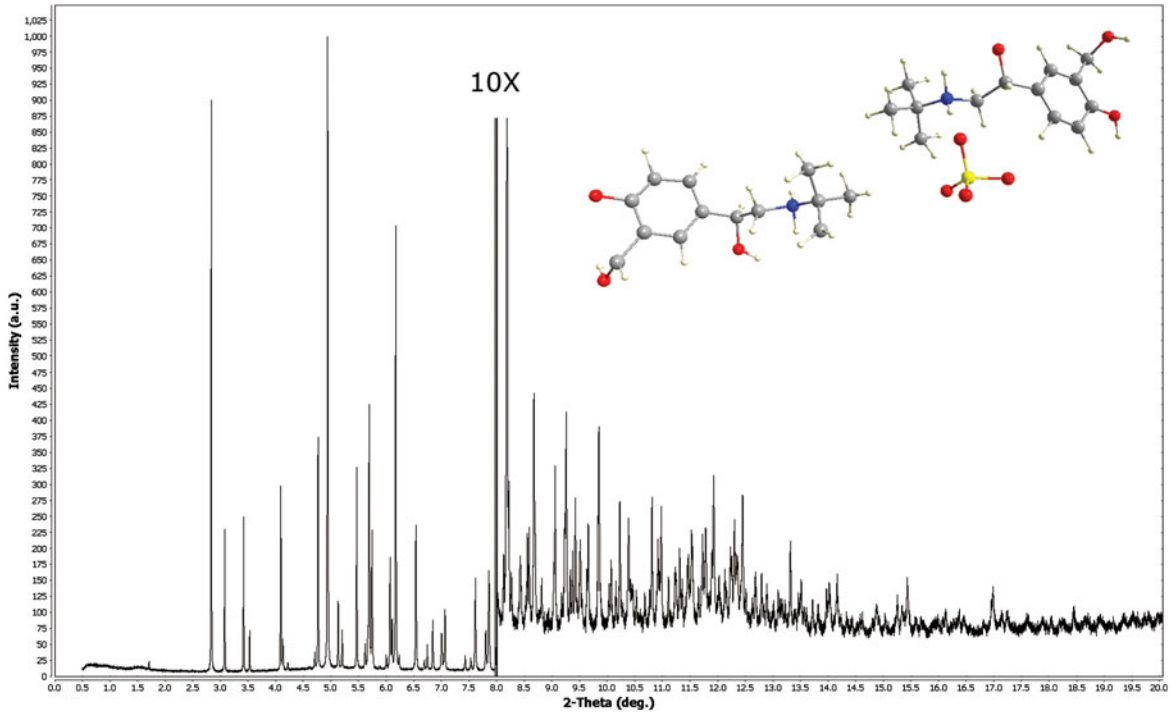

Figure 1. (Color online) Powder X-ray diffraction pattern of albuterol sulfate.

[a)]Author to whom correspondence should be addressed. Electronic mail: zhong@icdd.com
Data was submitted via Genie (http://www.icdd.com/websubmission/launch.html), the ICDD® Web Submission Page.

https://doi.org/10.1017/S0885715614000232 Published online by Cambridge University Press