Powder X-ray diffraction of ibandronate sodium monohydrate, $C_9H_{22}NNaO_7P_2(H_2O)$

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Ibandronate sodium monohydrate (marketed as Boniva) is an important pharmaceutical used in the prevention and treatment of osteoporosis. Commercial ibandronate sodium monohydrate crystallizes in the triclinic space group $P1(2)$, with $a = 5.97639(5)$ Å, $b = 9.19265(7)$ Å, $c = 14.85368(15)$ Å, $\alpha = 98.0829(11)°$, $\beta = 99.2075(15)°$, $\gamma = 93.6981(7)°$, $V = 794.361(13)$ Å^3, and $Z = 2$. Previous structure determination did not include hydrogens (Malpezzi et al., 2012). In this work, the sample was ordered from United States Pharmacopeia (USP). 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.

Malpezzi, L., Elisabetta Maccaroni, E., Carcano, G. and Ventimiglia, G. (**2012**). "Structural and thermal characterization of sodium ibandronate monohydrate," J. Thermal. Anal. Calorim. **109**, 373–379. CSD Refcode YEHJOM.

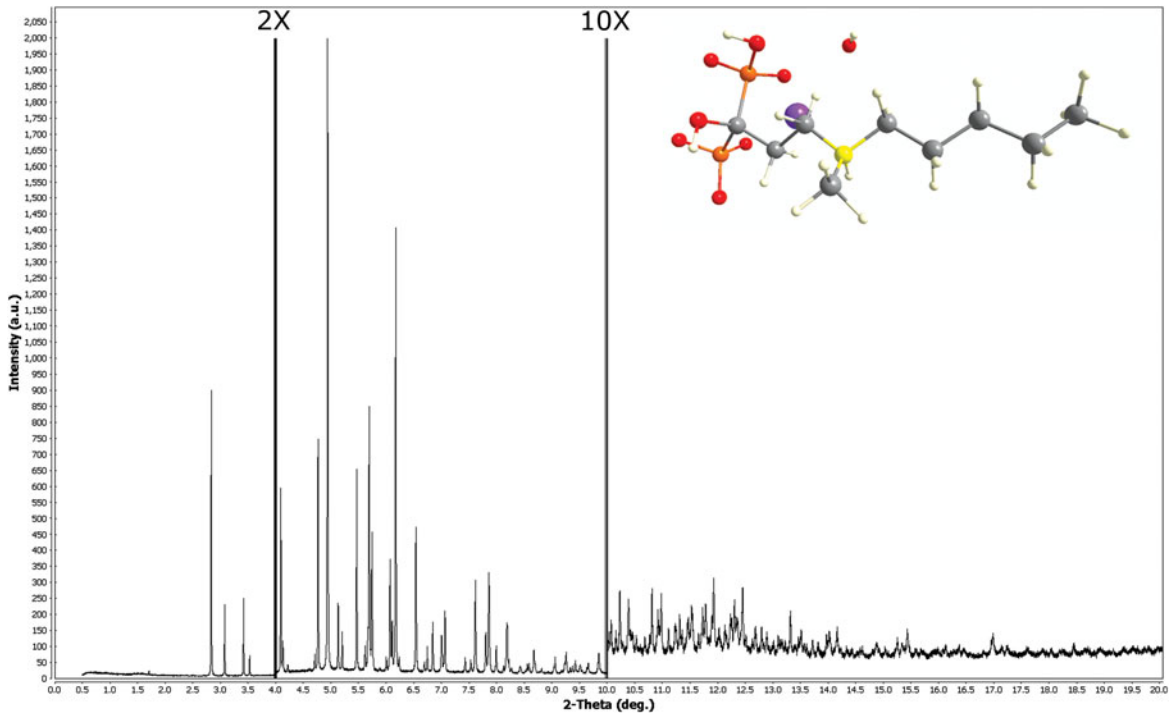


Figure 1. (Color Online) Powder X-ray diffraction pattern of ibandronate sodium monohydrate.

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