CRYSTAL STRUCTURES OF LARGE-VOLUME COMMERCIAL PHARMACEUTICALS

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As part of a continuing project, the room-temperature crystal structures of several commercial pharmaceutical APIs have been solved using synchrotron X-ray powder diffraction data (11-BM at APS), and optimized using density functional techniques. All of the structures presented have features which made their solution and refinement non-routine. The molecules to be discussed include: 1. terazosin hydrochloride dihydrate (Hytrin), which was originally solved (but only approximately) using data contained in the Powder Diffraction File database. 2. bretylium tosylate (Bretylol and others), which exhibited significant decomposition in the beam. 3. oxybutynin hydrochloride hemihydrate (Dytropan and Lyrinel XL), which has not been described as a hemihydrate, and which exhibits X-ray induced photoreduction of a triple bond. 4. levocetirizine dihydrochloride (Xyzal), which solves and refines better in $P2_1/n$ rather than the true space group $P2_1$. The presentation may also include progress (or lack thereof) on febuxostat Form G (Uloric and Adenuric), as well as other new structures as they are solved.