Structure determination of racemic trichlormethiazide from powder diffraction data

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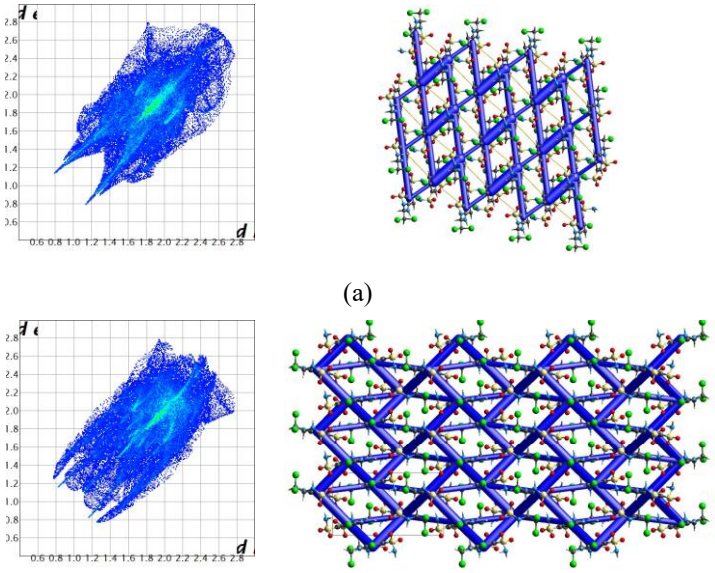
Trichlormethiazide is a thiazide derivative, an important group of diuretic drugs, which is used in the treatment of hypertension. The Cambridge Structural Database (CSD) contains only one report (KIKCUD) associated with this pharmaceutical [1], corresponding to the orthorhombic form of anhydrous *S*-Trichlormethiazide. The PDF-4/Organics database contains two entries. One is the calculated pattern of the CSD entry (PDF 02-094-5865) and the other is an experimental unindexed pattern (PDF 00-039-1828). In this contribution the structure of racemic Trichlormethiazide was determined from laboratory X-ray powder diffraction data. This material was also characterized by FT-IR, TGA and DSC. The structure was determined with DASH [2] and refined by the Rietveld method with TOPAS-Academic [3]. The final unit-cell parameters are ***a*** = 8.4389(6), ***b*** = 8.8929(7), ***c*** = 9.7293(8) Å, α = 91.315(3)°, β = 106.113(2)°, γ = 97.1580(17)°, V = 694.73(9) Å^3, Z = 2. The refinement converged to R_p = 0.0512, R_{wp} = 0.0694, and *GoF* = 2.704. In the crystal structure, the molecules form chains along the **a**-axis connected by cyclic N-H···N and N-H···Cl hydrogen bonds. The chains are connected by additional cyclic N-H···Cl hydrogen bonds to form layers almost parallel to the ***ab*** plane. The fingerprint plots and energy frameworks diagrams of *S* and racemic forms clearly show the different intermolecular interactions and their topologies. A detailed discussion will be present in this work.



(a)

(b)

Figure 1. Fingerprint plots and energy frameworks diagram (along *b*) for (a) *S*- and (b) racemic trichlormethiazide.

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2. David, W., Shankland, K., van de Streek, J., Pidcock, E., Motherwell, W.D.S., Cole, J. (2006). *J. Appl. Crystallogr*. **39**, 910.
3. Coelho, A.A. (2016) TOPAS-Academic version 6, Coelho Software, Brisbane, Australia.

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