Supplementary Material (ESI) for New Journal of Chemistry

Supplementary material

Polymorphic gabapentin: thermal behaviour, reactivity and interconversion of forms in solution and in the solid state.

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Form III crystals were obtained dissolving gabapentin Form II in ethyl –L-lactate and let evaporate at room temperature.

Form IV crystals were obtained in a co-crystallization attempt of gabapentin and morpholine. Gabapentin Form II was dissolved in a mixture of morpholine, water and ethanol (2:1:1) and the solution was heated at 80ºC for 30 min, allowing the solution to boil in the last 3 minutes. Crystals were obtained by slow evaporation at room temperature. Suitable crystal for single-crystal x-ray diffraction analysis was chosen as soon as they appeared in the solution (approximately 13h after). The remaining crystals formed were removed from the solution and were left to dry.

Crystal data for Form III were collected at room temperature on a Nonius CAD4 diffractometer; with Mo-Kα radiation, λ = 0.71073 Å, monochromator graphite. M = 171.24; monoclinic C2/c, a = 30.582(9), b = 5.932(3), c = 10.915(3) Å, β = 108.31(2)°, V=1879.9(12)Å3, Z = 8, D_c = 1.210 0.0177). SHELX97 was used for structure solution and refinement based on F^2. Non-hydrogen atoms were refined anisotropically. Hydrogen atoms bound to carbon atoms were added in calculated positions.

Crystal data for Form IV were collected at room temperature on a Bruker AXS-KAPPA APEX II diffractometer using graphite-monochromated Mo-Kα (radiation λ=0.71069 Å). $C_9H_{17}NO_2$, M = 171.24; monoclinic $P2_1/c$, a = 14.7361(17), b = 6.6656(12), c = 9.890(2) Å, β = 106.090(6), V = 933.4(3)$Å^3$, Z = 4, D_c = 1.219 g.cm^{-3}, R_1 (wR_2)= 0.0654 (0.1923) for 1750 observed independent reflections (Rint = 0.0782). SIR97 was used for structure solution and refinement based on F^2. Non-hydrogen atoms refined anisotropically. H_{NH} atoms found and refined. H_{CH} atoms added in calculated positions and refined riding on their C atoms.