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Comparative Crystal Structure Analysis of (2S, 3S)-2-morpholino-3-phenylpentan-3-ol hydrochloride and (2S, 3R)-2-morpholino-3-phenylpentan-3-ol hydrochloride

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Abstract : The crystal structure of the potential active (2*S*, 3*S*)-2-morpholino-3-phenylpentan-3-ol hydrochloride and (2*S*, 3*R*)-2-morpholino-3-phenylpentan-3-ol hydrochloride has been determined from single crystal X-ray diffraction data. The both compound are structurally diastereomers, but it adopts different crystal system. In compound I crystallizes in the monoclinic system space group C_12_1 with unit cell dimension a=12.9486 (15) Å, b=6.0083 (5) Å and c= 19.670 (18)Å [α=90°, β= 95.484 (5)° and γ= 90°] and for the compound II crystallizes in the orthoromic system space group $P2_12_12_1$ with unit cell dimension a= 5.8923 (9) Å, b=11.413 (2) Å and c= 22.659 (4)Å [α=90°, β= 90° and γ= 90°] In both the compound morpholino ring adopts chair conformation. The crystal packing is stabilized by intermolecular C-H...O hydrogen bond interaction.
Keywords: Morpholine; Diastereomers; Single Crystal Structure; X-ray diffraction.

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