Ab-initio Structure Determination of $C_{18}H_{19}N_4S$ from Powder X-Ray Diffraction

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The crystal structure of 1-(N-allythiacarbamoyl)-3-(4-methyl-phenyl)-5-(pyrol-2-yl)-2-pyrazoline, $C_{18}H_{19}N_4S$, has been solved by the method of simulated annealing from synchrotron x-ray powder diffraction data. Pyrazolines are known to display various biological functions, such as fungicidal, antibacterial activities, pharmacological properties such as anti-inflammatory agents and industrial applications. The powder sample was sealed in 1mm capillary and diffraction data was collected with curved imaging plate method using 12KeV x-rays at the BL01C2 beamline in National Synchrotron Radiation Research Center (NSRRC). The structure was determined while following these procedures: (1) determination of the unit cell parameters, (2) determination of the space group, (3) extraction process by Pawley method, (4) structure solution by simulated annealing using DASH (David et al., 1998) and (5) Rietveld refinement by GSAS (Larson &Von Dreele, 1990) programs. The title compound crystallizes in triclinic system with space group, *P* -1, unit cell parameters of a = 12.603(14), b = 9.094(8), c = 8.494(8)Å, α = 70.85(8)˚, β = 105.26(8)˚, γ = 109.10 (7)˚, Volume = 855.7Å^3 and Z=2. The final reliability factors of Rietveld refinement are R_{wp} = 0.039 R_p = 0.029 R_B = 0.118 and S = 1.041.

Keywords: ab-initio structure determination, drug design, synchron powder diffraction