

## Crystal Structure Determination from Synchrotron X-ray Powder Diffraction Data by Simulated Annealing

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The crystal structure of 1-(N-allylthiocarbamoyl)-3-(4-methylphenyl)-5-(pyrol-2-yl)-2-pyrazolines, C<sub>18</sub>H<sub>19</sub>N<sub>4</sub>S (P1A12) has been determined by the method of Simulated Annealing from synchrotron x-ray powder diffraction data. Pyrazolines are known to display various biological properties, such as fungicidal, antibacterial activities, pharmacological properties such as anti-inflammatory agents and industrial properties. The compound crystallizes in triclinic system space group, *P*-1, *Z*=2, unit cell parameters of *a*=13.228Å, *b*=9.019Å, *c*=8.489Å,  $\alpha$ =109.190°,  $\beta$ =113.057°,  $\gamma$ =95.742°, and *V*=855.02Å<sup>3</sup>. Figure 1 shows as XRD pattern and ORTEP diagram from Simulated Annealing.

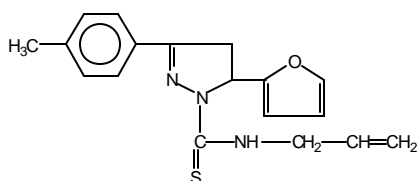
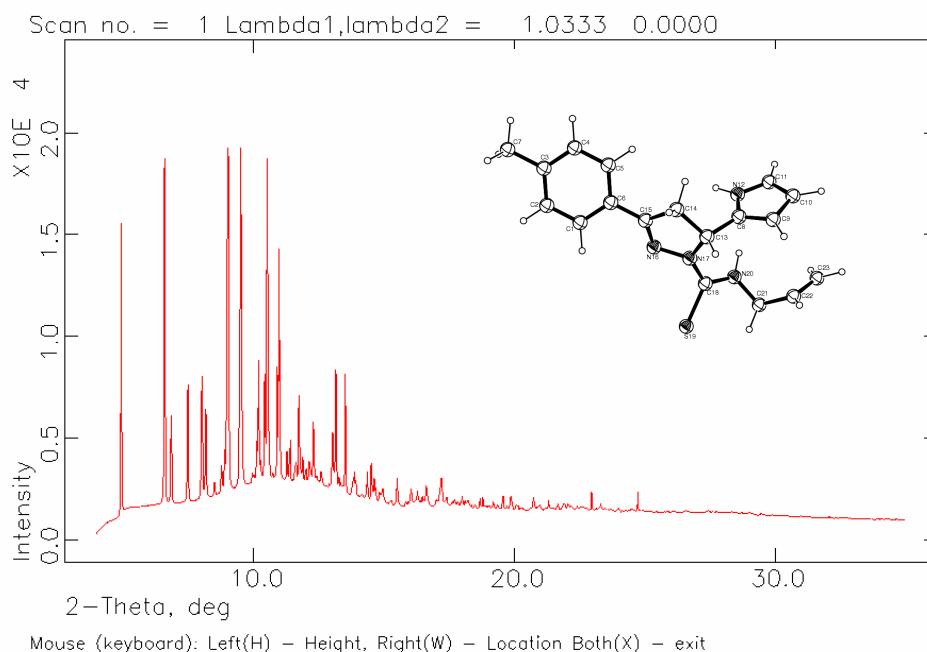


Diagram of P1A12



**Figure 1.** Powder diffraction pattern as a function diffraction angle  $2\theta$ , and ORTEP 3 of the compound P1A12.