Experimental. A prismatic crystal (0.1x0.1x0.2 mm) was selected and mounted on a MAR345 diffractometer with an image plate detector. Unit-cell parameters were determined from automatic 185 reflections (3 < θ < 31°) and refined by least-squares method. Intensities were collected with graphite monochromatized Mo Kα radiation. 16387 reflections were measured in the range 1.58 ≤ θ ≤ 32.35. 5891 of which were non-equivalent by symmetry (Rint(on I) = 0.076 ). 5116 reflections were assumed as observed applying the condition I > 2σ(I). Lorentz-polarization but no absorption corrections were made.

The structure was solved by Direct methods, using SHELXS computer program (Sheldrick, G.M., (1997), A computer program for automatic solution of crystal structure. UNIVER goettingen, Germany) and refined by full-matrix least-squares method with SHELX97 computer program (Sheldrick, G.M., (1997), A program for crystal structure refinement. Univer Goettinhen, Germany), using 16387 reflections, (very negative intensities were not assumed). The function minimized was Σ w ||Fo||² - ||Fc||² /P, where w = [σ²(I) +(0.0785P)²+5.2849P]⁻¹, and P = (||Fo||² + 2 ||Fc||² )/3, f, f' and f'' were taken from International Tables of X-Ray Crystallography (International Tables of X-Ray Crystallography, (1974), Ed. Kynoch press, Vol. IV, pp 99-100 and 149). 15H atoms were located from a difference synthesis and refined with an overall isotropic temperature factor and 7H atoms were computed and refined, using a riding model, with an isotropic temperature factor equal to 1.2 time the equivalent temperature factor of the atom which are linked. The final R(on F) factor was 0.077, wR(on ||F||²) = 0.181 and goodness of fit = 1.09 for all observed reflections. Number of refined parameters was 351. Max. shift/esd = 0.00, Mean shift/esd = 0.00. Max. and min. peaks in final difference synthesis was 0.562 and -0.767 e.Å⁻³, respectively.

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Table 1. Crystal data and structure refinement for xcpm80.

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Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\AA^2 \times 10^3$) for xcpm80. $U_{eq}$ is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

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Symmetry transformations used to generate equivalent atoms:
Table 4. Anisotropic displacement parameters (Å\(^2\) x 10\(^3\)) for xcpm80.
The anisotropic displacement factor exponent takes the form:
\[-2 \pi^2 \left[ h^2 a^* a^* U_{11} + ... + 2 h k a^* b^* U_{12} \right]\]

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for xcpm80.

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