The Structure of Compound 3b.
**X-Ray Analysis for Compound 3c**

The data were collected on a Bruker AXS smart X-ray diffractometer equipped with a CCD area detector and a graphite-monochromated Mo Kα radiation ($\lambda = 0.71073$ Å). A total of 18438 reflections, of which 4005 unique ($R_{int} = 0.0402$) were collected in a $\theta$ range of 1.39 to 26.41°. The data were corrected by empirical absorption. The structure was solved by direct method and refined anisotropically for all non-hydrogen atoms by full-matrix least squares. All calculations were performed using SHLEXTL (version 5.1) proprietary software package. Crystal data for 3c: $C_{23}H_{17}BrCl_2$ ($M = 444.18$), crystal size 0.41 x 0.22 x 0.15 mm, monoclinic, space group P2₁/c, $a = 11.0373(12)$ Å, $b = 6.0040(6)$ Å, $c = 29.402(3)$ Å, $\beta = 94.695(2)^\circ$, $V = 1948.5(4)$ Å$^3$, $Z = 4$, $Dx = 1.514$ mg/m$^3$, $\mu = 2.388$ mm$^{-1}$, $T = 295$ K, $R1 = 0.334$ (wR2 = 0.0846), GOF = 1.119, max/min $\Delta\rho = 0.557/-0.657$ e Å$^{-3}$. 
Table 1. Crystal data and structure refinement for 3c.

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| Largest diff. peak and hole                   | 0.557 and -0.657 eÅ⁻³
Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [Å^2 x 10^3] for 3c. 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 \([\text{Å}^2 \times 10^3]\) for 3c.

The anisotropic displacement factor exponent takes the form:

\[-2\pi^2 \left( \text{ha}^2 \text{U}_{11} + \ldots + 2\text{hka}^* \text{b}^* \text{U}_{12} \right)\]

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Table 5. Hydrogen coordinates ($x \times 10^4$) and isotropic displacement parameters ($\AA^2 \times 10^3$) for 3c.

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