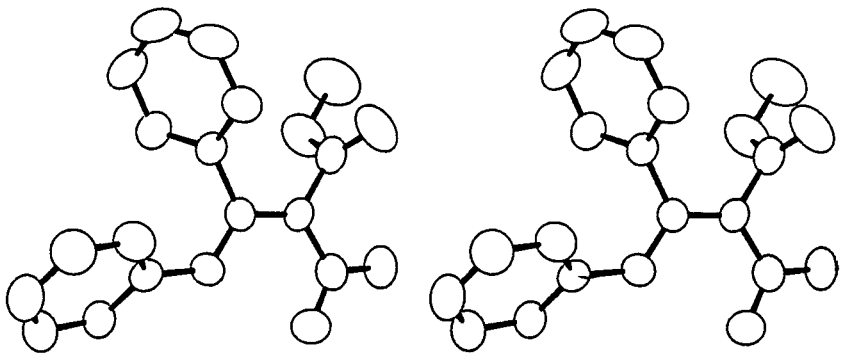
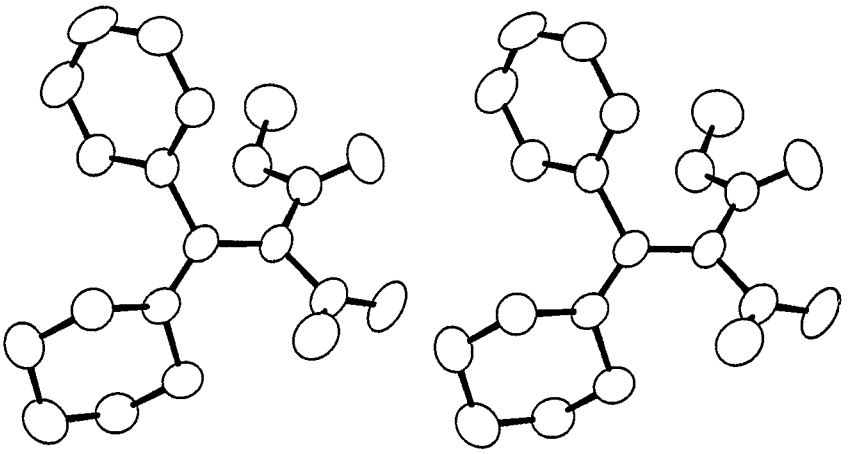


A stereoview of **7a**



A stereoview of **7b**

X-RAY CRYSTAL STRUCTURE ANALYSIS FOR 7a

Data were measured on a PW1100/20 Philips Four-Circle Computer-Controlled Diffractometer. MoK_{α} (λ=0.71069 Å) radiation with a graphite crystal monochromator in the incident beam was used. The unit cell dimensions were obtained by a least-squares fit of 24 centered reflections in the range of $10 \leq \theta \leq 14^{0}$. Intensity data were collected using the ω-2θ technique to a maximum 2θ of 46^{0}. The scan width, $\Delta\omega$, for each reflection was $1.00 + 0.35 \cdot \tan\theta$ with a scan speed of 3.0 deg/min. Background measurements were made for a total of 10 seconds at both limits of each scan. Three standard reflections were monitored every 60 minutes. No systematic variations in intensities were found.

Intensities were corrected for Lorentz and polarization effects. All non-hydrogen atoms were found by using the results of the SHELXS-86 direct method analysis (1). After several cycles of refinements (2) the positions of the hydrogen atoms were calculated, and added to the refinement process. Refinement proceeded to convergence by minimizing the function $\Sigma w(|F_o|-|F_c|)^2$. A final difference Fourier synthesis map showed several peaks less than 0.24 $e/Å^3$ scattered about the unit cell without a significant feature.

The discrepancy indices, $R=\Sigma||F_o|-|F_c||/\Sigma|F_o|$ and $R_w=\left[\Sigma w(|F_o|-|F_c|)^2/\Sigma w|F_o|^2\right]^{1/2}$ are presented with other pertinent crystallographic data in table I.

(1)Sheldrick G. M., Crystallographic Computing 3, Oxford University Press, pp. 175-189 (1985).

(2)All crystallographic computing was done on a VAX9000 computer at the hebrew University of Jerusalem, using the TEXSAN Structure Analysis Software.

X-RAY CRYSTAL STRUCTURE ANALYSIS FOR 7b

Data were measured on a PW1100/20 Philips Four-Circle Computer-Controlled Diffractometer. MoK_α (λ=0.71069 Å) radiation with a graphite crystal monochromator in the incident beam was used. The unit cell dimensions were obtained by a least-squares fit of 24 centered reflections in the range of $10 \leq \theta \leq 15^\circ$. Intensity data were collected using the ω-2θ technique to a maximum 2θ of 50°. The scan width, $\Delta\omega$, for each reflection was $0.80 + 0.35 \tan\theta$ with a scan speed of 3.0 deg/min. Background measurements were made for a total of 10 seconds at both limits of each scan. Three standard reflections were monitored every 60 minutes. No systematic variations in intensities were found.

Intensities were corrected for Lorentz and polarization effects. All non-hydrogen atoms were found by using the results of the SHELXS-86 direct method analysis (1). After several cycles of refinements (2) the positions of the hydrogen atoms were calculated, and added to the refinement process. Refinement proceeded to convergence by minimizing the function $\Sigma w(|F_o|-|F_c|)^2$. A final difference Fourier synthesis map showed several peaks less than 0.18 e/Å^3 scattered about the unit cell without a significant feature.

The discrepancy indices, $R=\Sigma||F_o|-|F_c||/\Sigma|F_c|$ and $R_w=[\Sigma w(|F_o|-|F_c|)^2/\Sigma w|F_o|^2]^{1/2}$ are presented with other pertinent crystalloraphic data in table I.

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