JOC The Journal of Organic Chemistry

J. Org. Chem., 1996, 61(21), 7326-7334, DOI:10.1021/jo960911k

TABLE S1

X-ray Crystal Structure Analysis of 3

Data were measured on an ENRAF-NONIUS CAD-4 Computer-Controlled Diffractometer. CuK_α (λ= 1.54178 Å) radiation with a graphite crystal monochromator in the incident beam was used. The standard CAD-4 centering, indexing, and data collection programs were used. The unit cell dimensions were obtained by a least-squares fit of 24 centered reflections in the range of $24 \leq \theta \leq 33°$.

Intensity data were collected using the θ-2θ technique to a maximum 2θ of 140°. The scan width, $\Delta\theta$, for each reflection was $0.80 + 0.15 \tan\cdot\theta$. An aperture with a height of 4 mm and a variable width, calculated as $(2.0 + 0.5 \tan\cdot\theta)$ mm, was located 173 mm from the crystal. Reflections were first measured with a scan of 8.24°/min. The rate of the final scan was calculated from the preliminary scan results so that the ratio $I/\sigma(I)$ would be at least 40 but the maximum scan time would not exceed 60 seconds. If in a preliminary scan $I/\sigma(I) < 2$, this measurement was used as the datum. Scan rates varied from 1.27 to 8.24°/min. Of the 96 steps in the scan, the first and the last 16 steps were considered to be background. During data collection the intensities of three standard reflections were monitored after every hour of X-ray exposure. No decay was observed. In addition, three orientation standards were checked after 100 reflections to check the effects of crystal movement. If the standard deviation of the h, k, and l values of any orientation reflection exceeded 0.06, a new orientation matrix was calculated on the basis of the recentering of the 24 reference reflections.

Intensities were corrected for Lorentz and polarization and absorption 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 0.8 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 $R_w = [\Sigma w(|F_o|-|F_c|)^2/\Sigma w|F_o|^2]^{1/2}$ are presented with other pertinent crystallographic data in the following Table.

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

(2) All crystallographic computing was done on a VAX 9000 computer at the Hebrew University of Jerusalem, using the TEXSAN structure Analysis Software.

Crystallographic Data for 3

formula	$C_{40}H_{44}S_2 \cdot 1/2\ C_5H_5N$
space group	Cmca
a, Å	25.424 (4)
b, Å	14.087 (2)
c, Å	11.274 (2)
V, Å^3	4037.5 (8)
Z	4
$\rho_{calcd.}$, g cm^{-3}	1.03
μ (CuK_α), cm^{-1}	13.42
no. of unique reflections	2017
no. of reflections with $I \geq 3\sigma_I$	1592
R	0.056
R_w	0.081

Table S2

X-ray Crystal Structure Analysis of 4

Data were measured on a PW1100/20 Philips Four-Circle 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 $10 \leq \theta \leq 14^\circ$. Intensity data were collected using the ω-2θ technique to a maximum 2θ of 46°. The scan width, $\Delta\omega$, for each reflection was 1.00 + 0.35 tan·θ 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 variatios 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 0.7 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 $R_w = [\Sigma w(|F_o|-|F_c|)^2 / \Sigma w|F_o|^2]^{1/2}$ are presented with other pertinent crystallographic data in the following Table .

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

(2) All crystallographic computing was done on a VAX 9000 computer at the Hebrew University of Jerusalem, using the TEXSAN Structure Analysis Software.

Crystallographic Data for 4

formula	$C_{40}H_{44}S_4$
space group	$P\bar{1}$
a, Å	13.378 (2)
b, Å	15.227 (3)
c, Å	11.719 (2)
α, deg.	104.44 (1)
β, deg.	110.02 (1)
γ, deg.	95.43 (1)
V, Å^3	2129.2 (8)
Z	2
$\rho_{calcd.}$, g cm^{-3}	1.02
μ (MoK_α), cm^{-1}	2.35
no. of unique reflections	5927
no. of reflections with $I \geq 3\sigma_I$	4099
R	0.062
R_w	0.086

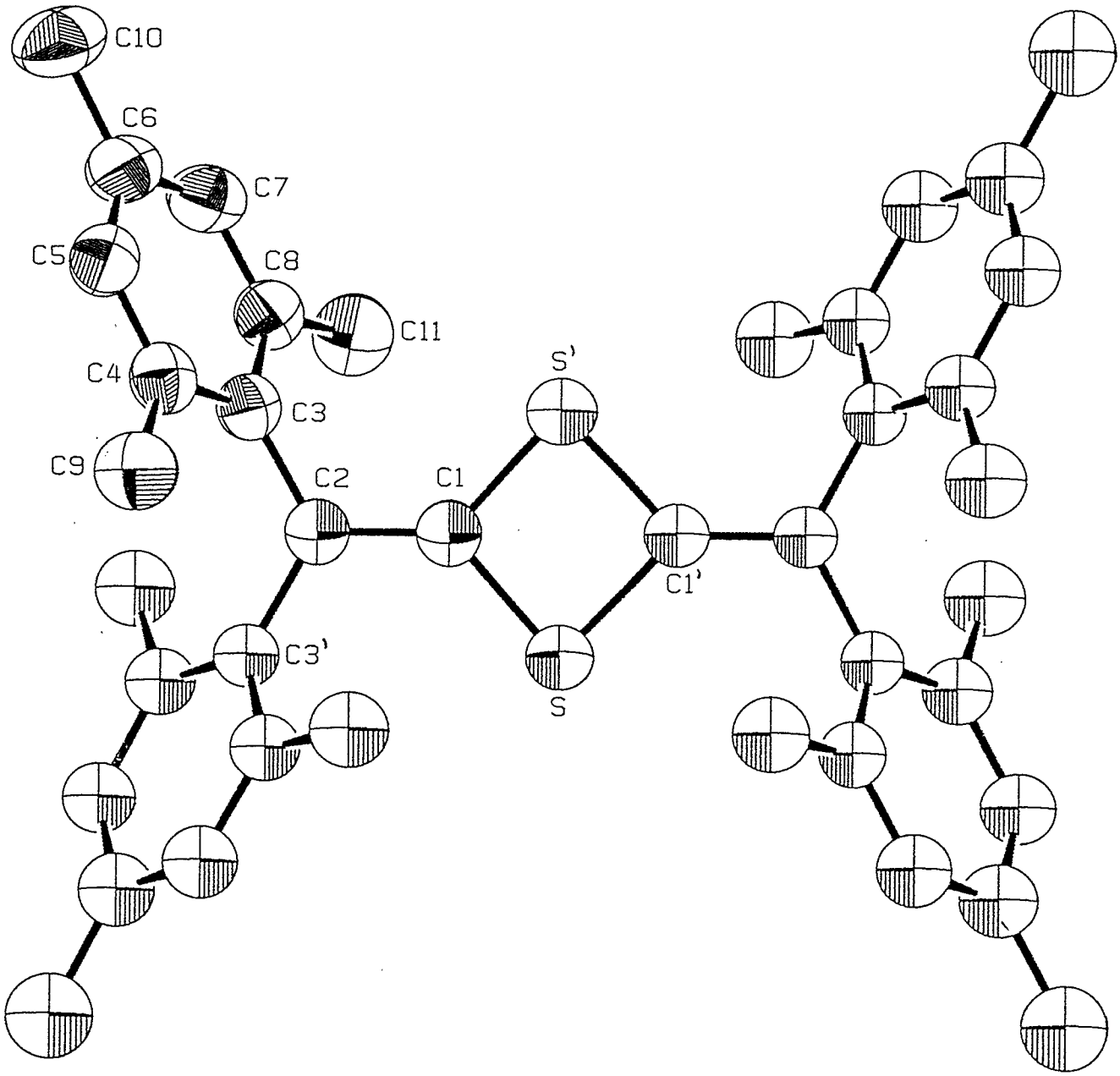

Figure S1

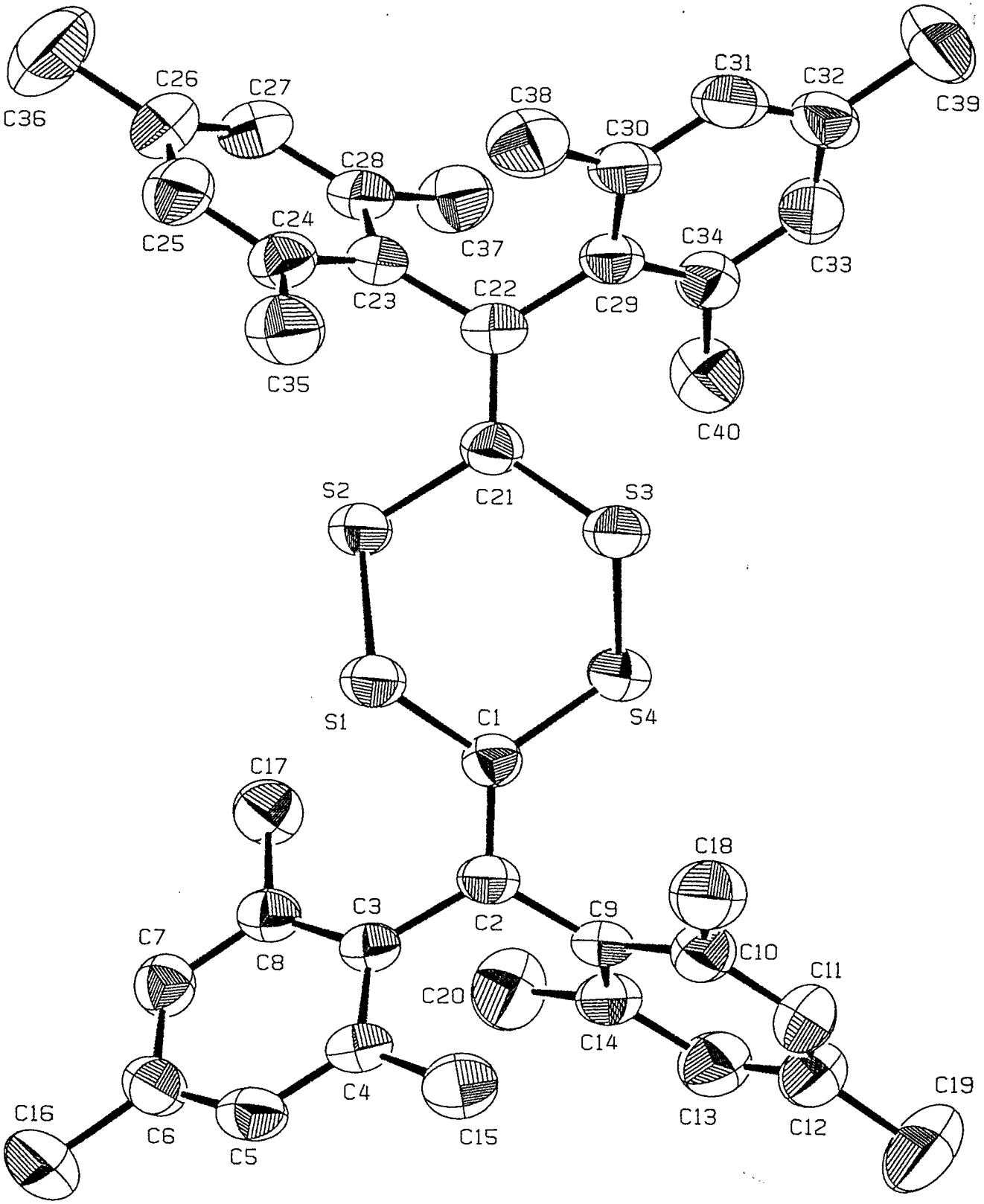
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Figure S2