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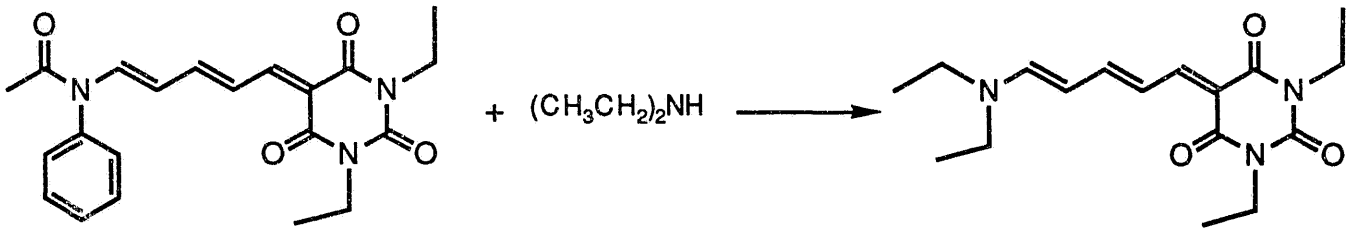
J-2620-M1

Synthesis of 1,3-diethyl-5-(5-(N,N'-diethylamino)penta-2,4-dienylidene) barbituric acid, **3**.



A **B** **3**

The synthesis of the starting material 1,3-diethyl-5-(5-acetanilidopenta-2,4-dienylidene) barbituric acid, **A**, has been reported previously.[9] 1.3g (3.41 mmol) of **A** was dissolved in 25ml of methylene chloride. While gently warming the solution, 0.9ml (8.72 mmol) of diethylamine was added with swirling, causing an immediate color change to magenta. Excess diethylamine and methylene chloride were removed under reduced pressure, resulting in an inky oil with a metallic greenish sheen. The oil was redissolved in 10ml of fresh methylene chloride. Diethyl ether (100 ml) was added dropwise, resulting in crystal precipitation. The crystals were filtered, washed with ether and dried in air. Yield 0.950 g (87%).

Characterizing data for **3**: ^{1}H NMR. δ 8.00 (d, J = 13.3 Hz, 1H), 7.72 (dd, J = 13.3, 13.2 Hz, 1H), 7.26 (dd, J = 13.2, 12.2 Hz, 1H), 7.05 (d, J = 12.3 Hz, 1H), 5.68 (dd, J = 12.3, 12.2 Hz, 1H), 4.00 (q, J = 7.0 Hz, 4H), 3.37 (m, 4H), 1.27 (m, 6H), 1.23 (t, J = 7.0 Hz, 3H), 1.22 (t, J = 7.0 Hz, 3H). Elemental Analysis: Calculated for $C_{17}H_{25}N_3O_3$: C, 63.93; H, 7.89; N, 13.16; Found: C, 63.92; H, 7.91; N, 13.19.

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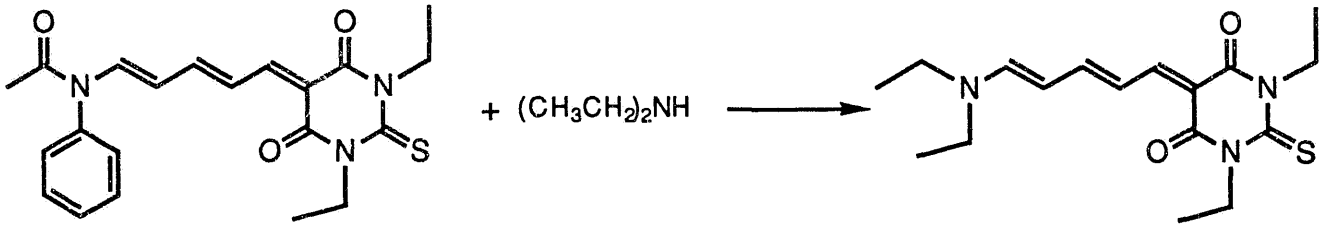
J-2620-M2

Synthesis of 1,3-diethyl-5-(5-(N,N'-diethylamino)penta-2,4-dienylidene)-2-thiobarbituric acid, **4**.



C **B** **4**

The synthesis of the starting material 1,3-diethyl-5-(5-acetanilidopenta-2,4-dienylidene)-2-thiobarbituric acid, **C**, has been reported previously.[9] 1.3g (3.27 mmol) of **C** was dissolved in 25ml of methylene chloride. While gently warming the solution, 0.9ml (8.72 mmol) of diethylamine was added with swirling, causing an immediate color change to magenta. Excess diethylamine and methylene chloride were removed under reduced pressure, resulting in an inky oil with metallic greenish-gold sheen. The oil was redissolved in 10ml of fresh methylene chloride. Diethyl ether (100 ml) was added dropwise, resulting in crystal precipitation. The crystals were filtered, washed with ether and dried in air. Yield 0.920 g (84%).

Characterizing data for **4**: ^{1}H NMR. δ 7.99 (d, J = 13.5 Hz, 1H), 7.79 (dd, J = 13.5, 12.3 Hz, 1H), 7.33 (dd, J = 12.4, 13.0 Hz, 1H), 7.18 (d, J = 12.2 Hz, 1H), 5.79 (dd, J = 12.2, 12.4 Hz, 1H), 4.57 (q, J = 6.9 Hz, 4H), 3.42 (q, J = 7.1 Hz, 4H), 1.30 (m, 12H). Elemental Analysis: Calculated for $C_{17}H_{25}N_3O_2S$: C, 60.87; H, 7.51; N, 12.53; S, 9.56. Found: C, 60.77; H, 7.56; N, 12.44; S, 9.63.

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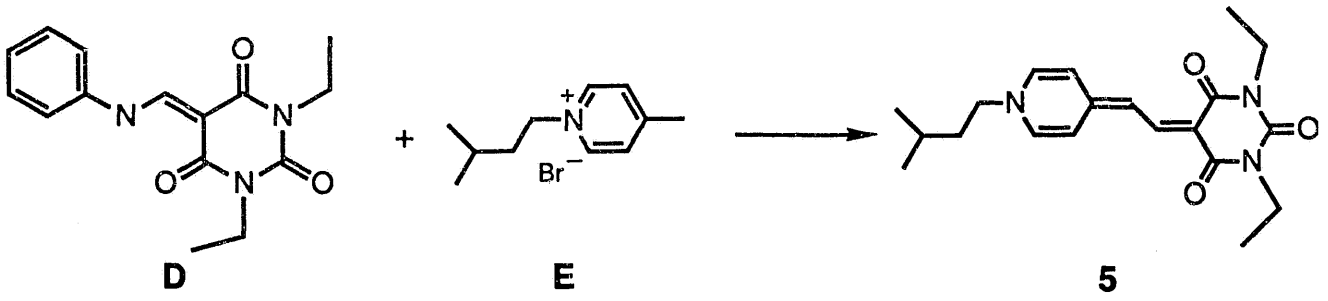
J-2620-M3

Synthesis of 1,3-diethyl-5-[(1-isopentyl-4-pyridylidene)-ethylene]-barbituric acid, **5**.



D **E** **5**

The synthesis of the starting material 1,3-diethyl-5-anilinylidene barbituric acid, **D**, has been reported previously.[9] 3.97g (16.2 mmol) of isopentyl-4-picolinium bromide, **E**, and 4.9g (17.1 mmol) of **D** were added to 50ml toluene while gently heating the solution. Then, 2.5ml of triethylamine was added and the reaction mixture refluxed for 2.5 hours at 110°C. Toluene was removed under vacuum and water was added to the remaining residue. An orange precipitate formed upon addition of the water. This precipitate was dissolved in toluene and dichloromethane and separated from the water layer. The solution was dried over Magnesium Sulfate, filtered and the remaining solvent removed under vacuum. The residue was recrystallized from toluene. Yield 1.98g (34.2%).

Characterizing data for 5: ^{1}H NMR. δ 8.38 (d, J = 15.0 Hz, 1H), 7.36 (d, J = 14.8 Hz, 1H), 7.36 (d, J = 7.2 Hz, 2H), 7.6 - 7.0 (very broad peak, due to hindered rotation, 2H), 4.00 (q, J = 7.0 Hz, 4H), 3.90 (m, 2H), 1.72 (m, 2H), 1.67 (m, 1H), 1.22 (t, J = 6.9 Hz, 6H), 0.98 (d, J = 6.6, 6H). Elemental Analysis: Calculated. for $C_{20}H_{27}N_3O_3$: C, 67.20; H, 7.61; N, 11.76; Found: C, 67.32; H, 7.60; N, 11.76.

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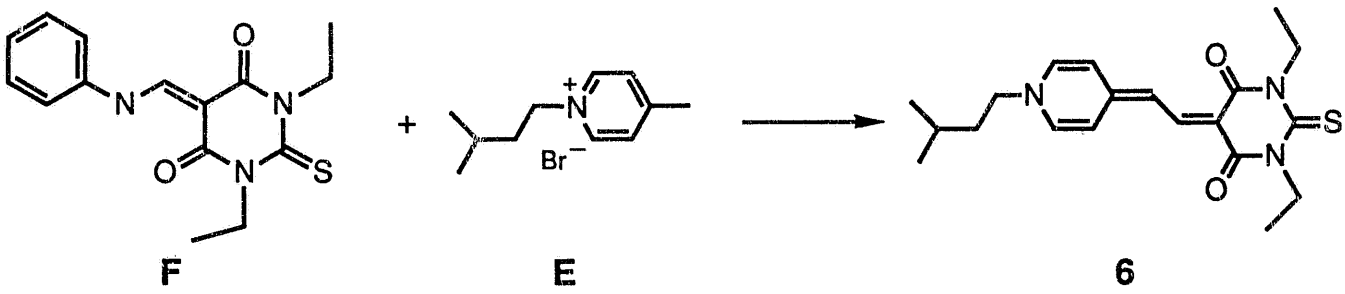
Synthesis of 1,3-diethyl-5-[(1-isopentyl-4-pyridylidene)-ethylene]-2-thiobarbituric acid, **6**.



F **E** **6**

The synthesis of the starting material 1,3-diethyl-5-anilinylidene-2-thiobarbituric acid, **F**, has been reported previously.[9] 3.60g (14.8 mmol) of isopentyl-4-picolinium bromide, **E**, and 4.48g (14.8 mmol) of **F** were added to 50ml toluene while gently heating the solution. Then, 2.5ml of triethylamine was added and the reaction mixture refluxed for 2 hours at 110°C. Toluene was removed under vacuum and water was added to the remaining residue. A red precipitate formed upon addition of the water. This precipitate was dissolved in toluene and dichloromethane and separated from the water layer. The solution was dried over Magnesium Sulfate, filtered and the remaining solvent removed under vacuum. The residue was recrystallized from toluene to give red crystals. Yield 2.43g (44%).

Characterizing data for 6: ^{1}H NMR. δ 8.36 (d, J = 15.3 Hz, 1H), 7.64 (d, J = 15.1 Hz, 1H), 7.49 (d, J = 7.3 Hz, 2H), 7.34 (broad peak, due to hindered rotation, 2H), 4.60 (q, J = 6.9 Hz, 4H), 3.98 (m, 2H), 1.75 (m, 2H), 1.63 (m, 1H), 1.31 (t, J = 6.9 Hz, 6H), 0.99 (d, J = 6.7, 6H). Elemental Analysis: Calculated. for $C_{20}H_{27}N_3O_2S$: C, 64.31; H, 7.29; N, 11.25; S, 8.58; Found: C, 64.21; H, 7.26; N, 11.28; S, 8.50.

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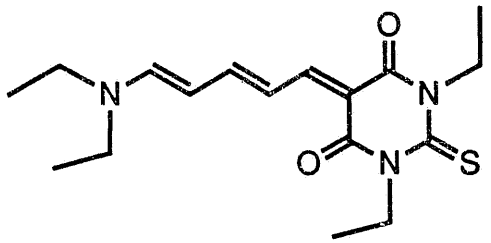
X-RAY CRYSTALLOGRAPHIC SUPPLEMENTARY MATERIAL FOR COMPOUND **4**



1,3-diethyl-5-(5-(N,N'-diethylamino)penta-2,4-dienylidene)-2-thiobarbituric acid

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Name	1,3-diethyl-5-(5-(N,N'-diethylamino)penta-2,4-dienylidene)-2-thiobarbituric acid
Formula	$C_{17}H_{25}N_3O_2S$
Formula Weight	335.46
Crystal System	triclinic
Space Group	$P\bar{1}$
Cell Dimensions a, Å	10.272 (2)
b, Å	10.288 (1)
c, Å	10.291 (2)
α, °	60.97 (1)
β, °	87.03 (1)
γ, °	70.57 (1)
V, Å^3	888.8 (3)
Z	2
Density, calc, g cm^{-3}	1.26
Crystal color, habit	red, irregular prism
Crystal size, mm^3	0.33 x 0.35 x 0.56
μ, cm^{-1}	1.86
μ r_{max}	0.71073
maximum 2θ (scan type)	28°
range of h,k, l	-13-13, -13-13, -13-13
# of reflections measured	8687
# of independent reflections	4292
# reflections, $F_o^2 > 0$	3973
# reflections, $F_o^2 > 3\sigma(F_o^2)$	3326
GOF, merge	1.01
R(merge) for refs meas. twice	0.019
secondary extinction (x 10^{-6})	2.16(29)
R, $F_o^2 > 0$	0.046
R, $F_o^2 > 3\sigma (F_o^2)$	0.038
GOF (number of parameters)	2.34, (309)
$(\Delta/\sigma)_{max}$ in final least squares	<0.005
Final Difference map:	
Maximum, eÅ^{-3}	+ 0.34
Minimum, eÅ^{-3}	- 0..28

Data were collected at 296 K.
Hydrogen positions were assumed, C-H 0.95 Å, and repositioned once near the end of refinement.
Structure solved using MULTAN 88.

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X-ray I.D. SRM31

Name of Compound Diethylamino-II-Thiobarbituric acid

Chemical Formula $C_{17}H_{25}N_3O_2S$ M. wt. 335.46

Crystal System Triclinic Space Group $P\bar{1}$ (# 2)

a=	10.272(2)	Å	α=	60.97(1)°	
b=	10.288(1)	Å	β=	87.03(1)°	
c=	10.291(2)	Å	γ=	70.57(1)°	
V=	888.8(3)	Å^3	Z=	2	
D_m	—	g cm^{-3}	D_x	1.26	g cm^{-3}

Radiation used MoKα Wavelength 0.71073 Å

Absorption Coefficient, μ= 1.86 cm^{-1} Temperature 296 °K

Type of Absorption Correction none (program used) —

Range of Transmission Factors —

Crystal Color red Crystal Shape (Habit) irregular prism

Crystal Size 0.33 mm × 0.35 mm × 0.56 mm

Source of Crystal synthesized by BGT

Type of Diffractometer Enraf-Nonius Cad-4

Data Collection method (diffraction geometry, scan type) θ-2θ scans

Lattice Parameters: Number of reflections 25 ; θ range 4° to 16°

θ range for data collection 1° to 28°

h_{min} -13 h_{max} 13 k_{min} -13 k_{max} 13 l_{min} -13 l_{max} 13

Number of reflections measured 8687

Number of independent reflections 4292

Number of reflections used in refinement 4292

Criterion for reflections used all used, F_o^2 positive and negative

Goodness of fit for merging data 1.01 (number of multiples 4292)

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R_{int} for duplicate reflections 0.019 (number of duplicates 3815)

Number of standard reflections 3 Interval 150 minutes

Variations of standards within counting statistics

How structure solved? Sharpened Patterson map gave vectors which were interpreted to give positions of ring atoms and the Si connected to them; remaining atoms found from subsequent Structure Factor - Fourier calculation.

How H atoms treated? all refined with isotropic displacement parameters

Refinement on F^2, $w=1/\sigma^2(F_o^2)$, one full matrix used.

R = 0.046 on F for 3973 reflections with $F_o^2 > 0$

R = 0.038 on F for 3326 reflections with $F_o^2 > 3\sigma(F_o^2)$

wR = 0.008 on F^2 for 4292 reflections

Goodness of Fit (S) = 2.34 for 4292 data and 309 parameters

$(\Delta/\sigma)_{max}$ in final least squares cycle < 0.005

$\Delta\rho_{max}$ +0.34 eÅ^{-3}, $\Delta\rho_{min}$ −0.28 eÅ^{-3} in final difference map.

Secondary Extinction parameter (if used) $2.16(29) \times 10^{-6}$

(Reference: Larson, A. C. (1967). *Acta Cryst.* 23, 644-665.)

Computer Programs

The CRYM Crystallographic Computing System

(Duchamp, D. J. (1964). Am. Crystallogr. Assoc. Meet., Bozeman, Montana, Paper B14, p. 29.)

ORTEP

(Johnson, C. K. (1976). *ORTEP*II. Report ORNL-3794. Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA.)

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MULTAN88

Debaerdemaeker, T., Germain, G., Main, P., Refaat, L. S., Tate, C. & Woolfson, M. M. (1988). *MULTAN 88. Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*, Univs. of York, England and Louvain, Belgium.

Scattering Factors and f', f'':

Cromer, D. T. (1974). *International Tables For X-ray Crystallography*, Vol. IV, pp. 149–151. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Cromer, D. T. & Waber, J. T. (1974). *International Tables For X-ray Crystallography*, Vol. IV, pp. 99–101. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Any additional Data:

Structure solved and refined by R. E. Marsh.

Weights w are calculated as $1/\sigma^2(F_o^2)$; variances ($\sigma^2(F_o^2)$) were derived from counting statistics plus an additional term, $(0.014I)^2$; variances of the merged data were obtained by propagation of error plus another additional term, $(0.014\bar{I})^2$.

Definitions:

$$R = \frac{\Sigma||F_o| - |F_c||}{\Sigma F_o}; \quad R_w = \frac{\Sigma w(F_o^2 - F_c^2)^2}{\Sigma w(F_o^2)^2}$$

$$S = \left\{\frac{\Sigma w(F_o^2 - F_c^2)^2}{n-p}\right\}^{\frac{1}{2}}$$

where n = number of data,

p = number of parameters refined.

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Legends for Figures.

Figure 1. An ORTEP drawing of the molecule with 50 % probability ellipsoids showing the numbering system. Hydrogen atoms are shown with arbitrary, small displacement parameters.

Figure 2. An ORTEP drawing of the contents of a unit cell with a unit cell outlined. Atoms are shown as 50 % probability ellipsoids; hydrogen atoms are as in Fig. 1. The view is perpendicular to the a c plane.

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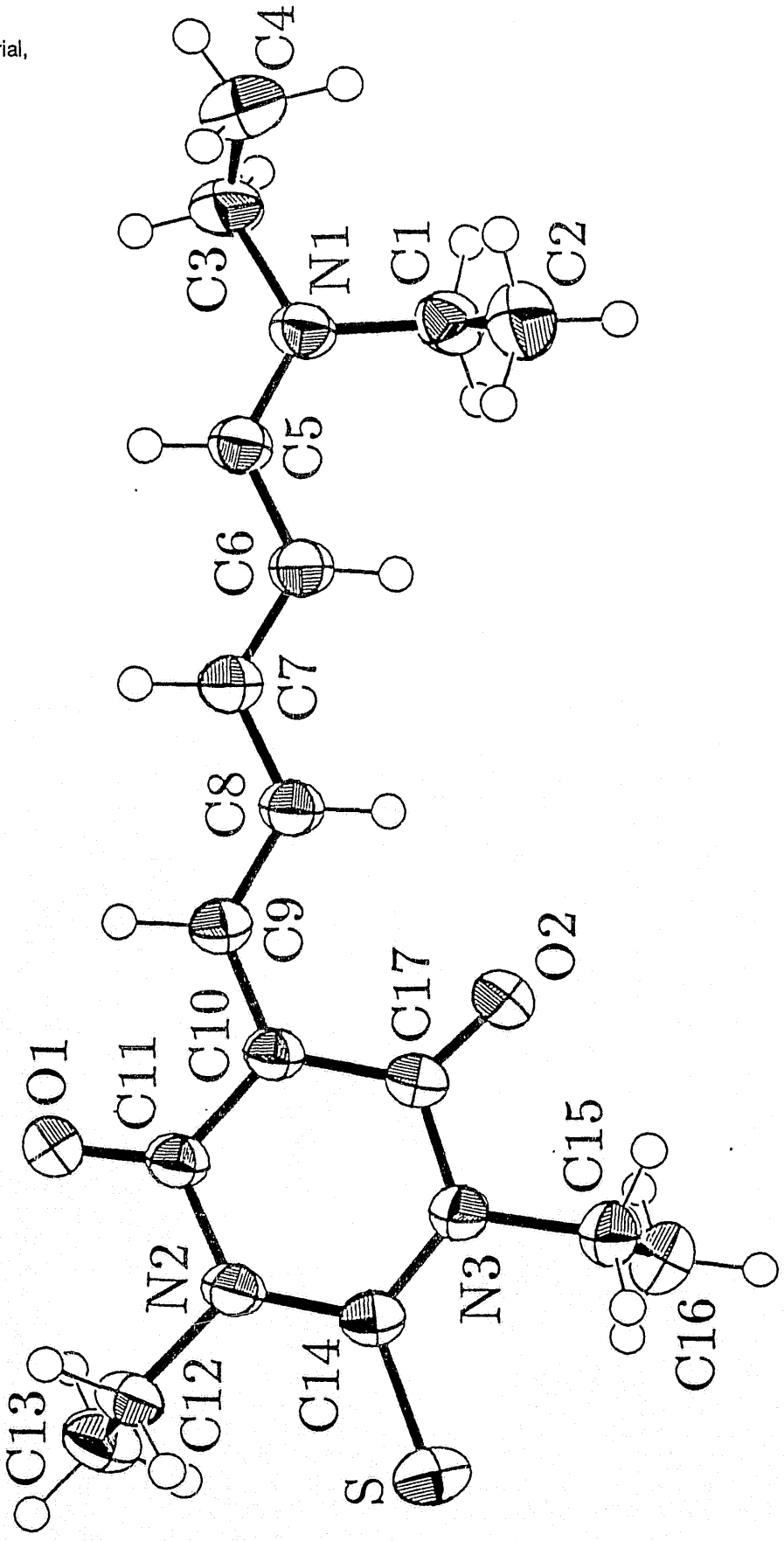

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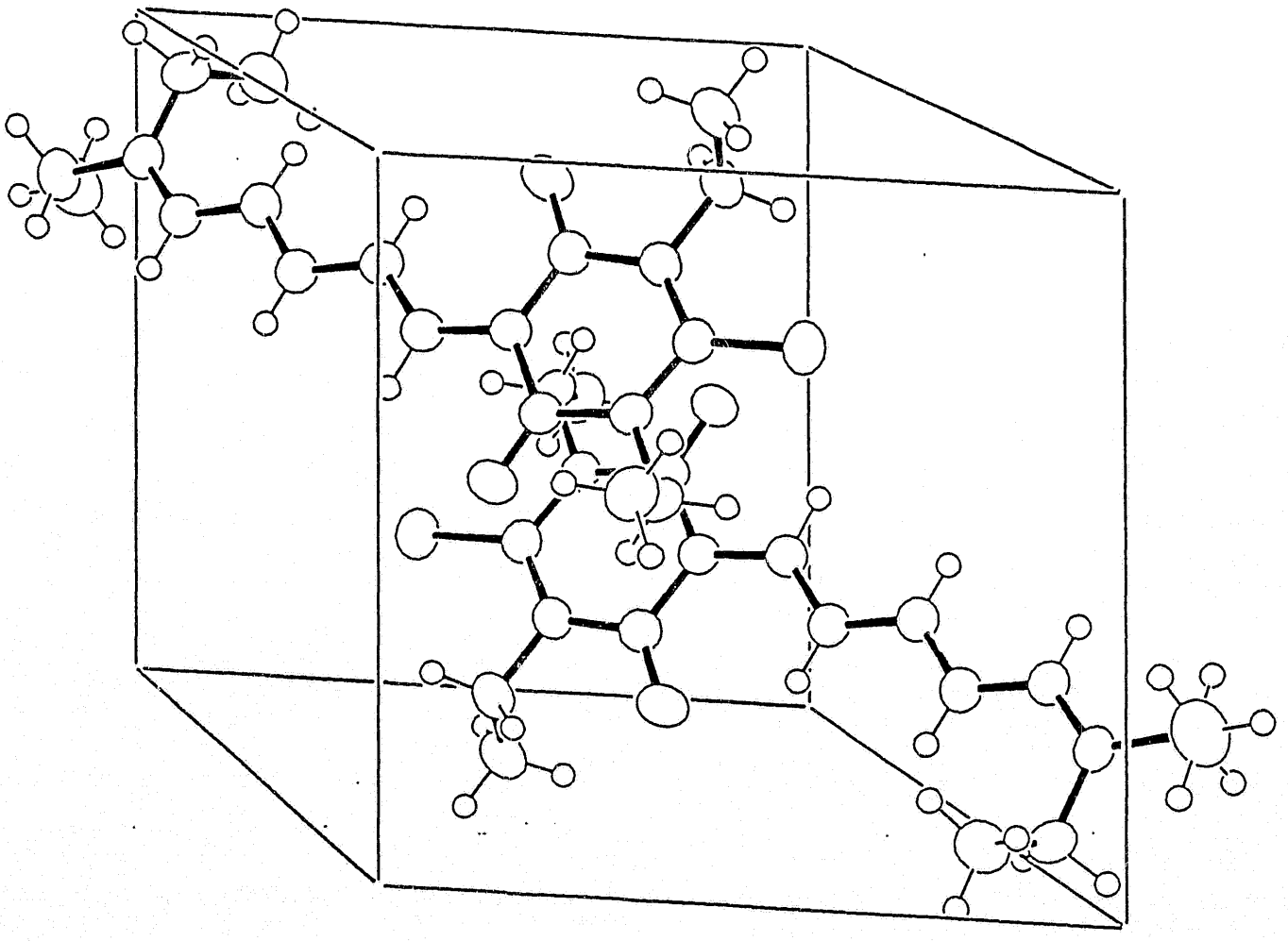

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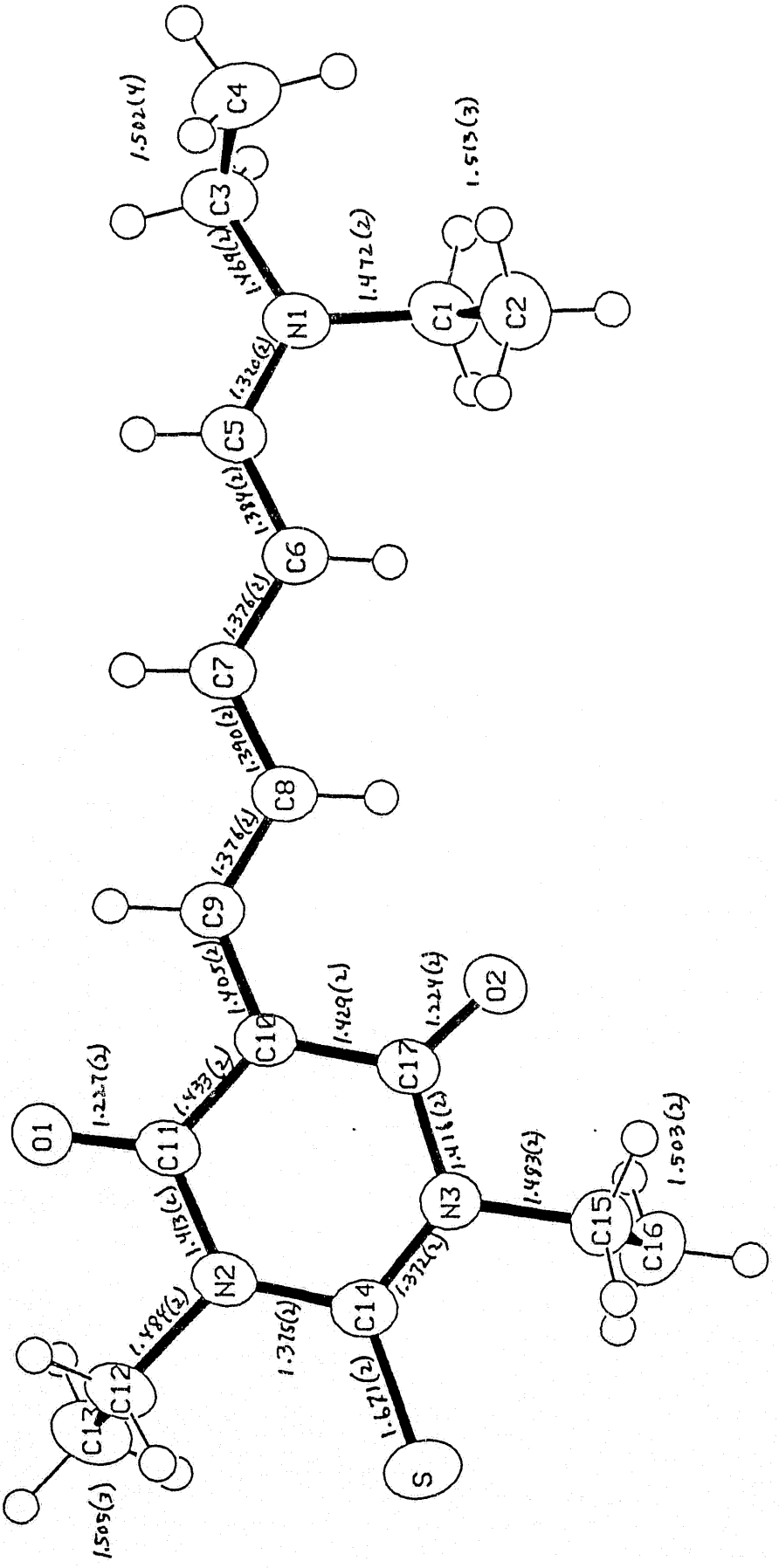
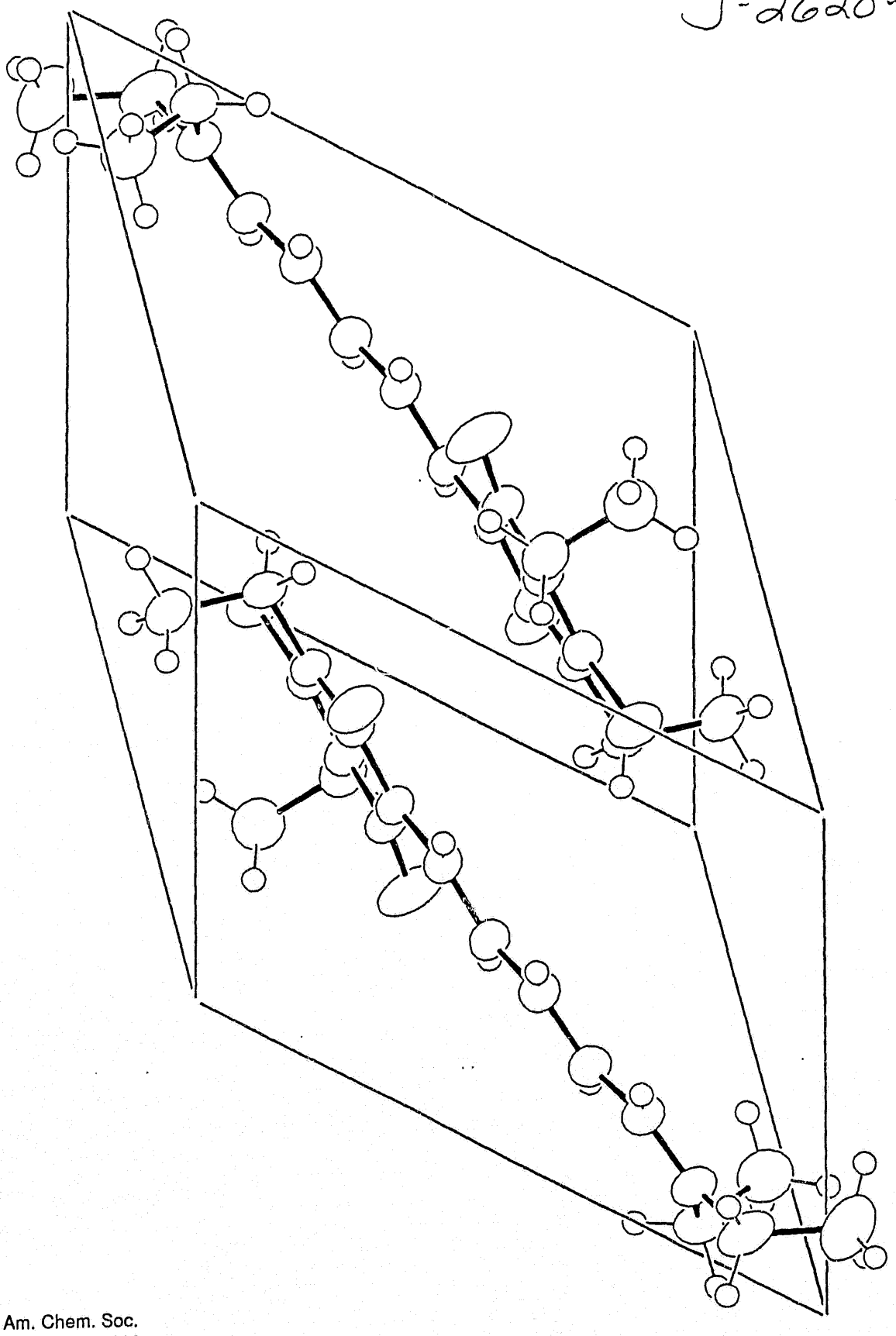
J-2620-M13



J-2620-M14



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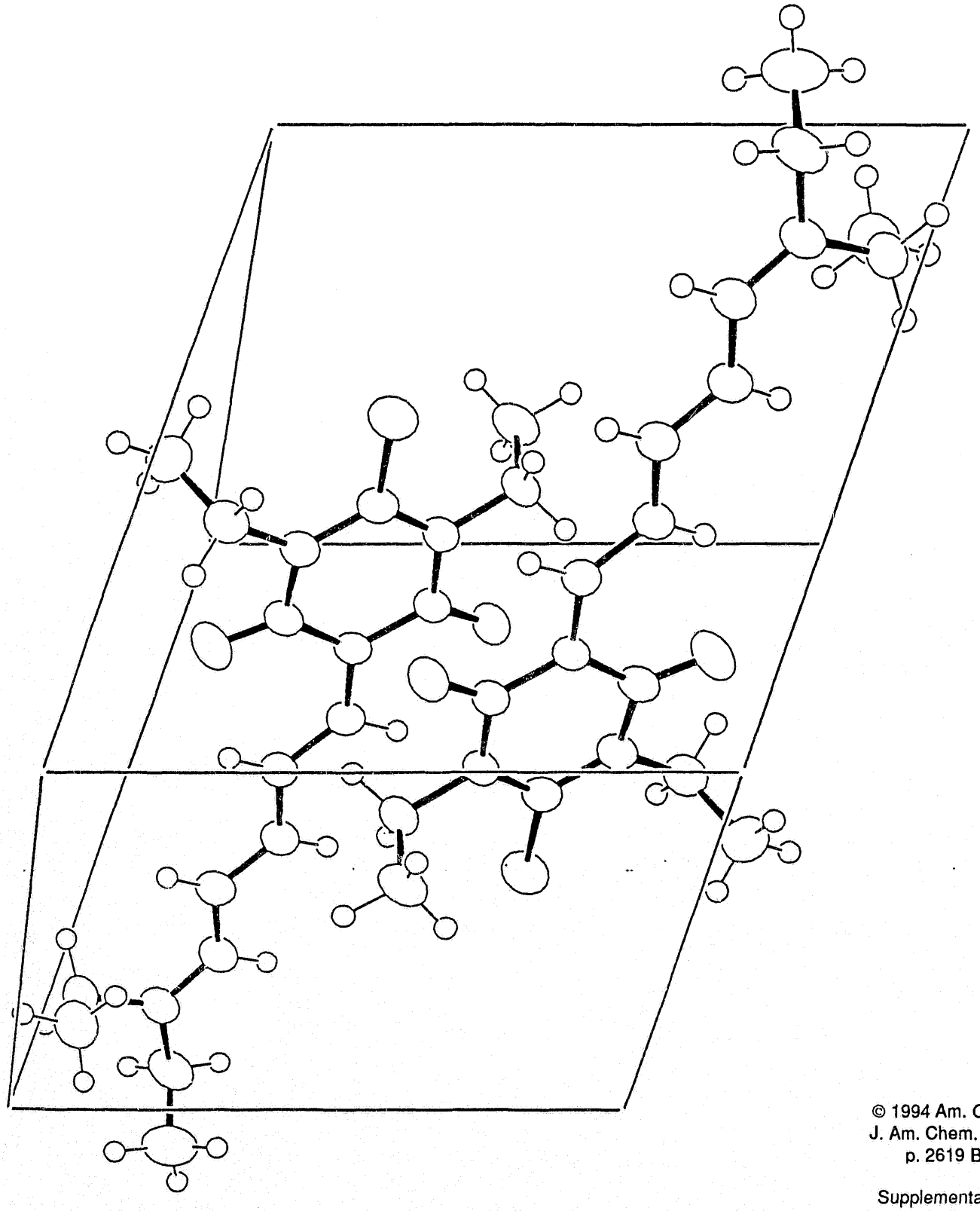
J-2620-M15



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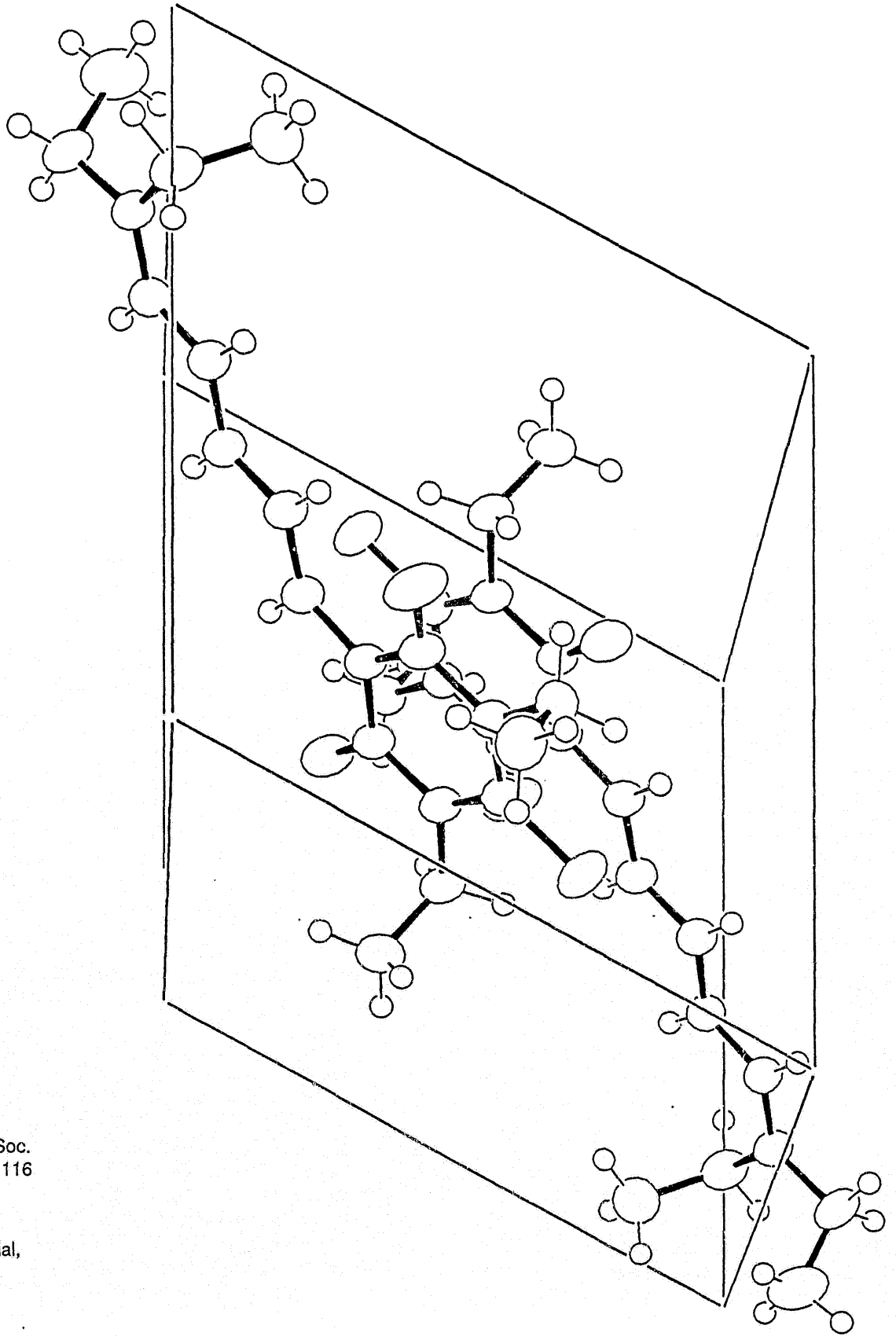
J-2620-M16



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J-2620-M17

Table 1. Final Parameters for Diethylamino-II-Thiobarbituric Acid.

x, y, z and $U_{eq}{}^{a} \times 10^4$

Atom	x	y	z	U_{eq} or B
N1	1804(1)	2209(1)	−602(1)	426(3)
C1	537(2)	2000(2)	70(2)	494(3)
C2	820(2)	621(2)	1657(2)	626(5)
C3	2260(2)	1608(2)	−1647(2)	581(4)
C4	2763(3)	−172(3)	−894(3)	804(6)
C5	2481(2)	2953(2)	−322(2)	405(3)
C6	2138(2)	3589(2)	618(2)	407(3)
C7	2908(2)	4327(2)	880(2)	408(3)
C8	2597(1)	4920(2)	1863(2)	400(3)
C9	3381(1)	5613(2)	2176(1)	382(3)
C10	3191(1)	6172(1)	3201(1)	361(3)
C11	4195(1)	6775(1)	3394(1)	374(3)
O1	5176(1)	6912(1)	2669(1)	540(2)
N2	4027(1)	7247(1)	4491(1)	370(2)
C12	5032(2)	7956(2)	4597(2)	434(3)
C13	4534(2)	9716(2)	3519(2)	555(4)
C14	2990(1)	7132(1)	5397(1)	381(3)
S	2876(.4)	7680(.5)	6697(.5)	589(1)
N3	2040(1)	6566(1)	5167(1)	385(2)
C15	881(2)	6410(2)	6085(2)	468(3)

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Table 1. (Cont.)

Atom	x	y	z	U_{eq} or B
C16	−396(2)	7887(2)	5390(2)	563(4)
C17	2044(1)	6140(2)	4049(2)	415(3)
O2	1068(1)	5782(2)	3876(1)	683(3)
H1A	26(16)	1858(17)	−612(17)	4.7(3)*
H1B	−37(17)	3036(20)	7(17)	5.0(4)*
H2A	−52(22)	593(22)	2024(22)	7.5(5)*
H2B	1261(19)	−372(23)	1636(20)	6.4(5)*
H2C	1366(18)	766(20)	2293(19)	5.7(4)*
H3A	1473(19)	2073(20)	−2414(19)	5.9(4)*
H3B	2980(18)	1968(20)	−2081(18)	5.4(4)*
H4A	3037(22)	−457(25)	−1598(25)	8.3(6)*
H4B	3605(23)	−595(25)	−158(24)	7.8(6)*
H4C	1962(22)	−524(24)	−433(23)	7.8(5)*
H5	3265(15)	3082(16)	−797(15)	3.4(3)*
H6	1366(15)	3483(16)	1141(15)	3.5(3)*
H7	3672(16)	4468(16)	388(16)	3.8(3)*
H8	1794(15)	4818(15)	2362(15)	3.4(3)*
H9	4209(16)	5710(16)	1666(15)	4.0(3)*
H12A	5155(14)	7689(16)	5619(16)	3.9(3)*
H12B	5936(15)	7383(16)	4392(15)	3.8(3)*

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Table 1. (Cont.)

Atom	x	y	z	U_{eq} or B
H13A	5243(17)	10188(19)	3583(17)	5.4(4)*
H13B	4385(16)	9946(18)	2499(19)	4.8(4)*
H13C	3676(18)	10261(19)	3812(18)	5.2(4)*
H15A	693(16)	5504(18)	6148(17)	4.8(4)*
H15B	1254(15)	6150(17)	7048(16)	4.0(3)*
H16A	−1145(20)	7736(21)	6008(20)	6.5(4)*
H16B	−234(18)	8779(22)	5335(20)	6.4(5)*
H16C	−719(19)	8160(22)	4398(22)	7.0(5)*

[a] $U_{eq} = \frac{1}{3}\sum_i \sum_j [U_{ij}(a_i^* a_j^*)(\vec{a}_i \cdot \vec{a}_j)]$

* Isotropic displacement parameter, B

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Table 2. Anisotropic Displacement Parameters for Diethylamino-II-Thiobarbituric Acid.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N1	506(7)	470(7)	409(6)	−233(5)	66(5)	−258(5)
C1	424(8)	571(9)	580(9)	−199(7)	26(7)	−336(8)
C2	676(12)	695(12)	615(11)	−366(10)	202(9)	−336(10)
C3	743(11)	776(12)	560(10)	−430(10)	195(9)	−484(9)
C4	954(17)	832(14)	1013(17)	−407(13)	375(15)	−706(14)
C5	467(8)	421(7)	388(7)	−201(6)	63(6)	−217(6)
C6	470(8)	403(7)	396(7)	−177(6)	67(6)	−220(6)
C7	448(8)	401(7)	416(7)	−158(6)	54(6)	−228(6)
C8	430(7)	391(7)	436(7)	−157(6)	53(6)	−238(6)
C9	398(7)	366(7)	424(7)	−138(6)	67(6)	−226(6)
C10	378(7)	346(6)	418(7)	−140(5)	55(5)	−226(6)
C11	388(7)	361(7)	430(7)	−145(6)	53(6)	−229(6)
O1	514(6)	748(7)	688(7)	−382(5)	258(5)	−513(6)
N2	382(6)	377(6)	422(6)	−157(5)	37(5)	−233(5)
C12	450(8)	475(8)	486(8)	−211(7)	16(6)	−284(7)
C13	690(11)	481(9)	587(10)	−300(8)	49(8)	−270(8)
C14	427(7)	341(7)	375(7)	−116(6)	25(6)	−188(6)
S	657(3)	779(3)	596(3)	−299(2)	139(2)	−511(2)
N3	438(6)	388(6)	400(6)	−186(5)	102(5)	−226(5)
C15	571(9)	504(9)	429(8)	−289(7)	190(7)	−253(7)
C16	534(9)	658(11)	570(10)	−220(8)	201(8)	−364(9)
C17	457(7)	431(7)	482(8)	−211(6)	104(6)	−288(7)
O2	627(7)	1116(10)	937(9)	−594(7)	403(6)	−816(8)

$U_{i,j}$ values have been multiplied by 10^4

The form of the displacement factor is:

$$\exp -2\pi^2(U_{11}h^2a^{*^2} + U_{22}k^2b^{*^2} + U_{33}\ell^2c^{*^2} + 2U_{12}hka^*b^* + 2U_{13}h\ell a^*c^* + 2U_{23}k\ell b^*c^*)$$

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Table 3. Complete Distances and Angles for Diethylamino-II-Thiobarbituric Acid.

	Distance(Å)		Distance(Å)
N1 –C1	1.472(2)	C7 –H7	0.925(16)
N1 –C3	1.469(2)	C8 –H8	0.957(15)
N1 –C5	1.320(2)	C9 –H9	0.984(16)
C1 –C2	1.513(3)	C12 –H12A	0.953(16)
C3 –C4	1.502(4)	C12 –H12B	0.995(16)
C5 –C6	1.384(2)	C13 –H13A	1.021(18)
C6 –C7	1.376(2)	C13 –H13B	0.965(18)
C7 –C8	1.390(2)	C13 –H13C	0.995(19)
C8 –C9	1.376(2)	C15 –H15A	0.985(17)
C9 –C10	1.405(2)	C15 –H15B	0.956(16)
C10 –C11	1.433(2)	C16 –H16A	0.98(2)
C10 –C17	1.429(2)	C16 –H16B	0.96(2)
C11 –O1	1.227(2)	C16 –H16C	0.96(2)
C11 –N2	1.413(2)		
N2 –C12	1.484(2)		
N2 –C14	1.375(2)		
C12 –C13	1.505(3)		
C14 –S	1.671(2)		
C14 –N3	1.372(2)		
N3 –C15	1.483(2)		
N3 –C17	1.416(2)		
C15 –C16	1.503(3)		
C17 –O2	1.224(2)		
C1 –H1A	0.989(17)		
C1 –H1B	1.003(18)		
C2 –H2A	0.96(2)		
C2 –H2B	0.98(2)		
C2 –H2C	0.976(19)		
C3 –H3A	0.97(2)		
C3 –H3B	0.933(19)		
C4 –H4A	0.91(3)		
C4 –H4B	1.00(3)		
C4 –H4C	1.01(2)		
C5 –H5	0.934(16)		
C6 –H6	0.941(16)		

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Table 3. (Cont.)

	Angle(°)		Angle(°)
C3 –N1 –C1	117.4(1)	H2A –C2 –C1	108.7(14)
C5 –N1 –C1	121.6(1)	H2B –C2 –C1	108.8(13)
C5 –N1 –C3	121.0(1)	H2C –C2 –C1	109.6(11)
C2 –C1 –N1	113.9(2)	H2B –C2 –H2A	106.1(18)
C4 –C3 –N1	113.0(2)	H2C –C2 –H2A	109.4(18)
C6 –C5 –N1	126.2(1)	H2C –C2 –H2B	114.1(17)
C7 –C6 –C5	123.1(1)	H3A –C3 –N1	107.4(12)
C8 –C7 –C6	123.3(1)	H3B –C3 –N1	106.7(12)
C9 –C8 –C7	124.1(1)	H3A –C3 –C4	110.1(12)
C10 –C9 –C8	128.3(1)	H3B –C3 –C4	109.8(12)
C11 –C10 –C9	118.2(1)	H3B –C3 –H3A	109.8(17)
C17 –C10 –C9	121.9(1)	H4A –C4 –C3	108.2(16)
C17 –C10 –C11	120.0(1)	H4B –C4 –C3	107.3(14)
O1 –C11 –C10	124.4(1)	H4C –C4 –C3	107.9(14)
N2 –C11 –C10	117.1(1)	H4B –C4 –H4A	107.9(21)
N2 –C11 –O1	118.4(1)	H4C –C4 –H4A	110.7(21)
C12 –N2 –C11	115.7(1)	H4C –C4 –H4B	114.7(20)
C14 –N2 –C11	124.4(1)	H5 –C5 –N1	118.5(10)
C14 –N2 –C12	119.9(1)	H5 –C5 –C6	115.3(10)
C13 –C12 –N2	111.3(1)	H6 –C6 –C5	119.3(10)
S –C14 –N2	121.7(1)	H6 –C6 –C7	117.6(10)
N3 –C14 –N2	116.7(1)	H7 –C7 –C6	120.9(10)
N3 –C14 –S	121.6(1)	H7 –C7 –C8	115.8(10)
C15 –N3 –C14	120.5(1)	H8 –C8 –C7	117.4(9)
C17 –N3 –C14	124.5(1)	H8 –C8 –C9	118.5(9)
C17 –N3 –C15	115.0(1)	H9 –C9 –C8	118.3(10)
C16 –C15 –N3	112.3(1)	H9 –C9 –C10	113.4(9)
N3 –C17 –C10	117.0(1)	H12A –C12 –N2	106.3(10)
O2 –C17 –C10	125.1(1)	H12B –C12 –N2	106.4(9)
O2 –C17 –N3	117.9(1)	H12A –C12 –C13	113.4(10)
H1A –C1 –N1	105.2(10)	H12B –C12 –C13	112.2(9)
H1B –C1 –N1	106.6(10)	H12B –C12 –H12A	106.9(13)
H1A –C1 –C2	111.4(10)	H13A –C13 –C12	110.7(10)
H1B –C1 –C2	112.0(11)	H13B –C13 –C12	111.2(11)
H1B –C1 –H1A	107.3(14)	H13C –C13 –C12	109.9(11)

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Table 3. (Cont.)

	Angle(°)
H13B –C13 –H13A	108.5(15)
H13C –C13 –H13A	104.8(15)
H13C –C13 –H13B	111.6(15)
H15A –C15 –N3	104.9(10)
H15B –C15 –N3	104.9(10)
H15A –C15 –C16	110.8(10)
H15B –C15 –C16	113.2(10)
H15B –C15 –H15A	110.4(14)
H16A –C16 –C15	110.2(12)
H16B –C16 –C15	111.9(12)
H16C –C16 –C15	111.6(13)
H16B –C16 –H16A	105.8(18)
H16C –C16 –H16A	108.6(18)
H16C –C16 –H16B	108.6(18)

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Table 4. Intermolecular Distances Less than 3.5 Å for Diethylamino-II-Thiobarbituric Acid.

	Distance(Å)		Distance(Å)
C1 –C8	3.481(2)	C8 –H1A	3.191(17)
C3 –O1	3.344(2)	C8 –H1B	2.822(18)
C5 –O1	3.307(2)	C8 –H16A	3.32(2)
C9 –C12	3.452(2)	C8 –H12A	3.000(16)
C10 –N2	3.477(2)	C8 –H12B	3.479(16)
C11 –C11	3.440(2)	C9 –H4C	3.37(2)
C11 –N2	3.441(2)	C9 –H1A	3.474(17)
O1 –C14	3.458(2)	C9 –H12A	2.903(16)
O1 –N3	3.473(2)	C9 –H12B	3.274(16)
C15 –O2	3.465(2)	C10 –H2B	3.04(2)
O2 –O2	3.312(2)	C10 –H12A	3.345(16)
C1 –H8	3.189(15)	C10 –H12B	3.094(16)
N1 –H13B	3.493(18)	C11 –H2B	3.24(2)
N1 –H15A	3.286(17)	C11 –H4B	3.25(3)
N1 –H15B	3.422(16)	O1 –H4B	2.85(3)
C1 –H4C	3.31(2)	O1 –H3B	2.437(19)
C2 –H16C	3.48(2)	O1 –H5	2.440(16)
C2 –H4C	3.23(2)	N2 –H2B	3.46(2)
C2 –H16B	3.43(2)	N2 –H2C	3.437(19)
C3 –H15A	3.327(17)	C12 –H3B	3.200(19)
C3 –H16C	3.18(2)	C12 –H13A	3.208(18)
C3 –H12B	3.222(16)	C13 –H2C	3.180(19)
C4 –H2A	3.31(2)	C13 –H3B	3.296(19)
C4 –H13A	3.360(18)	C13 –H4A	3.16(3)
C4 –H13B	3.308(18)	C13 –H12A	3.303(16)
C5 –H13B	3.110(18)	C13 –H13A	3.055(18)
C5 –H15A	3.419(17)	C13 –H13C	3.398(19)
C5 –H15B	2.948(16)	C14 –H2C	3.432(19)
C6 –H13B	3.285(18)	S –H4A	3.21(3)
C6 –H13C	3.323(19)	S –H2A	3.43(2)
C6 –H15B	3.260(16)	S –H9	3.441(16)
C6 –H1B	3.181(18)	S –H16B	3.41(2)
C6 –H16A	3.30(2)	S –H13A	3.283(18)
C7 –H1B	3.074(18)	N3 –H2B	3.36(2)
C7 –H12A	3.462(16)	C15 –H8	3.405(15)

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Table 4. (Cont.)

	Distance(Å)		Distance(Å)
C16 –H2A	3.32(2)	H3A –H12B	3.30(3)
C16 –H3A	3.29(2)	H3B –H15A	3.23(3)
C16 –H2C	3.262(19)	H3B –H16C	3.49(3)
C16 –H6	3.377(16)	H3B –H12B	2.45(3)
C16 –H8	3.349(15)	H3B –H13A	3.31(3)
C16 –H16B	3.42(2)	H3B –H13B	2.92(3)
C17 –H2B	3.06(2)	H4A –H16C	3.15(3)
C17 –H1A	3.474(17)	H4A –H13A	2.60(3)
C17 –H12B	3.117(16)	H4A –H13B	2.89(3)
O2 –H1A	3.018(17)	H4B –H9	3.16(3)
O2 –H3A	2.70(2)	H4B –H13B	3.23(3)
O2 –H15A	2.579(17)	H4B –H5	3.20(3)
O2 –H12B	3.394(16)	H4B –H13B	3.06(3)
H1A –H1A	3.41(2)	H4C –H9	3.38(3)
H1A –H2A	3.46(3)	H5 –H13B	3.25(2)
H1A –H2B	2.87(3)	H5 –H15A	3.46(2)
H1A –H4C	2.72(3)	H5 –H15B	2.91(2)
H1A –H8	2.92(2)	H5 –H9	3.15(2)
H1B –H6	2.98(2)	H6 –H13C	3.28(2)
H1B –H8	2.58(2)	H6 –H6	3.30(2)
H2A –H16B	3.02(3)	H6 –H15B	3.22(2)
H2A –H16C	2.78(3)	H6 –H16A	2.60(3)
H2A –H3A	3.37(3)	H7 –H7	3.19(2)
H2A –H4A	3.18(3)	H7 –H9	2.98(2)
H2A –H4C	2.66(3)	H8 –H15A	2.94(2)
H2A –H16B	3.13(3)	H8 –H16A	2.63(3)
H2B –H16C	3.43(3)	H8 –H12A	3.30(2)
H2B –H4C	3.26(3)	H8 –H12B	3.42(2)
H2C –H13B	2.92(3)	H9 –H12A	3.11(2)
H2C –H13C	2.67(3)	H12A –H13A	2.59(2)
H2C –H16B	3.49(3)	H12A –H13C	3.03(3)
H2C –H16A	2.80(3)	H13A –H13A	2.79(3)
H2C –H16B	2.83(3)	H13A –H13C	2.72(3)
H3A –H15A	2.91(3)	H13C –H16A	2.79(3)
H3A –H16C	2.37(3)	H13C –H13C	3.48(3)

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Table 4. (Cont.)

	Distance(Å)
H16B –H16B	2.47(3)

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Table 5. Observed and Calculated Structure Factors for Diethylamino-II-Thiobarbituric Acid

The columns contain, in order, ℓ, $10F_{obs}$, $10F_{calc}$ and $10\sigma F_{obs}$. A minus sign preceding F_{obs} indicates that F^2_{obs} is negative.

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-12 1 1

1	18	17	2
2	13	15	2
3	7	3	3
4	27	23	1

-11 1 1

1	-10	5	2
2	8	3	3
3	27	25	1
4	17	17	2
5	1	0	6
6	18	18	2
7	8	2	3

-11 2 1

1	17	18	2
2	6	3	4
3	31	32	1
4	54	51	1
5	7	7	3
6	16	14	2

-11 3 1

1	11	9	2
2	8	13	3
3	-6	1	3
4	7	6	3
5	10	4	3
6	32	31	1

-10 1 1

1	11	10	2
2	15	17	1
3	13	15	2
4	34	31	1
5	49	50	1
6	-9	4	2
7	19	17	2
8	26	27	1

-10 2 1

1	10	11	2
2	37	34	1
3	32	35	1
4	24	30	1
5	48	46	1
6	3	4	5
7	-10	3	2
8	13	14	2

-10 3 1

1	16	18	2
2	-4	3	4
3	32	32	1
4	58	62	1
5	26	29	1
6	9	6	3
7	-2	2	6
8	45	39	1

-10 4 1

1	9	8	3
2	21	21	1
3	27	28	1
4	29	24	1
5	19	19	2
6	33	35	1
7	15	18	2

-10 5 1

2	16	13	2
3	52	50	1
4	36	39	1
5	5	4	4

-9 1 1

1	21	23	1
2	69	66	1
3	15	14	1
4	96	99	1
5	86	91	1
6	49	53	1
7	39	39	1
8	22	22	1
9	13	5	2

-9 2 1

1	8	13	2
2	25	27	1
3	2	12	5
4	30	26	1
5	5	3	3
6	17	13	1
7	-10	4	2
8	10	9	2
9	77	73	1

-9 3 1

1	23	18	1
2	31	30	1
3	58	61	1
4	73	73	1
5	43	43	1
6	13	12	2
7	84	83	1
8	6	4	4
9	29	27	1

-9 4 1

1	17	14	2
2	10	6	2
3	4	0	4
4	50	48	1
5	22	23	1
6	41	37	1
7	30	32	1
8	33	32	1
9	27	23	1

-9 5 1

1	9	11	3
2	24	23	1
3	11	9	2
4	38	39	1
5	29	27	1
6	-6	6	4
7	32	27	1
8	41	41	1

-9 6 1

2	13	12	2
3	19	17	2
4	39	38	1
5	42	43	1
6	9	2	3
7	-1	9	6

-8 1 1

1	-7	9	2
2	37	36	1
3	45	40	1
4	45	54	1
5	82	85	1
6	71	70	1
7	-5	5	3
8	55	54	1
9	20	23	1
10	57	53	1

-8 2 1

1	32	35	1
2	11	12	2
3	-6	2	2
4	105	108	1
5	122	126	1
6	16	17	1
7	44	44	1
8	55	59	1
9	17	19	2
10	16	12	2

-8 3 1

1	18	20	1
2	21	21	1
3	61	59	1
4	21	20	1
5	22	19	1
6	7	0	3
7	56	58	1
8	18	19	1
9	46	44	1
10	-8	3	3

-8 4 1

1	31	33	1
2	23	27	1
3	-3	2	4
4	65	61	1
5	80	81	1
6	53	54	1
7	8	3	3
8	56	53	1
9	12	13	2
10	11	8	2

-8 5 1

1	15	16	2
2	2	1	5
3	34	30	1
4	23	20	1
5	12	4	2
6	72	75	1
7	16	16	2
8	15	13	2
9	-12	3	2

-8 6 1

1	12	2	2
2	2	5	5
3	41	39	1
4	20	19	1
5	30	33	1
6	8	1	3
7	64	62	1
8	29	26	1
9	-4	4	4

-8 7 1

2	24	19	1
3	39	39	1
4	52	50	1
5	8	4	3
6	1	5	7
7	-5	4	4
8	17	21	2

-7 1 1

1	125	126	1
2	71	69	1
3	99	99	1
4	31	33	1
5	8	16	2
6	61	67	1
7	48	45	1
8	43	42	1
9	13	5	2
10	50	47	1

-7 2 1

1	110	108	1
2	99	101	1
3	103	103	1
4	125	126	1
5	42	46	1
6	79	77	1
7	53	57	1
8	7	13	3
9	39	37	1
10	38	35	1
11	-7	3	3

-7 3 1

1	52	53	1
2	18	26	1
3	18	21	1
4	42	43	1
5	48	50	1
6	52	52	1
7	86	86	1
8	42	40	1
9	18	15	1
10	16	18	2
11	-11	5	2

-7 4 1

1	28	33	1
2	71	70	1
3	34	32	1
4	25	22	1
5	64	63	1
6	25	24	1
7	6	7	3
8	97	94	1
9	40	36	1
10	-8	8	3
11	28	26	1

-7 5 1

1	22	21	1
2	18	19	1
3	16	10	1
4	108	106	1
5	72	73	1
6	64	67	1
7	14	9	2
8	34	31	1
9	3	6	5
10	25	22	1

-7 6 1

1	27	29	1
2	32	34	1

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Diethylamino-II-Thiobarbituric Acid

3	14	4	2
4	16	14	1
5	100	98	1
6	0	2	7
7	32	31	1
8	36	36	1
9	12	15	2
10	36	34	1

-7 7 1

1	-5	6	4
2	56	56	1
3	15	4	2
4	43	38	1
5	69	69	1
6	19	20	1
7	46	45	1
8	-8	9	3
9	21	20	1

-7 8 1

2	49	48	1
3	42	40	1
4	45	44	1
5	32	31	1
6	0	0	8
7	8	8	3
8	7	2	4

-6 1 1

1	39	35	0
2	115	108	1
3	163	168	1
4	33	33	1
5	32	35	1
6	84	86	1
7	75	72	1
8	90	91	1
9	11	12	2
10	55	55	1
11	12	15	2

-6 2 1

1	207	201	1
2	174	173	1
3	60	63	1
4	5	3	3
5	23	21	1
6	94	97	1
7	20	18	1
8	70	71	1
9	76	75	1
10	-5	6	4
11	-6	9	3

-6 3 1

1	84	78	1
2	25	25	1
3	18	22	1
4	39	38	1
5	92	91	1
6	16	11	1
7	44	43	1
8	92	91	1
9	120	120	1
10	6	12	3
11	16	15	2

-6 4 1

1	43	44	1
2	16	19	1
3	54	56	1
4	48	49	1
5	62	62	1
6	193	195	1
7	33	35	1
8	14	3	2
9	26	27	1
10	24	22	1
11	-10	4	2

-6 5 1

1	41	45	1
2	44	45	1
3	9	2	2
4	15	8	1
5	67	66	1
6	129	129	1
7	19	20	1
8	99	95	1
9	33	34	1
10	12	12	2
11	54	51	1

-6 6 1

1	11	14	2
2	22	24	1
3	128	125	1
4	47	48	1
5	16	3	1
6	26	20	1
7	12	10	2
8	17	17	1
9	17	16	1
10	56	53	1
11	24	23	1

-6 7 1

1	8	7	3
2	-6	2	3
3	46	44	1
4	98	97	1
5	137	137	1
6	51	52	1
7	14	13	2
8	35	36	1
9	-10	0	2
10	14	9	2

-6 8 1

1	10	13	3
2	6	4	4
3	12	8	2
4	34	29	1
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6	40	42	1
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9	58	54	1
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-6 9 1

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7	-7	6	3
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-5 1 1

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3	126	115	1
4	133	135	1
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6	9	9	2
7	128	127	1
8	-5	3	3
9	16	13	1
10	78	77	1
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-5 2 1

1	16	9	1
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3	87	81	1
4	127	128	1
5	118	121	1
6	140	142	1
7	158	162	1
8	71	71	1
9	60	59	1
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11	23	22	1
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-5 3 1

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6	74	75	1
7	221	223	2
8	21	22	1
9	49	48	1
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-5 4 1

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4	168	171	1
5	16	11	1
6	95	94	1
7	96	98	1
8	14	14	1
9	53	48	1
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-5 5 1

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5	206	207	1
6	160	157	1
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6	212	214	2
7	54	54	1
8	-10	5	2
9	-6	1	3
10	51	49	1
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-5 7 1

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4	50	45	1
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7	30	34	1
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9	24	26	1
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7	12	17	2
8	7	15	3
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6	12	13	2
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-5 10 1

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6	22	25	1
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8	282	283	2
9	70	68	1
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11	35	32	1
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2	137	129	1
3	46	40	0
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5	61	62	0
6	92	87	1
7	119	117	1

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8	120	121	1
9	45	45	1
10	47	48	1
11	-8	3	2
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-4 3 l

1	11	9	1
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3	37	37	0
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6	196	196	1
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8	23	20	1
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-4 4 l

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3	103	103	1
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5	76	78	1
6	341	343	3
7	264	266	2
8	96	99	1
9	34	35	1
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-4 5 l

1	64	65	1
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3	18	19	1
4	74	73	1
5	48	52	1
6	62	58	1
7	105	106	1
8	67	69	1
9	69	69	1
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11	67	65	1
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-4 6 l

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5	112	113	1
6	98	98	1
7	99	102	1
8	65	68	1
9	66	68	1
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11	89	85	1
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-4 7 l

1	59	59	1
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3	70	70	1
4	42	40	1
5	118	119	1
6	115	118	1
7	52	52	1
8	31	34	1
9	11	7	2
10	28	32	1
11	56	50	1
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-4 8 l

1	10	15	2
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3	7	4	3
4	28	29	1
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6	10	4	2
7	11	7	2
8	55	55	1
9	36	34	1
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-4 9 l

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5	27	25	1
6	-12	3	1
7	48	50	1
8	13	14	2
9	27	25	1
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-4 10 l

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4	18	20	2
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6	-9	2	2
7	16	21	2
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6	139	138	1
7	15	11	1
8	71	71	1
9	48	50	1
10	10	3	2
11	11	3	2
12	17	18	2

-3 2 l

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4	70	71	0
5	26	27	0
6	106	104	1
7	396	401	3
8	146	146	1
9	85	86	1
10	43	41	1
11	23	23	1
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-3 3 l

1	291	290	2
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3	275	281	2
4	108	111	1
5	107	106	1
6	121	118	1
7	299	297	2
8	224	224	2
9	21	22	1
10	-3	3	4
11	-8	3	3
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-3 4 l

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4	92	94	1
5	40	37	0
6	61	62	1
7	100	102	1
8	64	63	1
9	97	97	1
10	71	71	1
11	6	11	3
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6	186	183	1
7	103	105	1
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9	49	51	1
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11	9	20	2
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-3 6 l

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4	32	34	1
5	91	90	1
6	55	55	1
7	14	13	1
8	-8	8	2
9	37	39	1
10	21	19	1
11	12	17	2
12	33	27	1
13	-6	7	4

-3 7 l

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5	18	14	1
6	64	64	1
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8	60	61	1
9	79	78	1
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-3 8 l

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6	89	87	1
7	41	41	1
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-3 11 l

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-2 3 l

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9	24	33	1
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9	64	63	1
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12	28	25	1
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6	110	109	1
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9	93	93	1
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11	107	111	1
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3	136	128	1
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8	110	109	1
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12	28	23	1

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2	109	116	1
3	56	54	0
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7	65	63	1
8	62	61	1
9	76	75	1
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12	28	30	1
13	16	15	2

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-4	151	152	1
-3	35	36	1
-2	63	59	1
-1	133	131	1
0	56	57	0
1	186	187	1
2	50	41	0
3	83	81	0
4	58	58	0
5	66	69	0
6	87	90	1
7	77	76	1
8	195	197	1
9	66	65	1
10	90	92	1
11	50	48	1
12	15	20	2
13	44	43	1

3 6 1

-7	-8	6	3
-6	33	31	1
-5	29	25	1
-4	22	23	1
-3	34	34	1
-2	7	11	2
-1	14	16	1
0	314	304	2
1	111	109	1
2	46	44	0
3	95	96	1
4	70	67	0
5	90	92	1
6	218	217	2
7	5	9	2
8	147	150	1
9	168	166	1
10	-9	1	2
11	25	24	1
12	59	60	1
13	5	7	4

3 7 1

-6	-4	1	4
-5	-4	10	4
-4	26	30	1
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-2	19	19	1
-1	34	35	1
0	140	135	1
1	74	70	1
2	64	60	1
3	91	88	1
4	48	52	0
5	121	120	1
6	43	43	1
7	91	87	1
8	204	206	1
9	-9	0	2
10	45	46	1
11	63	64	1
12	39	37	1
13	40	38	1

3 8 1

-5	20	17	2
-4	16	14	2
-3	7	10	3
-2	-5	3	3
-1	102	104	1
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1	44	47	1
2	52	53	1
3	97	97	1
4	-4	1	3
5	115	115	1
6	276	275	2
7	165	166	1
8	35	37	1
9	63	65	1
10	44	42	1
11	-11	2	2
12	28	28	1
13	18	15	2

3 9 1

-4	-10	4	2
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-1	30	31	1
0	5	0	3
1	8	8	2
2	4	7	3
3	36	35	1
4	102	102	1
5	262	260	2
6	89	89	1
7	0	2	6
8	96	98	1
9	81	83	1
10	95	95	1
11	50	51	1
12	35	38	1
13	35	37	1

3 10 1

-3	44	42	1
-2	3	2	5
-1	12	11	2
0	6	7	3
1	19	17	1
2	43	40	1
3	72	70	1
4	176	176	1
5	43	42	1
6	-5	2	3
7	28	25	1
8	92	91	1
9	57	55	1
10	14	15	2
11	36	33	1
12	7	5	3

3 11 1

-1	-5	0	4
0	-5	5	4
1	7	10	3
2	26	26	1
3	18	16	1
4	165	162	1
5	117	119	1
6	52	54	1
7	5	5	4
8	12	8	2
9	63	63	1
10	37	35	1
11	70	58	1
12	84	77	1

3 12 1

1	-7	12	3
2	19	18	2
3	24	22	1
4	60	59	1
5	59	59	1
6	28	29	1
7	32	32	1
8	34	33	1
9	14	15	2
10	13	11	2
11	20	23	2

3 13 1

4	35	34	1
5	25	21	1
6	43	42	1
7	26	21	1
8	14	7	2
9	92	84	1

4 -9 1

0	4	14	4

4 -8 1

0	2	11	5
1	27	20	1
2	23	21	1

4 -7 1

0	16	16	1
1	-7	3	3
2	11	6	2
3	53	52	1
4	39	34	1

4 -6 1

0	32	34	1
1	-7	2	2
2	50	51	1
3	65	66	1
4	92	96	1
5	24	26	1

4 -5 1

0	14	12	1
1	37	38	1
2	19	18	1
3	23	16	1
4	48	58	1
5	32	34	1
6	-13	4	2

4 -4 1

0	132	132	1
1	60	60	1
2	167	166	1
3	35	32	1
4	43	41	1
5	12	17	2
6	14	12	2
7	5	11	4

4 -3 1

0	45	46	0
1	105	101	1
2	94	97	1
3	121	124	1
4	10	2	2
5	-9	2	2
6	24	21	1
7	26	25	1
8	4	1	5

4 -2 1

0	102	107	1
1	61	59	0
2	4	3	2
3	38	41	1
4	7	8	2
5	78	74	1
6	-1	7	6
7	46	43	1
8	43	44	1
9	12	9	2

4 -1 1

0	56	58	0
1	45	39	0
2	32	33	0
3	62	64	0
4	90	85	1
5	14	15	1
6	15	18	1
7	53	58	1
8	34	37	1

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9	11	9	2
10	16	17	2

4 0 l

-11	34	36	1
-10	57	56	1
-9	13	3	2
-8	10	7	2
-7	11	9	1
-6	58	60	1
-5	24	24	1
-4	64	47	0
-3	123	105	1
-2	387	375	3
-1	70	57	0
0	335	327	2
1	136	141	1
2	240	237	2
3	91	89	1
4	117	117	1
5	148	151	1
6	49	53	1
7	6	6	3
8	49	48	1
9	2	4	5
10	7	9	3

4 1 l

-11	54	54	1
-10	21	21	1
-9	3	3	4
-8	60	60	1
-7	11	10	2
-6	25	27	1
-5	58	60	0
-4	202	202	1
-3	429	407	3
-2	309	301	2
-1	135	130	1
0	243	234	2
1	30	32	0
2	66	63	0
3	78	76	0
4	95	97	1
5	33	33	0
6	20	17	1
7	101	102	1
8	21	22	1
9	30	29	1
10	31	31	1
11	-7	3	3

4 2 l

-10	49	49	1
-9	19	20	1
-8	9	11	2
-7	16	23	1
-6	56	55	1
-5	103	105	1
-4	59	49	0
-3	238	228	2
-2	89	91	1
-1	127	132	1
0	345	333	3
1	14	17	1
2	269	264	2
3	105	99	1
4	201	206	1
5	17	19	1
6	18	20	1
7	68	67	1
8	3	9	4
9	2	1	5
10	34	31	1
11	17	18	2

4 3 l

-10	9	10	3
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-8	53	53	1
-7	20	22	1
-6	84	82	1
-5	42	41	1
-4	154	151	1
-3	129	123	1
-2	116	119	1
-1	35	31	0
0	160	164	1
1	209	212	1
2	42	39	0
3	336	315	2
4	194	186	1
5	43	42	0
6	134	139	1
7	90	94	1
8	56	57	1
9	25	27	1
10	22	23	1
11	56	59	1
12	37	31	1

4 4 l

-9	10	3	3
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-6	-8	4	2
-5	62	63	1
-4	68	67	1
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-2	142	146	1
-1	180	183	1
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1	380	369	3
2	166	159	1
3	57	56	0
4	210	222	1
5	140	144	1
6	60	61	0
7	122	121	1
8	53	51	1
9	53	51	1
10	113	113	1
11	42	40	1
12	11	8	2

4 5 l

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-6	-6	0	3
-5	15	13	1
-4	18	17	1
-3	71	65	1
-2	31	35	1
-1	40	38	0
0	50	50	0
1	351	338	3
2	172	157	1
3	130	116	1
4	52	50	0
5	236	233	2
6	146	146	1
7	152	152	1
8	15	8	1
9	164	161	1
10	27	30	1
11	41	40	1
12	35	34	1

4 6 l

-7	-8	6	3
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-5	13	11	2
-4	24	25	1
-3	45	45	1
-2	21	17	1
-1	48	48	1
0	136	137	1
1	123	112	1
2	8	11	1
3	164	166	1
4	214	213	1
5	39	39	0
6	36	38	1
7	197	197	1
8	147	146	1
9	104	105	1
10	80	79	1
11	12	12	2
12	-11	1	2
13	45	42	1

4 7 l

-6	2	7	6
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-4	14	18	2
-3	47	47	1
-2	19	13	1
-1	94	96	1
0	152	153	1
1	155	157	1
2	23	25	1
3	73	75	1
4	10	8	1
5	168	166	1
6	351	356	3
7	275	278	2
8	100	95	1
9	39	42	1
10	9	12	2
11	14	17	2
12	9	14	3
13	13	11	2

4 8 l

-5	2	6	6
-4	-2	5	5
-3	64	64	1
-2	48	50	1
-1	92	89	1
0	10	15	2
1	84	88	1
2	14	15	1
3	104	103	1
4	75	73	1
5	26	21	1
6	179	176	1
7	36	33	1
8	44	48	1
9	4	14	4
10	91	91	1
11	35	37	1
12	-3	7	5
13	55	52	1

4 9 l

-4	31	33	1
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-1	5	3	4
0	44	41	1
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2	15	12	1
3	9	7	2
4	30	29	1
5	370	372	3
6	83	84	1
7	12	10	2
8	59	59	1
9	77	75	1
10	39	40	1
11	46	45	1
12	65	58	1
13	60	61	1

4 10 l

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2	21	22	1
3	40	40	1
4	62	61	1
5	151	145	1
6	117	119	1
7	28	32	1
8	23	22	1
9	29	27	1
10	39	42	1
11	27	20	1
12	-8	0	3

4 11 l

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1	24	25	1
2	43	43	1
3	35	37	1
4	10	7	2
5	26	26	1
6	-4	3	4
7	70	72	1
8	45	44	1
9	17	21	1
10	61	58	1
11	54	49	1
12	30	29	1

4 12 l

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3	78	76	1
4	36	35	1
5	20	21	1
6	17	15	1
7	49	48	1
8	28	30	1
9	57	55	1
10	121	113	1
11	39	32	1

4 13 l

3	-4	0	5
4	17	12	2
5	-4	6	5
6	14	13	2
7	42	39	1
8	11	12	2
9	8	5	3

5 -8 l

0	2	12	6
1	16	11	2

5 -7 l

0	-4	2	4

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3	13	5	2	0	226	230	2	5	146	145	1	12	26	23	1
				1	148	146	1	6	23	25	1				
5	-6	1		2	159	159	1	7	116	119	1	5	7	1	
				3	163	156	1	8	138	139	1				
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4	10	7	3	8	14	14	2	5	4	1		-2	163	162	1
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1	18	18	1					-6	12	9	2	3	70	70	1
2	15	12	1	-11	22	26	1	-5	50	48	1	4	138	142	1
3	91	94	1	-10	10	9	2	-4	47	45	1	5	7	0	2
4	20	18	1	-9	51	49	1	-3	69	69	1	6	270	264	2
5	15	15	2	-8	13	16	2	-2	114	113	1	7	68	67	1
				-7	111	111	1	-1	23	21	1	8	26	24	1
5	-4	1		-6	42	42	1	0	44	47	0	9	105	106	1
				-5	98	94	1	1	99	100	1	10	78	79	1
0	117	120	1	-4	173	176	1	2	140	124	1	11	6	10	3
1	28	29	1	-3	70	54	0	3	53	47	0	12	35	30	1
2	40	43	1	-2	141	129	1	4	144	136	1				
3	14	11	1	-1	183	186	1	5	128	129	1	5	8	1	
4	62	67	1	0	83	80	0	6	98	97	1				
5	-8	3	2	1	-3	3	2	7	28	26	1	-5	13	13	2
6	9	7	3	2	148	143	1	8	18	16	1	-4	48	45	1
				3	246	243	2	9	67	66	1	-3	106	102	1
5	-3	1		4	109	105	1	10	64	65	1	-2	47	46	1
				5	126	128	1	11	50	49	1	-1	34	32	1
0	84	84	1	6	42	42	1	12	11	15	2	0	23	22	1
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2	52	53	1	8	23	25	1	5	5	1		2	82	84	1
3	-1	7	5	9	31	26	1					3	20	21	1
4	23	19	1	10	11	11	2	-8	35	33	1	4	41	41	1
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7	13	16	2					-5	15	18	1	7	84	86	1
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5	-2	1		-9	30	28	1	-3	8	6	2	9	12	16	2
				-8	9	13	2	-2	39	40	1	10	28	30	1
0	58	53	0	-7	18	22	1	-1	3	3	3	11	104	98	1
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2	56	58	1	-5	125	124	1	1	274	261	2				
3	90	92	1	-4	14	11	1	2	-3	5	2	5	9	1	
4	54	56	1	-3	215	208	1	3	27	24	0				
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6	25	23	1	-1	126	126	1	5	107	102	1	-3	43	38	1
7	5	4	4	0	25	18	0	6	176	170	1	-2	44	43	1
8	-2	6	5	1	92	96	1	7	196	198	1	-1	24	23	1
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5	-1	1		3	163	171	1	9	175	175	1	1	74	70	1
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3	75	76	1	8	28	22	1	5	6	1		6	60	60	1
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9	-6	1	4					-3	47	47	1	12	27	20	1
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6	74	75	1	3	18	16	1	2	64	65	0	9	82	80	1
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8	107	108	1	5	25	19	1	4	31	35	1	11	19	18	2
9	-10	3	2	6	-2	1	6	5	76	76	1				
10	64	65	1					6	55	54	1		6 5 1		
11	129	124	1		6 -3 1			7	17	16	1				
12	61	56	1					8	56	54	1	-8	27	26	1
				0	123	120	1	9	52	49	1	-7	21	19	1
	5 11 1			1	16	15	1	10	7	9	3	-6	-7	9	3
				2	98	96	1					-5	29	29	1
-1	-2	5	6	3	47	52	1		6 2 1			-4	-9	4	2
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7	57	52	1	0	74	69	1	-4	41	48	1	4	30	30	1
8	17	20	1	1	83	88	1	-3	25	26	1	5	40	45	1
9	-4	1	4	2	58	59	1	-2	155	158	1	6	44	42	1
10	62	60	1	3	-5	8	3	-1	134	137	1	7	18	14	1
11	57	49	1	4	25	21	1	0	189	186	1	8	130	127	1
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	5 12 1			6	-8	0	2	2	195	188	1	10	55	56	1
				7	15	12	2	3	251	236	2	11	-3	2	5
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2	8	4	3					5	25	27	1				
3	10	14	2		6 -1 1			6	39	42	1		6 6 1		
4	16	9	2					7	109	111	1				
5	-9	7	2	0	152	146	1	8	82	79	1	-7	25	22	1
6	-9	2	2	1	68	68	1	9	73	72	1	-6	-11	2	2
7	39	36	1	2	16	18	1	10	16	10	2	-5	17	18	1
8	17	19	2	3	120	116	1					-4	32	35	1
9	7	1	3	4	74	74	1		6 3 1			-3	155	155	1
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11	65	61	1	6	57	57	1	-9	-11	2	2	-1	169	167	1
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1	87	84	1
2	62	59	1
3	55	64	1
4	130	138	1
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7	13	12	2
8	64	58	1
9	6	6	3
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9 7 1

-5	12	15	2
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2	14	18	1
3	99	96	1
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8	13	13	2
9	51	51	1
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9 8 1

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6	38	40	1					6	43	41	1				
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11 2 1

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7	24	26	1

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12 9 1

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13 3 1

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