

# MARDER 2524-2526

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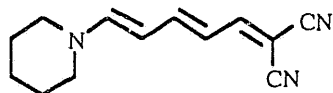
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JACS 4907

## SUPPLEMENTARY MATERIAL FOR COMPOUND 1

1,1-dicyano-6-(1-piperidinyl)-1,3,5-hexatriene



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p. 2524 Marder

Supplementary material,  
page 1

wps code	Pip-II-DCV
Name	1,1-dicyano-6-(1-piperidiny1)-1,3,5-hexatriene
Formula	C <sub>13</sub> H <sub>15</sub> N <sub>3</sub>
Formula Weight	213.28
Crystal System	triclinic
Space Group	$\bar{P}1$
Cell Dimensions	a, Å
	b, Å
	c, Å
	$\alpha$ , °
	$\beta$ , °
	$\gamma$ , °
	V, Å <sup>3</sup>
	Z
Density, calc, g cm <sup>-3</sup>	1.11
Crystal color, habit	thin orange, parallelepiped
Crystal size, mm <sup>3</sup>	0.07 x 0.09 x 0.21
$\mu$ , cm <sup>-1</sup>	0.063
$\mu_{\text{rmax}}$	0.0132
maximum $2\theta$ (scan type)	25°
range of h,k, l	-6-6, -12-12, -14-14
# of reflections measured	4551
# of independent reflections	2244
# reflections, $F_0^2 > 0$	1801
# reflections, $F_0^2 > 3\sigma(F_0^2)$	791
GOF, merge	???
R(merge) for refs meas. twice	0.081
secondary extinction (x 10 <sup>-6</sup> )	0.9(4)
R, $F_0^2 > 0$	0.171
R, $F_0^2 > 3\sigma(F_0^2)$	0.077
GOF (number of parameters)	1.62, (1.46)
$(\Delta/\sigma)_{\text{max}}$ in final least squares	0.01
Final Difference map:	
Maximum, eÅ <sup>-3</sup>	+ 0.42
Minimum, eÅ <sup>-3</sup>	- 0.40

Data was collected at 294 K.  
Hydrogen positions were assumed, C-H 0.95 Å, and repositioned once near the end of refinement.  
Structure solved using MULTAN 88.

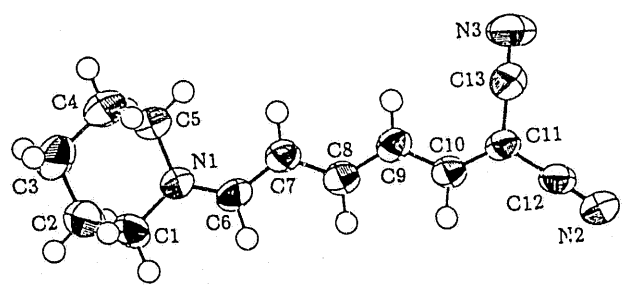


Figure 1

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Figure 1: An ORTEP drawing of the molecule with 50% probability ellipsoids showing the numbering system. Hydrogen atoms are drawn as circles of arbitrary small size.

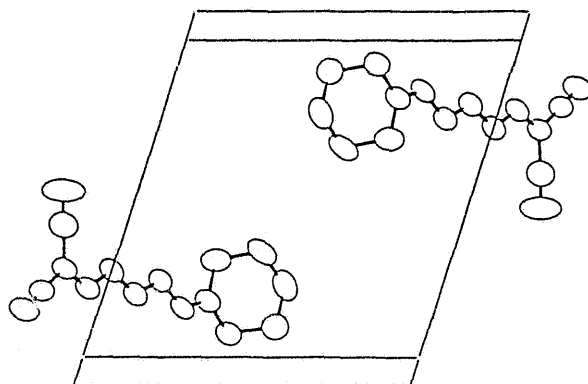


Figure 2.

Schaefer, Tiemann and Marder

Figure 2: An ORTEP drawing of the contents of a unit cell, with a unit cell outlined. Hydrogen atoms are not shown.

Table 1. Final Heavy Atom Parameters for  
1-(6,6-Dicyanohexa-1,3,5-triene)piperidine.

Atom	$x, y, z$ and $U_{eq}^a \times 10^4$			$U_{eq}$
	$x$	$y$	$z$	
N1	2912(8)	3116(4)	2228(3)	652(12)
C1	1552(10)	4066(5)	1385(4)	761(16)
C2	1615(11)	5378(5)	1585(5)	873(18)
C3	434(12)	5267(6)	2886(6)	990(20)
C4	1887(12)	4262(6)	3747(5)	989(20)
C5	1872(10)	2984(5)	3503(4)	846(18)
C6	4811(10)	2427(5)	1870(4)	648(15)
C7	6269(10)	1517(5)	2540(4)	612(15)
C8	8225(10)	905(5)	1973(4)	625(14)
C9	9884(10)	1(5)	2519(4)	613(15)
C10	11787(10)	-533(5)	1851(4)	620(15)
C11	13653(9)	-1376(5)	2252(4)	580(15)
C12	15538(10)	-1837(5)	1451(4)	635(16)
N2	17041(9)	-2173(4)	779(4)	884(15)
C13	13805(10)	-1836(5)	3504(5)	772(18)
N3	13880(10)	-2165(6)	4504(4)	1251(22)

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

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p. 2524 Marder

Supplementary material,  
page 5

Table 2. Heavy Atom Distances and Angles for  
1-(6,6-Dicyanohexa-1,3,5-triene)piperidine.

		Distance(Å)			Angle(°)
N1	-C1	1.463(7)	C5	-N1 -C1	113.2(4)
N1	-C5	1.469(7)	C6	-N1 -C1	122.7(4)
N1	-C6	1.311(7)	C6	-N1 -C5	124.0(4)
C1	-C2	1.517(8)	C2	-C1 -N1	110.2(4)
C2	-C3	1.518(8)	C3	-C2 -C1	109.3(5)
C3	-C4	1.531(9)	C4	-C3 -C2	109.8(5)
C4	-C5	1.502(8)	C5	-C4 -C3	110.0(5)
C6	-C7	1.369(7)	C4	-C5 -N1	110.8(5)
C7	-C8	1.384(7)	C7	-C6 -N1	129.5(5)
C8	-C9	1.376(7)	C8	-C7 -C6	120.2(5)
C9	-C10	1.381(7)	C9	-C8 -C7	126.9(5)
C10	-C11	1.365(7)	C10	-C9 -C8	121.6(5)
C11	-C12	1.428(7)	C11	-C10 -C9	128.3(5)
C11	-C13	1.422(8)	C12	-C11 -C10	122.3(5)
C12	-N2	1.147(7)	C13	-C11 -C10	120.9(5)
C13	-N3	1.131(8)	C13	-C11 -C12	116.8(5)
			N2	-C12 -C11	177.9(6)
			N3	-C13 -C11	177.6(6)

Table S1. Assigned Hydrogen Atom Parameters for  
1-(6,6-Dicyanohexa-1,3,5-triene)piperidine.

$x, y$  and  $z \times 10^4$

Atom	$x$	$y$	$z$	$B$
H1A	-164	3792	1509	6.9
H1B	2357	4127	580	6.9
H2A	643	5976	1060	7.9
H2B	3315	5673	1421	7.9
H3A	-1293	5014	3038	9.0
H3B	547	6080	3021	9.0
H4A	1072	4166	4559	9.0
H4B	3590	4541	3634	9.0
H5A	171	2669	3685	7.6
H5B	2887	2386	3998	7.6
H6	5237	2580	1017	5.8
H7	5946	1309	3399	5.6
H8	8430	1129	1115	5.6
H9	9721	-258	3375	5.6
H10	11797	-280	1002	5.6

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p. 2524 Marder

Supplementary material,  
page 7



Table S2. Anisotropic Displacement Parameters for  
1-(6,6-Dicyanohexa-1,3,5-triene)piperidine.

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{12}$	$U_{13}$	$U_{23}$
N1	744(33)	741(33)	553(27)	149(27)	-188(24)	-296(24)
C1	965(46)	773(42)	710(37)	195(35)	-428(33)	-333(32)
C2	1113(50)	800(44)	762(40)	141(36)	-297(35)	-263(34)
C3	1274(57)	820(46)	1017(48)	116(41)	-150(43)	-532(39)
C4	1327(59)	1117(54)	750(42)	218(45)	-272(38)	-596(40)
C5	977(47)	963(47)	549(35)	215(36)	-71(31)	-228(33)
C6	779(44)	744(42)	561(33)	55(34)	-168(30)	-383(31)
C7	689(41)	653(39)	573(33)	5(33)	-144(30)	-281(31)
C8	703(41)	663(38)	619(33)	-35(32)	-205(30)	-297(30)
C9	649(41)	685(43)	609(35)	3(33)	-142(30)	-327(31)
C10	735(41)	680(39)	563(34)	6(32)	-218(30)	-301(30)
C11	601(39)	704(40)	478(32)	-10(32)	-108(28)	-233(29)
C12	767(44)	680(40)	485(33)	10(33)	-181(30)	-175(30)
N2	1084(42)	1044(39)	602(30)	284(32)	-194(28)	-381(28)
C13	716(42)	907(46)	680(39)	79(33)	-72(34)	-264(37)
N3	1194(47)	1904(60)	566(32)	306(39)	-194(30)	-268(36)

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

The form of the displacement factor is:

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

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p. 2524 Marder

Supplementary material,  
page 8

Table S3. Complete Distances and Angles for  
1-(6,6-Dicyanohexa-1,3,5-triene)piperidine.

		Distance(Å)			Angle(°)
N1	-C1	1.463(7)	C5	-N1 -C1	113.2(4)
N1	-C5	1.469(7)	C6	-N1 -C1	122.7(4)
N1	-C6	1.311(7)	C6	-N1 -C5	124.0(4)
C1	-C2	1.517(8)	C2	-C1 -N1	110.2(4)
C1	-H1A	0.949	H1A	-C1 -N1	109.1
C1	-H1B	0.951	H1B	-C1 -N1	108.9
C2	-C3	1.518(8)	H1A	-C1 -C2	109.8
C2	-H2A	0.954	H1B	-C1 -C2	109.4
C2	-H2B	0.944	H1B	-C1 -H1A	109.4
C3	-C4	1.531(9)	C3	-C2 -C1	109.3(5)
C3	-H3A	0.945	H2A	-C2 -C1	109.2
C3	-H3B	0.952	H2B	-C2 -C1	110.0
C4	-C5	1.502(8)	H2A	-C2 -C3	108.9
C4	-H4A	0.953	H2B	-C2 -C3	109.9
C4	-H4B	0.946	H2B	-C2 -H2A	109.6
C5	-H5A	0.950	C4	-C3 -C2	109.8(5)
C5	-H5B	0.950	H3A	-C3 -C2	109.9
C6	-C7	1.369(7)	H3B	-C3 -C2	109.2
C6	-H6	0.953	H3A	-C3 -C4	109.4
C7	-C8	1.384(7)	H3B	-C3 -C4	108.8
C7	-H7	0.952	H3B	-C3 -H3A	109.8
C8	-C9	1.376(7)	C5	-C4 -C3	110.0(5)
C8	-H8	0.952	H4A	-C4 -C3	108.9
C9	-C10	1.381(7)	H4B	-C4 -C3	109.6
C9	-H9	0.951	H4A	-C4 -C5	109.1
C10	-C11	1.365(7)	H4B	-C4 -C5	109.6
C10	-H10	0.952	H4B	-C4 -H4A	109.6
C11	-C12	1.428(7)	C4	-C5 -N1	110.8(5)
C11	-C13	1.422(8)	H5A	-C5 -N1	109.0
C12	-N2	1.147(7)	H5B	-C5 -N1	108.9
C13	-N3	1.131(8)	H5A	-C5 -C4	109.4
			H5B	-C5 -C4	109.2
			H5B	-C5 -H5A	109.5
			C7	-C6 -N1	129.5(5)
			H6	-C6 -N1	115.3
			H6	-C6 -C7	115.2
			C8	-C7 -C6	120.2(5)
			H7	-C7 -C6	119.9
			H7	-C7 -C8	119.9
			C9	-C8 -C7	126.9(5)

Table S3. (Cont.)

			Angle(°)
H8	-C8	-C7	116.4
H8	-C8	-C9	116.7
C10	-C9	-C8	121.6(5)
H9	-C9	-C8	119.1
H9	-C9	-C10	119.3
C11	-C10	-C9	128.3(5)
H10	-C10	-C9	115.8
H10	-C10	-C11	115.9
C12	-C11	-C10	122.3(5)
C13	-C11	-C10	120.9(5)
C13	-C11	-C12	116.8(5)
N2	-C12	-C11	177.9(6)
N3	-C13	-C11	177.6(6)

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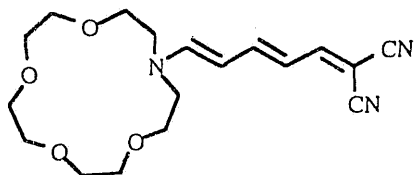
Supplementary material,  
page 10

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J-2526-m11

SUPPLEMENTARY MATERIAL FOR COMPOUND 2

1,1-dicyano-6-(N-aza-15-crown-5)-1,3,5-hexatriene



wps code	aza-15-crown-5 DCV
Name	1,1-dicyano-6-(N-aza-15-crown-5)-1,3,5-hexatriene
Formula	$C_{18}H_{12}N_3O_4$
Formula Weight	347.41
Crystal System	Monoclinic
Space Group	$P2_1/c$ , #14
Cell Dimensions	a, Å
	b, Å
	c, Å
	$\alpha$ , °
	$\beta$ , °
	$\gamma$ , °
	V, Å <sup>3</sup>
	Z
Density, calc, g cm <sup>-3</sup>	1.248
Crystal color, habit	orange-red, chunky rectangles
Crystal size, mm <sup>3</sup>	0.19 x 0.22 x 0.22
$\mu$ , cm <sup>-1</sup>	0.832
$\mu_{rmax}$	0.015
maximum 2 $\theta$ (scan type)	25°
range of h,k, l	-16 - 16, -10 - 10, 0 - 17
# of reflections measured	6974
# of independent reflections	2517
# reflections, $F_0^2 > 0$	2971
# reflections, $F_0^2 > 3\sigma(F_0^2)$	2215
GOF, merge	1.48
R(merge) for refs meas. twice	0.034
secondary extinction (x 10 <sup>-6</sup> )	1.48 (10)
R, $F_0^2 > 0$	0.054
R, $F_0^2 > 3\sigma(F_0^2)$	0.0358
GOF (number of parameters)	1.48, (327)
$(\Delta/\sigma)_{max}$ in final least squares	0.03
Final Difference map:	
Maximum, eÅ <sup>-3</sup>	+ 0.19
Minimum, eÅ <sup>-3</sup>	- 0.21

Data was collected at 225 K.  
Hydrogen atoms were refined isotropically  
Structure solved using MULTAN 88.

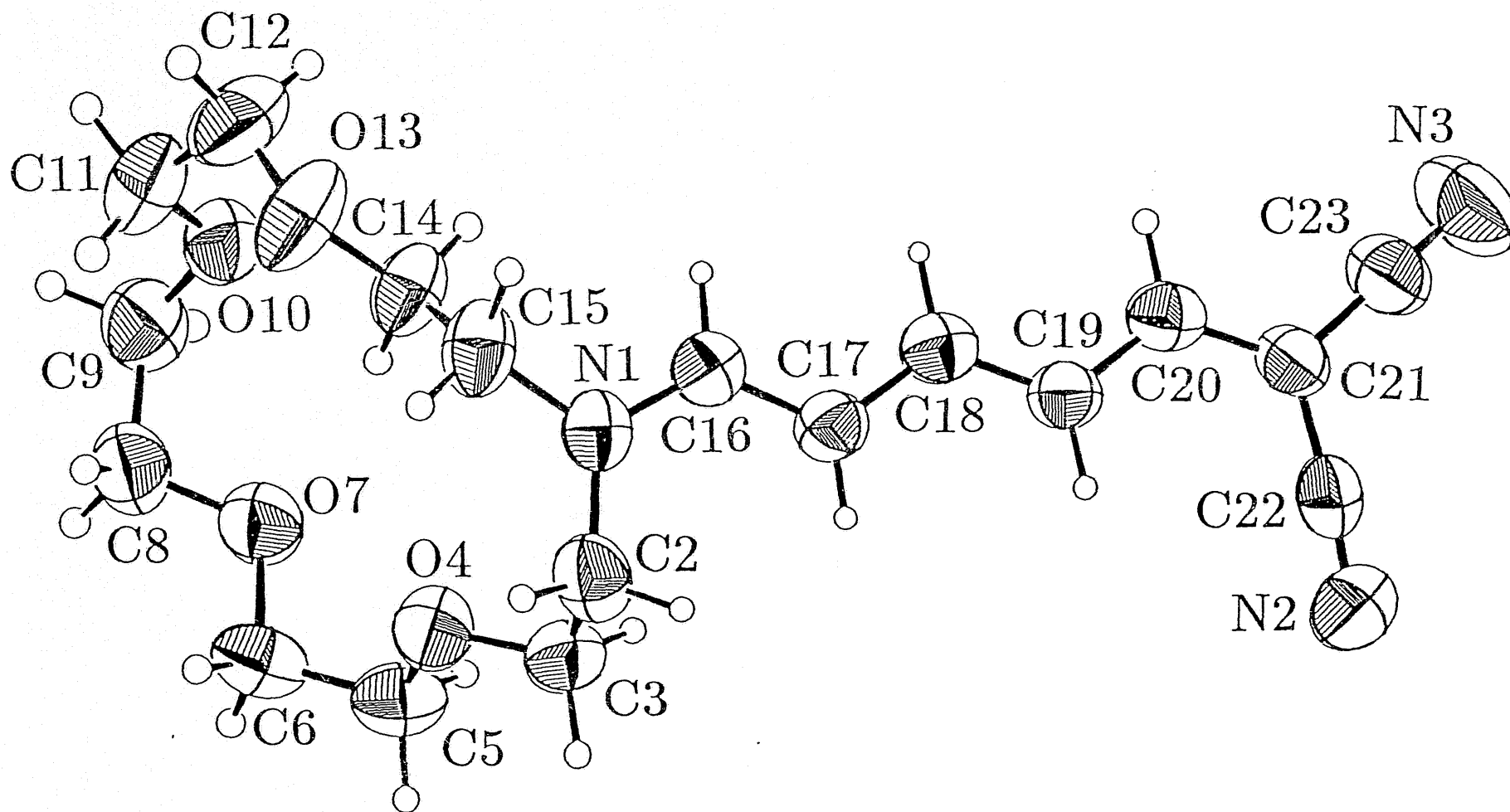


Figure 1: An ORTEP drawing of the molecule with 75% probability ellipsoids showing the numbering system. Hydrogen atoms are shown with thermal parameters one-tenth of their actual value.

J-2524 m13

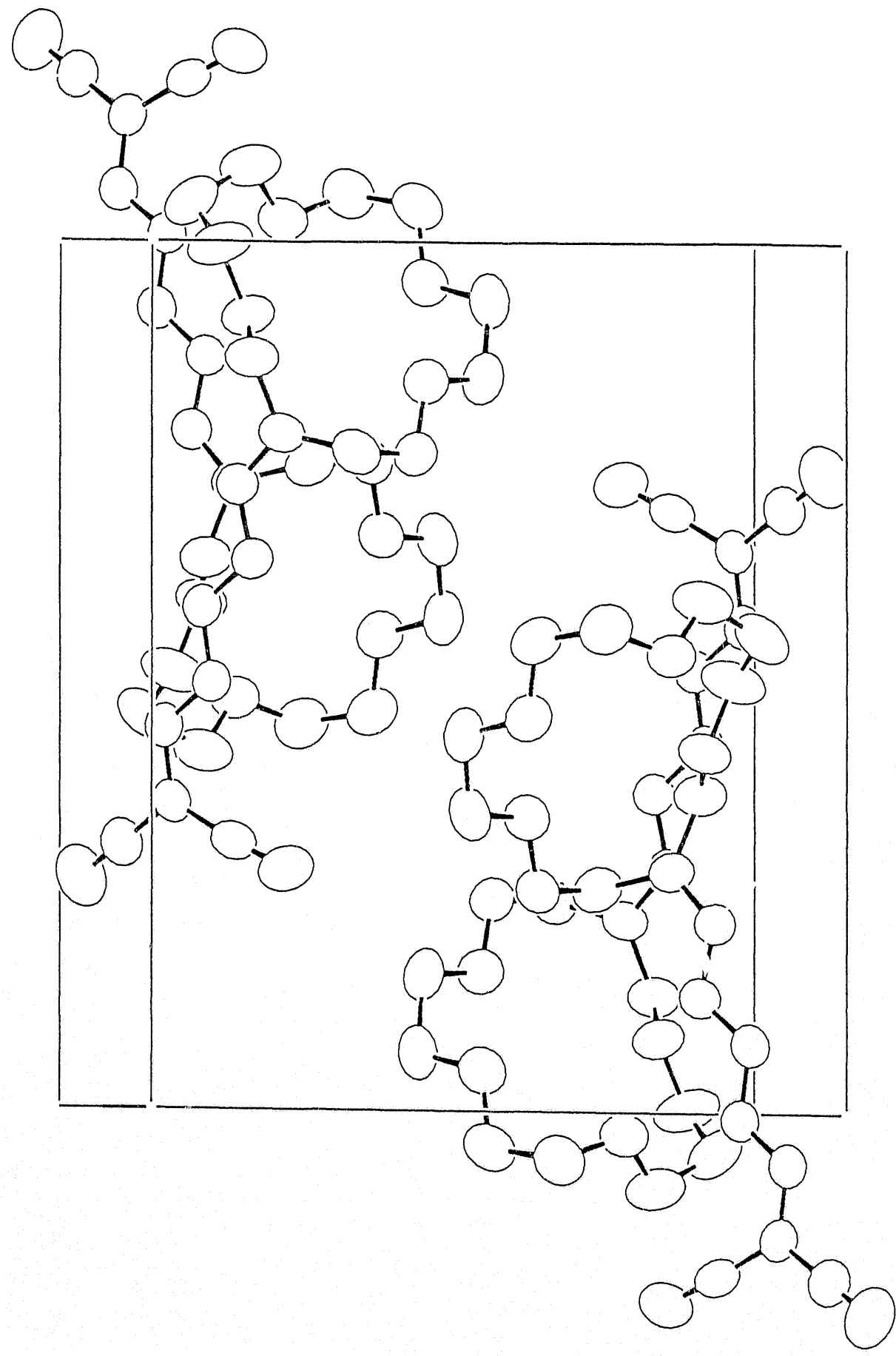


Figure 2: An ORTEP drawing of the contents of a unit cell, with a unit cell outlined. Atoms are shown as 75% probability ellipsoids; hydrogen atoms are not shown. The view is perpendicular to the  $a$   $b$  plane.

Table 1. Final Refined Parameters for  
Azo-15-Crown-5-Cyanine.

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

Atom	$x$	$y$	$z$	$U_{eq}$ or $B$
N1	2403(1)	7783(1)	4137(1)	341(3)
C2	3389(1)	7570(1)	3565(2)	401(4)
C3	4406(2)	7550(1)	4668(2)	394(4)
O4	4630(1)	8389(1)	5173(1)	406(3)
C5	5588(2)	8429(1)	6220(2)	423(5)
C6	5741(2)	9330(1)	6723(2)	431(5)
O7	4919(1)	9528(1)	7528(1)	448(3)
C8	4841(2)	10415(1)	7776(2)	476(5)
C9	3936(2)	10555(1)	8609(2)	489(5)
O10	2905(1)	10260(1)	7900(1)	418(3)
C11	2331(2)	10875(1)	6985(2)	514(5)
C12	1369(2)	10462(1)	6101(3)	579(6)
O13	1631(1)	9962(1)	4991(1)	568(4)
C14	2090(2)	9144(1)	5368(2)	421(5)
C15	1973(2)	8660(1)	4013(2)	420(5)
C16	1860(1)	7187(1)	4720(2)	316(4)
C17	2088(1)	6329(1)	4844(2)	325(4)
C18	1459(1)	5784(1)	5524(2)	318(4)
C19	1618(1)	4921(1)	5690(2)	318(4)
C20	1030(1)	4409(1)	6479(2)	332(4)



Table 1. (Cont.)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{eq}$ or <i>B</i>
C21	1182(1)	3547(1)	6700(2)	340(4)
C22	1987(1)	3103(1)	6087(2)	406(4)
N2	2652(1)	2784(1)	5574(2)	616(5)
C23	567(1)	3065(1)	7542(2)	434(5)
N3	71(1)	2674(1)	8213(2)	670(5)
H2A	3300(12)	6990(10)	3120(16)	2.8(4)*
H2B	3481(13)	7997(11)	2876(18)	3.4(4)*
H3A	4299(13)	7147(10)	5469(18)	3.2(4)*
H3B	5019(13)	7315(10)	4263(17)	3.3(4)*
H5A	5486(13)	8032(10)	7016(19)	3.6(4)*
H5B	6224(14)	8230(10)	5835(17)	3.3(4)*
H6A	6477(14)	9362(10)	7315(18)	3.8(4)*
H6B	5694(14)	9728(11)	5921(19)	4.1(4)*
H8A	5563(15)	10634(11)	8344(19)	4.4(4)*
H8B	4672(14)	10735(11)	6886(20)	4.1(4)*
H9A	4117(15)	10214(12)	9504(20)	4.9(5)*
H9B	3904(14)	11196(12)	8830(18)	4.3(4)*
H11A	2050(14)	11354(12)	7542(20)	4.8(5)*
H11B	2811(16)	11109(12)	6382(22)	5.8(6)*
H12A	970(14)	10113(12)	6704(20)	4.4(5)*

Table 1. (Cont.)

Atom	x	y	z	$U_{eq}$ or $B$
H12B	895(16)	10923(13)	5659(21)	5.6(5)*
H14A	2848(15)	9193(10)	5800(18)	3.9(4)*
H14B	1669(14)	8856(11)	6033(19)	4.1(4)*
H15A	1169(15)	8628(10)	3570(18)	3.8(4)*
H15B	2352(14)	8957(11)	3348(19)	4.1(4)*
H16	1237(12)	7383(9)	5106(16)	2.4(3)*
H17	2673(12)	6095(9)	4480(16)	2.4(3)*
H18	874(12)	6059(9)	5926(15)	1.9(3)*
H19	2168(12)	4649(9)	5248(16)	2.6(3)*
H20	472(13)	4676(10)	6935(16)	3.1(4)*

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

\* Isotropic displacement parameter,  $B$

Table 2. Anisotropic Displacement Parameters for  
Azo-15-Crown-5-Cyanine.

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{12}$	$U_{13}$	$U_{23}$
N1	380(8)	302(8)	334(8)	-22(6)	36(7)	21(6)
C2	487(11)	402(11)	340(11)	-77(9)	144(9)	-25(9)
C3	400(10)	381(10)	426(12)	28(9)	145(9)	-14(9)
O4	384(7)	402(7)	409(7)	11(5)	-3(6)	-2(6)
C5	317(10)	549(12)	394(11)	66(9)	36(9)	-20(10)
C6	304(10)	589(13)	403(11)	-37(9)	69(9)	-29(10)
O7	467(7)	437(8)	477(8)	-44(6)	185(6)	-42(6)
C8	526(13)	433(12)	491(13)	-103(9)	151(11)	-57(10)
C9	534(12)	493(13)	455(12)	-75(10)	123(10)	-102(10)
O10	465(7)	351(6)	452(8)	-8(6)	121(6)	35(6)
C11	684(14)	343(11)	518(13)	81(10)	108(12)	7(10)
C12	546(13)	483(13)	695(16)	199(11)	66(12)	-35(12)
O13	761(9)	362(7)	535(9)	180(7)	-23(7)	-1(6)
C14	490(12)	317(10)	429(12)	73(9)	1(10)	20(9)
C15	497(12)	322(10)	408(12)	2(9)	-20(10)	57(9)
C16	315(9)	332(10)	291(10)	-1(8)	20(8)	-22(7)
C17	318(9)	322(10)	338(10)	6(8)	63(8)	-33(8)
C18	284(9)	362(10)	298(9)	11(7)	23(8)	-34(8)
C19	291(9)	337(10)	333(10)	5(7)	73(8)	-23(8)
C20	276(9)	381(10)	340(10)	7(7)	51(8)	-21(8)
C21	284(9)	362(10)	381(10)	-27(7)	79(8)	41(8)
C22	406(11)	291(9)	534(12)	-41(8)	117(9)	70(9)
N2	631(11)	403(10)	894(14)	82(8)	363(11)	56(9)
C23	334(10)	460(11)	511(12)	-13(8)	76(9)	95(9)
N3	533(10)	744(13)	771(13)	-82(9)	216(10)	279(11)

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

The form of the displacement factor is:

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

Table 3. Complete Distances and Angles for  
Azo-15-Crown-5-Cyanine.

Distance(Å)		Distance(Å)	
N1 -C2	1.463(2)	C18 -C19	1.369(2)
N1 -C15	1.469(2)	C18 -H18	0.978(14)
N1 -C16	1.330(2)	C19 -C20	1.394(2)
C2 -C3	1.508(3)	C19 -H19	0.962(15)
C2 -H2A	1.002(16)	C20 -C21	1.372(2)
C2 -H2B	0.964(17)	C20 -H20	0.976(15)
C3 -O4	1.411(2)	C21 -C22	1.424(2)
C3 -H3A	1.026(16)	C21 -C23	1.422(2)
C3 -H3B	0.983(16)	C22 -N2	1.146(2)
O4 -C5	1.426(2)	C23 -N3	1.144(3)
C5 -C6	1.492(3)		
C5 -H5A	1.016(17)		
C5 -H5B	0.978(16)		
C6 -O7	1.419(2)		
C6 -H6A	0.993(17)		
C6 -H6B	0.990(17)		
O7 -C8	1.413(2)		
C8 -C9	1.503(3)		
C8 -H8A	1.026(18)		
C8 -H8B	0.989(18)		
C9 -O10	1.421(2)		
C9 -H9A	1.011(19)		
C9 -H9B	1.026(18)		
O10 -C11	1.416(2)		
C11 -C12	1.491(3)		
C11 -H11A	1.018(18)		
C11 -H11B	0.97(2)		
C12 -O13	1.412(3)		
C12 -H12A	0.990(18)		
C12 -H12B	0.98(2)		
O13 -C14	1.421(2)		
C14 -C15	1.502(3)		
C14 -H14A	0.963(17)		
C14 -H14B	1.002(17)		
C15 -H15A	1.017(17)		
C15 -H15B	0.976(18)		
C16 -C17	1.370(2)		
C16 -H16	0.963(15)		
C17 -C18	1.394(2)		
C17 -H17	0.932(15)		

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p. 2524 Marder

Supplementary material,  
page 19

Table 3. (Cont.)

	Angle(°)		Angle(°)
C15 -N1 -C2	119.7(1)	H9B -C9 -H9A	110.2(14)
C16 -N1 -C2	121.1(1)	C11 -O10 -C9	113.4(1)
C16 -N1 -C15	119.2(1)	C12 -C11 -O10	109.5(2)
C3 -C2 -N1	112.7(1)	H11A -C11 -O10	110.3(10)
H2A -C2 -N1	109.3(9)	H11B -C11 -O10	109.8(12)
H2B -C2 -N1	108.0(10)	H11A -C11 -C12	108.2(10)
H2A -C2 -C3	107.8(9)	H11B -C11 -C12	109.1(12)
H2B -C2 -C3	108.9(10)	H11B -C11 -H11A	109.9(16)
H2B -C2 -H2A	110.2(13)	O13 -C12 -C11	114.5(2)
O4 -C3 -C2	108.6(1)	H12A -C12 -C11	109.1(11)
H3A -C3 -C2	110.6(9)	H12B -C12 -C11	107.1(12)
H3B -C3 -C2	109.4(9)	H12A -C12 -O13	110.3(11)
H3A -C3 -O4	110.6(9)	H12B -C12 -O13	105.7(12)
H3B -C3 -O4	111.5(9)	H12B -C12 -H12A	110.0(16)
H3B -C3 -H3A	106.3(13)	C14 -O13 -C12	115.8(1)
C5 -O4 -C3	112.3(1)	C15 -C14 -O13	104.6(1)
C6 -C5 -O4	108.5(1)	H14A -C14 -O13	111.0(10)
H5A -C5 -O4	108.6(10)	H14B -C14 -O13	109.9(10)
H5B -C5 -O4	109.9(10)	H14A -C14 -C15	111.3(10)
H5A -C5 -C6	110.7(10)	H14B -C14 -C15	110.7(10)
H5B -C5 -C6	111.1(10)	H14B -C14 -H14A	109.3(14)
H5B -C5 -H5A	107.9(13)	C14 -C15 -N1	114.7(2)
O7 -C6 -C5	108.8(1)	H15A -C15 -N1	107.7(10)
H6A -C6 -C5	106.8(10)	H15B -C15 -N1	106.8(10)
H6B -C6 -C5	110.4(10)	H15A -C15 -C14	109.8(10)
H6A -C6 -O7	110.1(10)	H15B -C15 -C14	110.7(10)
H6B -C6 -O7	110.1(10)	H15B -C15 -H15A	106.8(14)
H6B -C6 -H6A	110.5(14)	C17 -C16 -N1	127.7(2)
C8 -O7 -C6	112.6(1)	H16 -C16 -N1	115.9(9)
C9 -C8 -O7	108.2(2)	H16 -C16 -C17	116.4(9)
H8A -C8 -O7	109.9(10)	C18 -C17 -C16	121.1(1)
H8B -C8 -O7	110.9(10)	H17 -C17 -C16	120.8(9)
H8A -C8 -C9	108.8(10)	H17 -C17 -C18	118.1(9)
H8B -C8 -C9	109.2(10)	C19 -C18 -C17	125.2(2)
H8B -C8 -H8A	109.7(14)	H18 -C18 -C17	115.5(8)
O10 -C9 -C8	112.5(2)	H18 -C18 -C19	119.3(8)
H9A -C9 -C8	107.9(11)	C20 -C19 -C18	123.5(2)
H9B -C9 -C8	108.3(10)	H19 -C19 -C18	118.8(9)
H9A -C9 -O10	107.1(11)	H19 -C19 -C20	117.8(9)
H9B -C9 -O10	110.8(10)	C21 -C20 -C19	125.4(2)

Supplementary material,  
page 20

Table 3. (Cont.)

	Angle(°)
H20 -C20 -C19	118.6(9)
H20 -C20 -C21	116.0(9)
C22 -C21 -C20	119.9(1)
C23 -C21 -C20	122.5(2)
C23 -C21 -C22	117.6(1)
N2 -C22 -C21	176.7(2)
N3 -C23 -C21	179.6(2)

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p. 2524 Marder

Supplementary material,  
page 21

Table 4. Intermolecular Distances Less Than 3.5 Å for  
Azo-15-Crown-5-Cyanine.

	Distance(Å)		Distance(Å)
C2 -H3A	3.409(16)	C17 -H15B	3.389(17)
C2 -H5A	3.346(17)	C17 -H8A	3.316(18)
C3 -H5A	3.225(17)	C18 -H15A	3.171(17)
C3 -H8B	3.369(18)	C18 -H15B	2.805(17)
C3 -H9B	3.154(17)	C18 -C20	3.366(2)
O4 -H6B	3.130(17)	C18 -H20	3.161(15)
O4 -H8B	2.682(18)	C19 -H15B	3.124(17)
C5 -H3B	3.357(16)	C19 -H9A	3.484(19)
C5 -H8B	3.250(18)	C19 -H20	3.369(15)
C6 -H6B	3.218(17)	C19 -H6A	2.920(17)
C6 -H8B	3.453(18)	C20 -H15B	3.390(17)
O7 -H2A	3.219(15)	C20 -H18	3.110(14)
O7 -H3B	3.327(16)	C20 -H12A	3.454(18)
O7 -H9A	2.952(19)	C20 -H6A	3.111(17)
C8 -H2B	3.365(17)	C21 -H18	3.340(14)
C8 -H9A	2.905(19)	C21 -H6A	3.162(17)
C8 -H3A	3.279(16)	C22 -H11A	3.072(18)
C9 -H17	3.203(15)	C22 -H11B	3.28(2)
C9 -H19	2.931(15)	C22 -H5A	3.353(17)
C9 -H8A	3.457(18)	C22 -H5B	3.409(16)
C9 -H9A	3.019(19)	C22 -H6A	2.982(17)
C9 -H3A	3.332(16)	N2 -H11A	3.111(18)
O10 -C17	3.375(2)	N2 -H11B	2.73(2)
O10 -C19	3.375(2)	N2 -H9B	2.948(17)
O10 -H17	2.658(15)	N2 -H11A	3.206(18)
O10 -H19	2.595(15)	N2 -H3B	2.865(16)
C11 -N2	3.334(3)	N2 -H5B	2.637(16)
C11 -H19	3.308(15)	N2 -H5A	3.018(17)
C12 -H20	3.434(15)	N2 -H6A	3.270(17)
O13 -H20	3.119(15)	C23 -H11A	3.244(18)
O13 -H12A	3.361(18)	C23 -H12B	3.37(2)
O13 -H12B	3.38(2)	C23 -H15A	3.464(17)
C14 -H2A	3.340(16)	C23 -H16	3.183(15)
C15 -C18	3.447(2)	N3 -H11A	3.350(18)
C15 -H18	3.104(14)	N3 -H12B	3.26(2)
C16 -H2B	3.377(17)	N3 -H15A	2.931(17)
C16 -C23	3.431(2)	N3 -H16	3.351(15)
C16 -N3	3.400(2)	N3 -H14B	3.019(17)
C16 -N3	3.454(2)	N3 -H16	2.526(15)
C17 -H2B	3.320(17)	N3 -H18	2.961(14)

Table 4. (Cont.)

	Distance(Å)		Distance(Å)
H2A -H3A	3.32(2)	H12B -H15A	2.87(3)
H2A -H5A	3.07(2)	H14B -H17	3.37(2)
H2A -H14A	2.89(2)	H15A -H18	2.58(2)
H2A -H14B	2.92(2)	H15A -H20	3.13(2)
H2B -H3A	2.71(2)	H15B -H18	2.72(2)
H2B -H5A	3.18(2)	H15B -H20	3.28(2)
H2B -H8A	2.80(2)	H18 -H20	3.20(2)
H2B -H8B	3.01(2)		
H3A -H8A	2.62(2)		
H3A -H8B	3.46(2)		
H3A -H9B	2.67(2)		
H3B -H5A	2.41(2)		
H3B -H8B	3.29(2)		
H3B -H9B	2.72(2)		
H5A -H9B	3.11(2)		
H5B -H8B	3.13(2)		
H5B -H11B	2.83(3)		
H5B -H9B	3.20(2)		
H6A -H15B	3.12(2)		
H6A -H9A	3.36(3)		
H6A -H19	2.70(2)		
H6B -H6B	2.41(2)		
H6B -H8B	2.78(3)		
H6B -H11B	3.39(3)		
H6B -H14A	3.15(2)		
H6B -H15B	3.16(3)		
H8A -H15B	3.35(3)		
H8A -H9A	2.45(3)		
H8A -H17	2.86(2)		
H8A -H19	3.29(2)		
H9A -H17	2.71(2)		
H9A -H19	2.64(2)		
H9A -H9A	2.33(3)		
H9A -H9B	3.48(3)		
H9B -H19	3.04(2)		
H11A -H19	3.04(2)		
H12A -H12B	3.38(3)		
H12A -H15A	3.27(3)		
H12A -H20	2.49(2)		
H12B -H14B	3.34(3)		

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 J. Am. Chem. Soc. v. 115  
 p. 2524 Marder

Supplementary material,  
 page 23



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:

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:

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

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

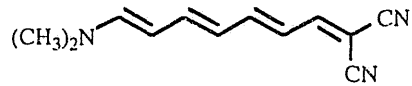
where  $n$  = number of data,

$p$  = number of parameters refined.

5/12/93

## SUPPLEMENTARY MATERIAL FOR COMPOUND 4

1,1-dicyano-8-(dimethylamino)-octa-1,3,5,7-tetraene



wps code	Me2N-III-DCV
Name	1,1-dicyano-8-(dimethylamino)-octa-1,3,5,7-tetraene
Formula	C <sub>12</sub> H <sub>13</sub> N <sub>3</sub>
Formula Weight	199.25
Crystal System	Monoclinic
Space Group	P2 <sub>1</sub> /c, #14
Cell Dimensions a, Å	9.242 (6)
b, Å	16.096 (7)
c, Å	8.188 (3)
α, °	90.0
β, °	105.38 (4)
γ, °	90.0
V, Å <sup>3</sup>	1174.4 (0)
Z	4
Density, calc, g cm <sup>-3</sup>	1.13
Crystal color, habit	dark, wide blade
Crystal size, mm <sup>3</sup>	0.19 x 0.36 x 0.70
μ, cm <sup>-1</sup>	0.65
μ <sub>r</sub> max	0.455
maximum 2θ (scan type)	25°
range of h, k, l	-9 - 9, -19 - 19, 0 - 11
# of reflections measured	4672
# of independent reflections	2060
# reflections, F <sub>o</sub> <sup>2</sup> > 0	1797
# reflections, F <sub>o</sub> <sup>2</sup> > 3σ(F <sub>o</sub> <sup>2</sup> )	1390
GOF, merge	1.02
R(merge) for refs meas. twice	0.025
secondary extinction (x 10 <sup>-6</sup> )	1.9 (4)
R, F <sub>o</sub> <sup>2</sup> > 0	0.065
R, F <sub>o</sub> <sup>2</sup> > 3σ(F <sub>o</sub> <sup>2</sup> )	0.051
GOF (number of parameters)	2.66, (137)
(Δ/σ) <sub>max</sub> in final least squares	0.02
Final Difference map:	
Maximum, eÅ <sup>-3</sup>	+ 0.21
Minimum, eÅ <sup>-3</sup>	- 0.19

Data was collected at 225 K.  
Hydrogen atoms were refined isotropically  
Structure solved using MULTAN 88.

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p. 2524 Marder

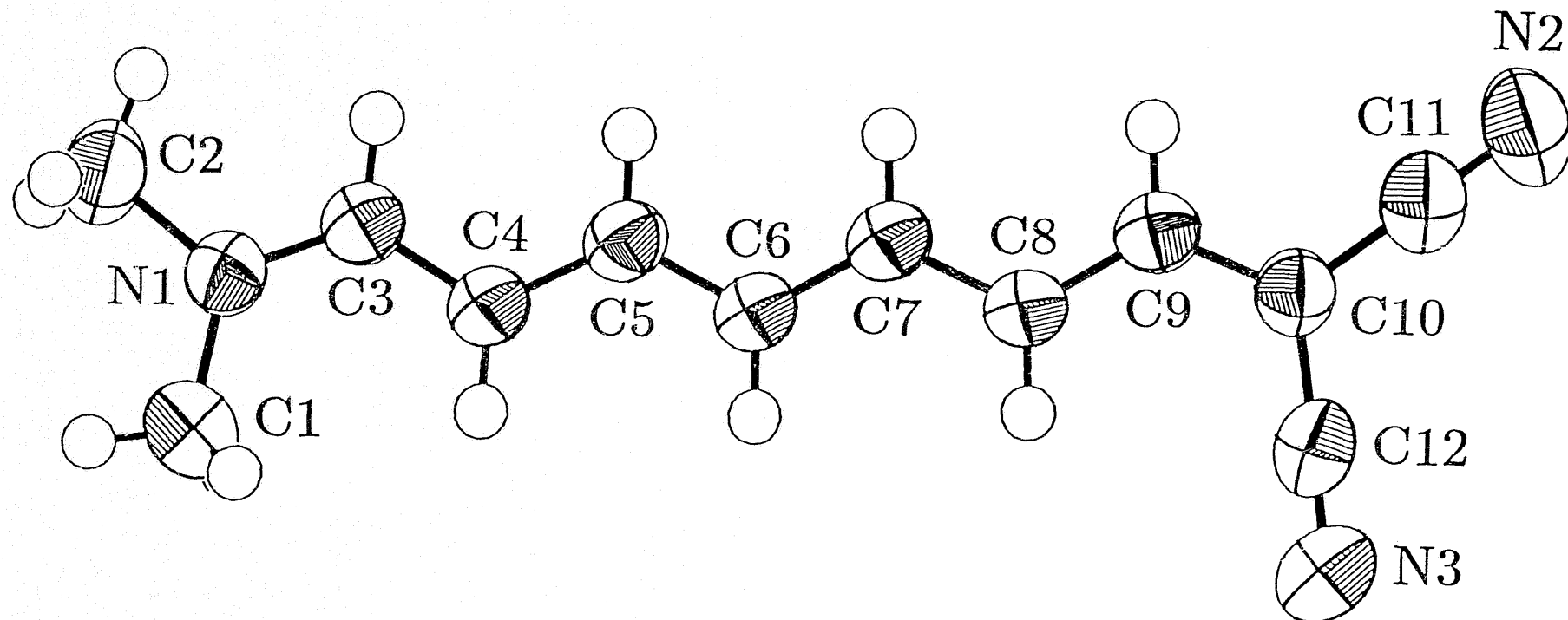


Figure 1: An ORTEP drawing of the molecule with 50% probability ellipsoids showing the numbering system. Hydrogen atoms are shown as spheres of small, arbitrary size.

Supplementary material,  
page 28

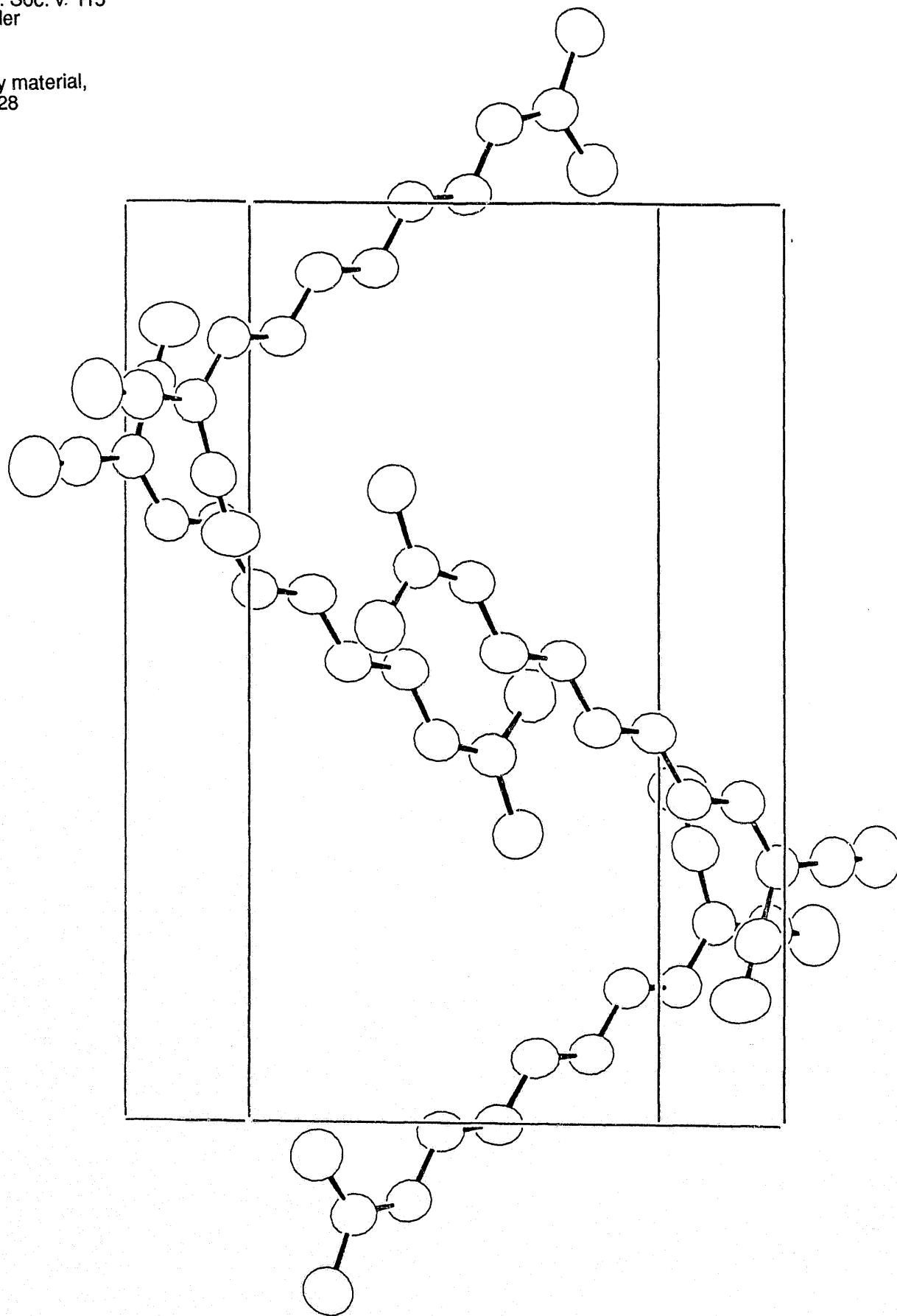


Figure 2: An ORTEP drawing of the contents of a unit cell, with a unit cell outlined. Atoms are shown as 50% probability ellipsoids; Hydrogen atoms are not shown.

J  
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r  
a  
r  
y

Table 1. Final Refined Parameters for  
2-Aza-2-Methyl-10,10-Dicyanodec-3,5,7,9-tetraene.

Atom	$x, y, z$ and $U_{eq}^a \times 10^4$			
	$x$	$y$	$z$	$U_{eq}$
C1	7476(3)	367(2)	4559(3)	863(6)
C2	7098(3)	1864(1)	3920(3)	842(6)
N1	6555(2)	1015(1)	3588(2)	668(4)
C3	5258(2)	858(1)	2499(2)	633(5)
C4	4574(2)	96(1)	2126(2)	638(5)
C5	3216(2)	15(1)	924(2)	629(5)
C6	2436(2)	-712(1)	456(2)	642(5)
C7	1092(2)	-761(1)	-788(2)	619(5)
C8	292(2)	-1477(1)	-1341(2)	614(5)
C9	-1012(2)	-1498(1)	-2636(2)	615(5)
C10	-1820(2)	-2191(1)	-3319(2)	630(5)
C11	-3158(3)	-2130(1)	-4650(3)	745(6)
N2	-4234(2)	-2071(1)	-5728(3)	1013(6)
C12	-1325(2)	-2999(1)	-2733(3)	705(6)
N3	-883(2)	-3640(1)	-2245(3)	971(7)

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

Table 2. Assigned Hydrogen Atom Parameters for  
2-Aza-2-Methyl-10,10-Dicyanodec-3,5,7,9-tetraene.

Atom	$x, y$ and $z \times 10^4$			$B$
	$x$	$y$	$z$	
H1 A	8353	610	5262	7.0
H1 B	7725	-17	3793	7.0
H1 C	6915	96	5222	7.0
H2 A	7973	1924	3527	7.0
H2 B	7324	1961	5099	7.0
H2 C	6334	2230	3325	7.0
H3	4730	1321	1903	6.0
H4	5051	-385	2708	6.0
H5	2778	509	367	6.0
H6	2844	-1209	1017	6.0
H7	676	-254	-1308	6.0
H8	668	-1985	-797	6.0
H9	-1398	-976	-3108	6.0

**Table 3. Anisotropic Displacement Parameters for  
2-Aza-2-Methyl-10,10-Dicyanodec-3,5,7,9-tetraene.**

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{12}$	$U_{13}$	$U_{23}$
C1	749(15)	897(16)	865(15)	40(13)	78(12)	40(13)
C2	729(15)	760(14)	1008(17)	-111(12)	180(13)	-171(13)
N1	628(11)	593(10)	738(11)	-1(8)	101(9)	-74(8)
C3	640(13)	571(12)	660(12)	31(10)	125(11)	-37(10)
C4	681(13)	540(12)	658(12)	24(10)	115(11)	-29(9)
C5	695(13)	535(11)	650(12)	12(10)	164(11)	-25(9)
C6	694(13)	516(11)	684(13)	17(10)	127(11)	-6(9)
C7	666(13)	522(11)	664(12)	26(10)	170(11)	-18(9)
C8	636(13)	531(11)	650(12)	34(10)	126(11)	13(9)
C9	634(13)	572(12)	649(12)	40(10)	190(11)	7(10)
C10	578(13)	631(13)	678(13)	-23(10)	163(11)	-65(10)
C11	664(15)	798(16)	776(15)	-64(12)	198(13)	-127(12)
N2	723(13)	1210(17)	998(15)	-60(12)	37(12)	-185(13)
C12	715(14)	671(15)	733(14)	-102(12)	200(11)	-115(12)
N3	1094(17)	666(13)	1110(16)	-42(12)	215(13)	-56(12)

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

The form of the displacement factor is:

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



Table 4. Complete Distances and Angles for  
2-Aza-2-Methyl-10,10-Dicyanodec-3,5,7,9-tetraene.

		Distance(Å)			Angle(°)
C1	-N1	1.446(3)	C2	-N1 -C1	116.8(2)
C2	-N1	1.455(3)	C3	-N1 -C1	122.1(2)
N1	-C3	1.315(2)	C3	-N1 -C2	121.0(2)
C3	-C4	1.376(3)	C4	-C3 -N1	127.2(2)
C4	-C5	1.380(3)	C5	-C4 -C3	121.3(2)
C5	-C6	1.374(3)	C6	-C5 -C4	126.2(2)
C6	-C7	1.383(3)	C7	-C6 -C5	123.8(2)
C7	-C8	1.379(3)	C8	-C7 -C6	126.0(2)
C8	-C9	1.378(3)	C9	-C8 -C7	123.8(2)
C9	-C10	1.375(3)	C10	-C9 -C8	127.1(2)
C10	-C11	1.419(3)	C11	-C10 -C9	121.7(2)
C10	-C12	1.420(3)	C12	-C10 -C9	120.9(2)
C11	-N2	1.145(3)	C12	-C10 -C11	117.4(2)
C12	-N3	1.142(3)	N2	-C11 -C10	179.1(2)
C1	-H1 A	0.946	N3	-C12 -C10	177.9(2)
C1	-H1 B	0.951	H1 A	-C1 -N1	108.7
C1	-H1 C	0.951	H1 B	-C1 -N1	108.4
C2	-H2 A	0.951	H1 C	-C1 -N1	108.3
C2	-H2 B	0.945	H1 B	-C1 -H1 A	110.6
C2	-H2 C	0.949	H1 C	-C1 -H1 A	110.7
C3	-H3	0.952	H1 C	-C1 -H1 B	110.1
C4	-H4	0.953	H2 A	-C2 -N1	108.3
C5	-H5	0.953	H2 B	-C2 -N1	108.5
C6	-H6	0.950	H2 C	-C2 -N1	108.3
C7	-H7	0.953	H2 B	-C2 -H2 A	110.6
C8	-H8	0.952	H2 C	-C2 -H2 A	110.3
C9	-H9	0.953	H2 C	-C2 -H2 B	110.8
			H3	-C3 -N1	116.6
			H3	-C3 -C4	116.2
			H4	-C4 -C3	119.2
			H4	-C4 -C5	119.5
			H5	-C5 -C4	116.9
			H5	-C5 -C6	116.9
			H6	-C6 -C5	118.0
			H6	-C6 -C7	118.2
			H7	-C7 -C6	117.2
			H7	-C7 -C8	116.8
			H8	-C8 -C7	117.8
			H8	-C8 -C9	118.3
			H9	-C9 -C8	116.5
			H9	-C9 -C10	116.4

Table 5. Intermolecular Distances Less Than 3.5 Å for  
2-Aza-2-Methyl-10,10-Dicyanodec-3,5,7,9-tetraene.

Distance(Å)			Distance(Å)		
C1	-H9	2.889	H1 C	-H9	2.480
C2	-N2	3.375(3)	H1 C	-H1 C	3.474
C2	-H6	3.103	H1 C	-H4	2.832
C2	-H8	2.894	H2 A	-H2 B	3.251
C3	-H1 C	3.443	H2 A	-H8	2.842
C4	-H1 C	2.879	H2 A	-H6	3.145
C5	-H9	3.164	H2 A	-H8	2.623
C5	-H1 C	3.194	H2 B	-H2 C	3.285
C6	-H7	3.499	H2 B	-H6	3.444
C7	-H7	3.126	H2 B	-H6	3.076
C7	-H1 B	3.200	H2 B	-H8	2.468
C7	-H2 A	3.211	H2 C	-H6	2.639
C8	-H2 A	2.795	H2 C	-H8	3.224
C8	-H2 B	3.321	H5	-H9	2.958
C9	-H1 C	3.398	H7	-H7	2.871
C9	-H5	3.203			
C9	-H2 A	3.159			
C10	-H3	3.492			
C11	-C12	3.399(3)			
C11	-H2 C	3.392			
C11	-H3	3.256			
C11	-H3	3.210			
N2	-H4	2.999			
N2	-H2 B	3.038			
N2	-H2 C	3.120			
N2	-H3	3.499			
N2	-H2 C	2.714			
N2	-H3	2.757			
C12	-H8	3.484			
C12	-H5	3.268			
N3	-H1 B	2.762			
N3	-H5	3.017			
N3	-H7	2.882			
N3	-H1 A	2.747			
N3	-H2 B	3.432			
H1 A	-H7	3.352			
H1 A	-H9	2.862			
H1 B	-H9	2.897			
H1 B	-H5	3.406			
H1 B	-H7	2.847			

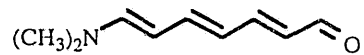
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J. Am. Chem. Soc. v. 115  
p. 2524 Marder

Supplementary material,  
page 33

JA9234907

## SUPPLEMENTARY MATERIAL FOR COMPOUND 5

7-dimethylamino-hepta-2,4,6-triene-1-al



wps code	Me2N-III-CHO
Name	7-dimethylamino-hepta-2,4,6-triene-1-al
Formula	C <sub>9</sub> H <sub>13</sub> NO
Formula Weight	151.21
Crystal System	Orthorhombic
Space Group	Pbca, #61
Cell Dimensions	
a, Å	8.189 (3)
b, Å	7.558 (2)
c, Å	28.295 (12)
α, °	90.0
β, °	90.0
γ, °	90.0
V, Å <sup>3</sup>	1751.2 (12)
Z	8
Density, calc, g cm <sup>-3</sup>	1.147
Crystal color, habit	orange plate
Crystal size, mm <sup>3</sup>	0.03 x 0.67 x 0.73
μ, cm <sup>-1</sup>	0.70
μ <sub>r</sub> max	0.511
maximum 2θ (scan type)	25°
range of h, k, l	0-9, 0-9, -33-33
# of reflections measured	3680
# of independent reflections	1545
# reflections, F <sub>0</sub> <sup>2</sup> > 0	1370
# reflections, F <sub>0</sub> <sup>2</sup> > 3σ(F <sub>0</sub> <sup>2</sup> )	904
GOF, merge	0.937
R(merge) for refs meas. twice	0.038
secondary extinction (x 10 <sup>-6</sup> )	0.32(6)
R, F <sub>0</sub> <sup>2</sup> > 0	0.063
R, F <sub>0</sub> <sup>2</sup> > 3σ(F <sub>0</sub> <sup>2</sup> )	0.035
GOF (number of parameters)	1.44, (153)
(Δ/σ) <sub>max</sub> in final least squares	0.01
Final Difference map:	
Maximum, eÅ <sup>-3</sup>	+ 0.21
Minimum, eÅ <sup>-3</sup>	- 0.23

Data was collected at 225 K.  
Hydrogen atoms were refined isotropically  
Structure solved using MULTAN 88.

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p. 2524 Marder

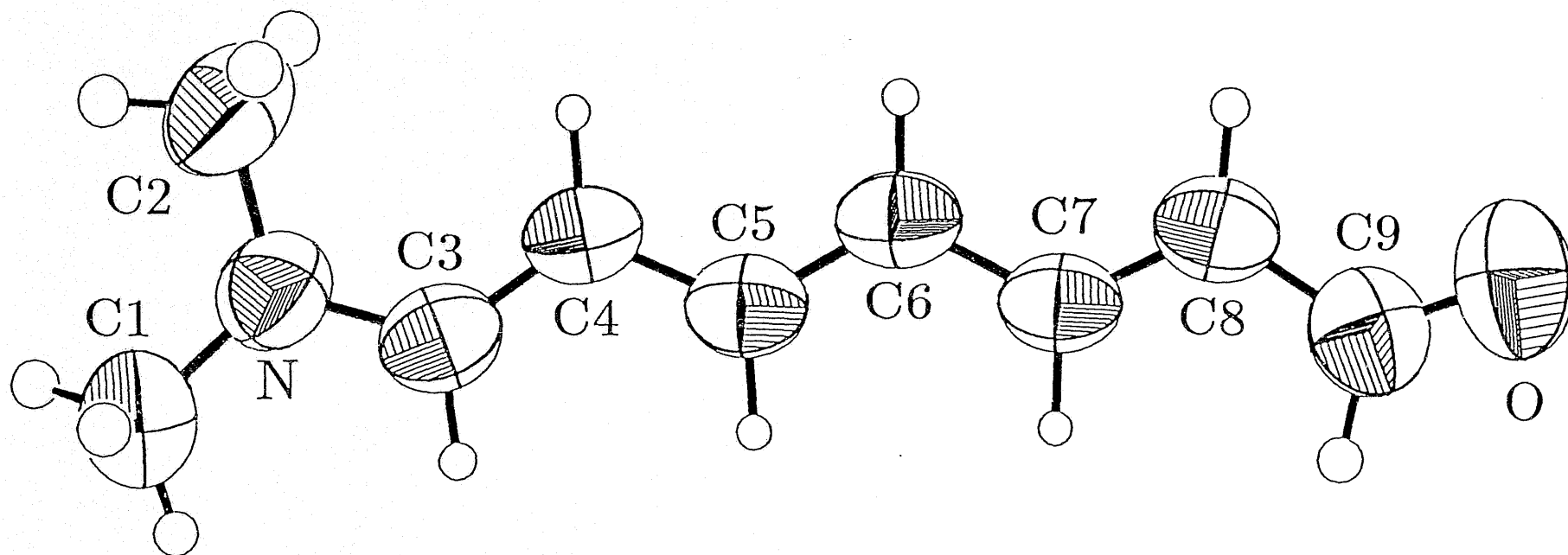
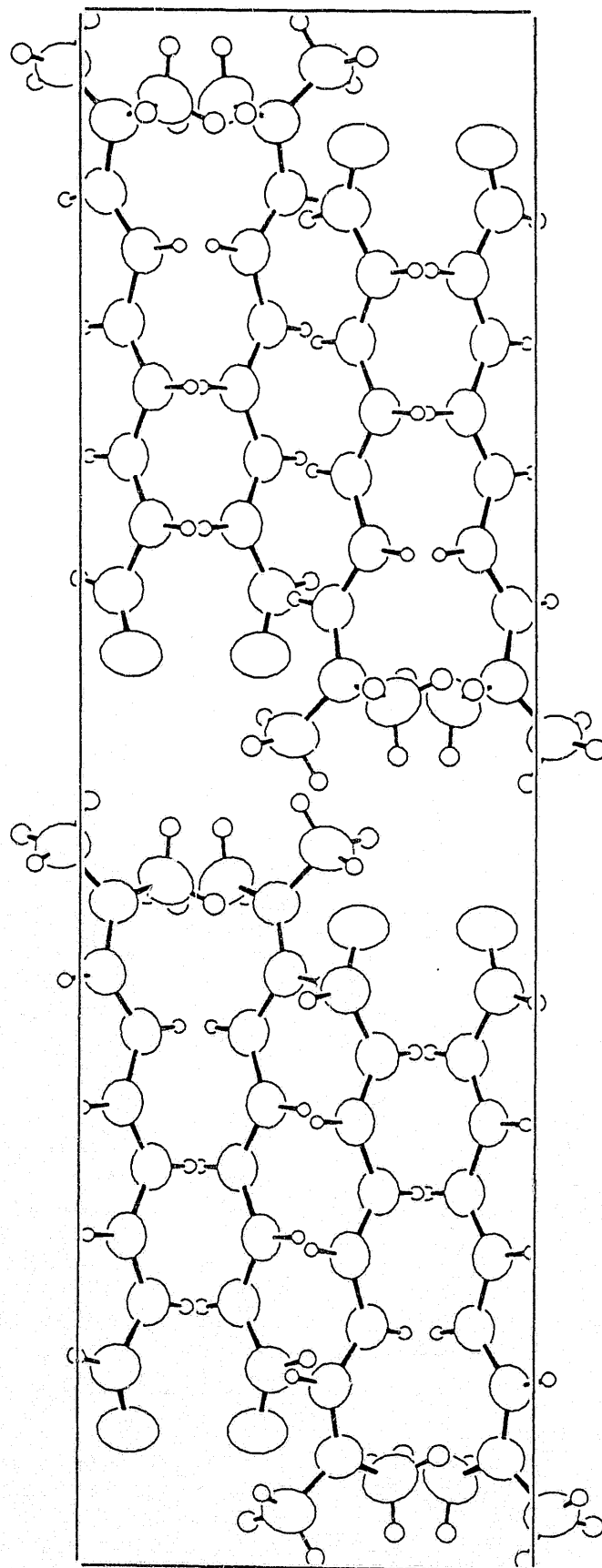


Figure 1: An ORTEP drawing of the molecule with 80% probability ellipsoids showing the numbering system. Hydrogen atoms are shown as one tenth actual size.



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p. 2524 Marder

Supplementary material,  
page 37

Figure 2: An ORTEP drawing of the contents of a unit cell, with a unit cell outlined. Atoms are shown as 70% probability ellipsoids; hydrogen atoms are shown at one-tenth actual size.

Table 1. Final Refined Parameters for  
Me<sub>2</sub>N - III - CHO.

$x, y, z$ and $U_{eq}^a \times 10^4$				
Atom	$x$	$y$	$z$	$U_{eq}$ or $B$
C1	10387(3)	2798(3)	364(1)	594(6)
C2	8157(3)	736(3)	581(1)	571(6)
N	9277(2)	2129(2)	719	452(4)
C3	9479(2)	2553(3)	1174(1)	410(4)
C4	8673(2)	1886(2)	1556(1)	391(4)
C5	9068(2)	2443(3)	2017(1)	390(4)
C6	8438(2)	1812(2)	2427(1)	389(4)
C7	8971(2)	2394(2)	2876(1)	382(4)
C8	8484(2)	1790(3)	3301(1)	418(5)
C9	9182(2)	2469(3)	3726(1)	493(5)
O	8912(2)	1955(2)	4127	683(4)
HC1a	10997(21)	3786(25)	476(6)	5.0(5)*
HC1b	11296(24)	1876(29)	292(6)	7.4(6)*
HC1c	9795(25)	3015(24)	69(7)	5.8(5)*
HC2a	7104(30)	915(29)	730(7)	8.0(7)*
HC2b	8585(26)	-387(30)	666(7)	8.0(7)*
HC2c	8068(22)	768(26)	235(7)	6.7(6)*
HC3	10325(18)	3397(21)	1232(5)	3.6(4)*
HC4	7856(18)	1029(20)	1519(4)	3.1(4)*
HC5	9914(19)	3340(20)	2048(5)	3.2(4)*

Table 1. (Cont.)

Atom	x	y	z	$U_{eq}$ or $B$
HC6	7619(21)	952(20)	2421(5)	3.3(4)*
HC7	9798(18)	3304(20)	2871(5)	3.0(4)*
HC8	7677(20)	914(23)	3330(5)	3.8(4)*
HC9	10025(21)	3421(23)	3656(6)	5.2(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,  $B$

Table 2. Anisotropic Displacement Parameters for  $\text{Me}_2\text{N} - \text{III} - \text{CHO}$ .

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{12}$	$U_{13}$	$U_{23}$
C1	676(14)	652(16)	453(12)	-60(14)	38(11)	-11(11)
C2	655(15)	522(14)	535(14)	-25(13)	-128(12)	-86(11)
N	507(9)	421(9)	427(8)	-2(8)	-22(7)	-40(7)
C3	402(10)	342(10)	487(11)	8(10)	-38(9)	-32(9)
C4	366(10)	329(11)	479(11)	-26(9)	-30(8)	-21(9)
C5	363(9)	302(11)	505(11)	14(10)	12(8)	-18(9)
C6	354(9)	309(10)	504(12)	-28(9)	5(9)	-24(9)
C7	345(9)	294(10)	506(11)	-3(9)	9(9)	-2(9)
C8	399(11)	342(11)	512(12)	-2(10)	14(9)	34(9)
C9	537(11)	449(12)	494(11)	51(11)	19(10)	31(10)
O	828(10)	759(10)	463(8)	52(9)	-14(7)	110(7)

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

The form of the displacement factor is:

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



Table 3. Complete Distances and Angles for  
Me<sub>2</sub>N - III - CHO.

Distance(Å)		Angle(°)	
C1 -N	1.446(3)	HC1a -C1 -N	111.8(11)
C1 -HC1a	0.953(18)	HC1b -C1 -N	110.6(11)
C1 -HC1b	1.04(2)	HC1c -C1 -N	109.8(12)
C1 -HC1c	0.98(2)	HC1b -C1 -HC1a	102.4(15)
C2 -N	1.450(3)	HC1c -C1 -HC1a	114.4(16)
C2 -HC2a	0.97(2)	HC1c -C1 -HC1b	107.5(16)
C2 -HC2b	0.95(2)	HC2a -C2 -N	110.1(13)
C2 -HC2c	0.979(19)	HC2b -C2 -N	110.3(13)
N -C3	1.338(2)	HC2c -C2 -N	107.3(11)
C3 -C4	1.363(2)	HC2b -C2 -HC2a	110.0(18)
C3 -HC3	0.956(15)	HC2c -C2 -HC2a	111.5(17)
C4 -C5	1.407(2)	HC2c -C2 -HC2b	107.7(17)
C4 -HC4	0.937(14)	C2 -N -C1	117.7(2)
C5 -C6	1.357(2)	C3 -N -C1	120.5(1)
C5 -HC5	0.973(15)	C3 -N -C2	120.8(2)
C6 -C7	1.413(2)	C4 -C3 -N	127.9(2)
C6 -HC6	0.934(15)	HC3 -C3 -N	114.5(9)
C7 -C8	1.347(2)	HC3 -C3 -C4	117.5(9)
C7 -HC7	0.966(14)	C5 -C4 -C3	120.8(2)
C8 -C9	1.427(2)	HC4 -C4 -C3	120.9(9)
C8 -HC8	0.939(16)	HC4 -C4 -C5	118.3(9)
C9 -O	1.219(2)	C6 -C5 -C4	126.8(2)
C9 -HC9	1.017(17)	HC5 -C5 -C4	117.2(9)
		HC5 -C5 -C6	115.9(9)
		C7 -C6 -C5	122.8(2)
		HC6 -C6 -C5	120.2(9)
		HC6 -C6 -C7	117.0(9)
		C8 -C7 -C6	127.3(2)
		HC7 -C7 -C6	115.1(9)
		HC7 -C7 -C8	117.5(9)
		C9 -C8 -C7	120.8(2)
		HC8 -C8 -C7	121.6(10)
		HC8 -C8 -C9	117.6(10)
		O -C9 -C8	126.7(2)
		HC9 -C9 -C8	111.1(10)
		HC9 -C9 -O	122.1(10)

Table 4. Intermolecular Distances Less Than 3.5 Å for Me<sub>2</sub>N - III - CHO.

	Distance(Å)		Distance(Å)
C1 -O	3.288(3)	C8 -HC3	3.148(15)
C1 -HC2a	3.28(2)	C8 -HC5	3.302(15)
C1 -HC2c	2.979(19)	C8 -HC8	3.260(16)
C1 -HC2c	3.427(19)	C8 -HC3	3.045(15)
C1 -HC1c	3.40(2)	C8 -HC5	3.082(15)
C2 -HC2b	3.27(2)	C9 -HC2a	3.08(2)
C2 -N	3.400(3)	C9 -HC4	3.274(14)
C2 -HC1c	3.49(2)	C9 -HC3	3.238(15)
C2 -HC9	3.155(17)	C9 -HC8	3.218(16)
C2 -HC1a	3.493(18)	C9 -HC2b	2.99(2)
C2 -HC1b	3.42(2)	C9 -HC3	3.106(15)
C2 -HC1c	3.44(2)	O -HC2a	2.76(2)
C2 -HC1b	3.19(2)	O -HC1a	2.978(18)
N -HC2a	3.08(2)	O -HC1b	2.70(2)
N -HC2b	3.01(2)	O -HC3	3.294(15)
N -HC9	3.364(17)	O -HC1c	2.76(2)
C3 -HC8	3.219(16)	O -HC2b	2.93(2)
C3 -HC2a	3.12(2)	O -HC1a	2.646(18)
C3 -HC2b	3.28(2)	O -HC3	2.942(15)
C3 -HC4	3.393(14)	HC1a -HC2a	3.09(3)
C3 -HC9	3.186(17)	HC1a -HC1b	3.26(3)
C4 -HC8	3.375(16)	HC1a -HC2c	2.65(3)
C4 -HC9	3.260(17)	HC1a -HC1c	2.94(3)
C4 -HC4	3.375(14)	HC1b -HC1c	3.04(3)
C4 -HC7	3.395(14)	HC1b -HC2a	3.40(3)
C4 -HC9	2.890(17)	HC1b -HC2c	2.74(3)
C5 -HC8	3.321(16)	HC1b -HC2b	2.94(3)
C5 -HC4	3.437(14)	HC1b -HC2c	2.55(3)
C5 -HC6	3.202(15)	HC1c -HC2a	3.27(3)
C5 -HC7	3.279(14)	HC1c -HC2b	3.46(3)
C6 -HC5	3.445(15)	HC1c -HC2c	3.17(3)
C6 -HC7	3.296(14)	HC1c -HC2a	3.06(3)
C6 -HC6	3.247(15)	HC1c -HC2c	2.96(3)
C6 -HC5	3.303(15)	HC1c -HC2b	3.17(3)
C6 -HC7	3.135(14)	HC1c -HC2c	3.46(3)
C7 -HC6	3.289(15)	HC1c -HC1c	3.04(3)
C7 -HC5	3.405(15)	HC2a -HC9	3.08(3)
C7 -HC6	3.253(15)	HC2a -HC2b	2.86(3)
C7 -HC8	3.248(16)	HC2a -HC3	3.10(3)
C7 -HC5	3.204(15)	HC2a -HC9	3.48(3)

Table 4. (Cont.)

Distance(Å)

HC2b -HC2c	3.43(3)
HC2b -HC9	2.41(3)
HC3 -HC8	2.96(2)
HC3 -HC4	3.38(2)
HC3 -HC8	2.80(2)
HC4 -HC7	3.49(2)
HC4 -HC9	2.98(2)
HC4 -HC5	3.39(2)
HC4 -HC7	3.30(2)
HC4 -HC9	2.67(2)
HC5 -HC6	3.23(2)
HC5 -HC8	3.10(2)
HC5 -HC6	3.05(2)
HC5 -HC6	3.20(2)
HC5 -HC8	2.97(2)
HC6 -HC7	3.03(2)
HC6 -HC7	3.09(2)
HC6 -HC7	3.03(2)
HC7 -HC8	3.11(2)
HC8 -HC9	3.05(2)

Table S4. Observed and Calculated Structure Factors for  
1-(6,6-Dicyanohexa-1,3,5-triene)piperidine

The columns contain, in order,  $\ell$ ,  $10F_{obs}$ ,  $10F_{calc}$  and  $10\left(\frac{F_{obs}^2 - F_{calc}^2}{\sigma F_{obs}^2}\right)$ . A minus sign preceding  $F_{obs}$  indicates that  $F_{obs}^2$  is negative.

1-(6,6-Dicyanohexa-1,3,5-triene)piperidine

				1	54	58	-9	3	-14	5	-6	9	-22	0	-13
	-6	1	1	2	24	13	11	4	-5	9	-3	10	-4	4	0
				3	47	43	9								
1	26	6	14	4	39	34	10	-3	1	1		-3	7	1	
				5	27	5	19								
	-6	2	1	6	-16	12	-12	1	68	63	15	1	55	53	5
				7	-11	6	-4	2	6	18	-10	2	92	88	10
1	21	2	10	8	-21	7	-14	3	58	57	0	3	35	35	0
				9	-8	4	-2	4	32	28	8	4	83	88	-11
	-5	1	1					5	38	32	10	5	22	15	7
					-4	3	1	6	60	59	3	6	24	31	-9
1	13	13	0					7	52	57	-12	7	-1	8	-2
2	37	39	-4	1	-3	3	0	8	-19	17	-19	8	-15	6	-8
3	44	24	28	2	72	71	3	9	9	27	-17	9	21	6	9
4	-8	4	-2	3	-24	16	-29	10	-21	15	-19				
5	-7	13	-6	4	-17	12	-14						-3	8	1
6	-22	3	-13	5	44	47	-5								
				6	-14	14	-11	-3	2	1					
	-5	2	1	7	-2	13	-4	1	24	20	4	1	11	16	-3
				8	-22	1	-14	2	-15	2	-8	2	3	20	4
1	28	21	8	9	-12	4	-4	3	53	50	7	4	23	27	-5
2	66	62	8					4	16	23	-9	5	43	44	-2
3	-13	9	-7		-4	4	1	5	-18	10	-14	6	-14	1	-6
4	20	23	-2					6	45	47	-3	7	-15	11	-10
5	21	2	11	1	21	1	12	7	14	22	-8	8	17	3	7
6	-8	8	-3	2	126	126	0	8	-17	6	-10	9	-28	7	-24
				3	24	31	-10	9	-10	22	-17				
	-5	3	1	4	39	43	-8	10	16	23	-7		-3	9	1
				5	15	17	-1								
1	24	1	15	6	-24	20	-30		-3	3	1	1	-21	1	-13
2	-9	8	-4	7	-13	1	-5					2	17	19	-2
3	13	12	0	8	16	11	3	1	46	34	26	3	-12	16	-11
4	-8	7	-3					2	25	33	-14	4	-10	13	-8
5	-11	8	-4		-4	5	1	3	64	62	7	5	19	30	-14
6	-21	0	-12					4	13	0	6	6	14	7	3
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Supplementary material, page 44

1-(6,6-Dicyanohexa-1,3,5-triene)piperidine

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Supplementary material, page 45

1-(6,6-Dicyanohexa-1,3,5-triene)piperidine

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Supplementary material, page 46

1-(6,6-Dicyanohexa-1,3,5-triene)piperidine

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7	57	58	0		-3	128	133	-25	-10	20	17	2				
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1-(6,6-Dicyanohexa-1,3,5-triene)piperidine

8	14	24	-11	-10	-11	19	-12	-8	-17	2	-8	1	48	33	29
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					3	4	1	-1	22	26	-5				
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1-(6,6-Dicyanohexa-1,3,5-triene)piperidine

0	-20	13	-16	4	49	39	19	0	40	22	29	12	-10	14	-8
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				7	13	5	4	3	22	12	10				
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	4	-3	1	2	33	13	25					0	31	14	16
				3	38	18	30		4	5	1	1	26	8	14
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Supplementary material, page 51

1-(6,6-Dicyanohexa-1,3,5-triene)piperidine

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4	66	64	4	3	27	2	19	2	19	0	8				
5	45	42	5	4	29	5	21	3	23	10	9	6	4	1	
6	31	8	21	5	22	7	12	4	12	2	3				
7	40	29	16	6	29	7	20	5	34	11	21	2	-12	1	-4
8	27	4	17	7	19	16	2	6	27	2	16	3	29	4	18
9	14	4	4	8	23	14	8	7	22	1	11	4	38	1	30
				9	32	22	12					5	18	3	7
	5 0 1			10	20	21	0								
								6	-3	1					

Table 5. Observed and Calculated Structure Factors for  
Azo-15-Crown-5-Cyanine

The columns contain, in order,  $\ell$ ,  $10F_{obs}$ ,  $10F_{calc}$  and  $10\left(\frac{F_{obs}^2 - F_{calc}^2}{\sigma F_{obs}^2}\right)$ . A minus sign preceding  $F_{obs}$  indicates that  $F_{obs}^2$  is negative.

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J. Am. Chem. Soc. v. 115  
p. 2524 Marder

Supplementary material,  
page 53

Azo-15-Crown-5-Cyanine

-14	0	1		8	95	87	14	10	-10	8	-2	7	24	3	11
				10	152	144	14								
2	81	66	20					6	0	1		-12	1	1	
4	53	56	-3	-3	0	1		0	154	155	-3	1	166	163	7
				2	1129	1108	18	2	307	308	-2	2	-7	11	-5
-13	0	1		4	428	425	7	4	437	427	17	3	64	59	10
				6	106	111	-12	6	77	78	-1	4	170	170	1
2	86	80	9	8	168	169	-4	8	150	149	1	5	208	210	-3
4	28	25	2	10	54	68	-21					6	25	12	10
6	-23	7	-9					7	0	1		7	67	74	-13
				-2	0	1		0	119	116	9	8	47	31	20
-12	0	1		2	419	437	-40	2	259	255	7				
				4	21	3	12	4	315	317	-3	-11	1	1	
2	104	105	-1	6	37	35	3	6	135	133	3	1	167	171	-12
4	110	120	-17	8	228	233	-11	8	78	66	17	2	37	32	7
6	134	147	-24	10	146	151	-9					3	64	67	-6
8	116	114	3					8	0	1		4	232	234	-4
				-1	0	1		0	50	56	-16	5	173	173	1
-11	0	1		2	344	341	6	2	227	213	30	6	-12	23	-17
				4	33	42	-16	4	282	296	-27	7	47	37	15
2	247	255	-14	6	94	100	-15	6	31	22	7	8	89	88	2
4	79	74	8	8	65	73	-13	8	10	5	1				
6	32	29	2	10	73	78	-7					-10	1	1	
8	86	93	-12					9	0	1		1	244	246	-3
				0	0	1		0	117	118	-2	2	48	49	-2
-10	0	1		2	427	444	-37	2	37	35	1	3	238	241	-8
				4	267	270	-8	4	233	231	4	4	63	52	24
2	262	267	-10	6	108	107	0	6	68	71	-4	5	56	57	-3
4	138	139	-2	8	106	100	11					6	145	147	-4
6	124	125	0	10	-16	30	-20	10	0	1		7	114	126	-30
8	12	14	0					0	29	34	-9	8	-5	3	0
				1	0	1		0	107	110	-6	9	146	138	17
-9	0	1		0	226	235	-42	2	36	49	-16				
				2	253	259	-17	4	12	25	-7	-9	1	1	
2	220	214	12	4	472	467	7	6				1	213	210	8
4	199	200	-2	6	32	32	0					2	55	49	14
6	476	483	-10	8	174	171	5	11	0	1		3	142	141	3
8	74	81	-11	10	97	90	12	0	17	21	-3	4	119	124	-14
10	55	53	1					2	30	46	-19	5	98	94	12
				0	444	453	-23	2	25	32	-5	6	70	72	-6
-8	0	1		2	2120	1956	75	4	134	140	-11	7	259	253	15
				4	362	370	-15	6				8	55	62	-13
2	278	282	-9	6	155	152	8	12	0	1		9	25	8	11
4	192	186	14	8	51	57	-8	0	53	46	13	10	4	14	-3
6	95	88	14	10	96	78	28	2	-17	13	-8				
8	161	164	-6					3	-16	32	-21	-8	1	1	
10	81	75	8	0	444	453	-23	0				1	95	93	4
				2	2120	1956	75	2	67	64	6	2	82	84	-7
-7	0	1		4	362	370	-15	4	72	70	3	3	63	60	7
				6	155	152	8	6				4	97	99	-4
2	23	22	0	8	51	57	-8	0	53	46	13	5	282	284	-6
4	58	49	16	10	96	78	28	2	-17	13	-8	6	96	98	-5
6	95	92	6					4	-16	32	-21	7	166	162	9
8	319	308	19	0	444	453	-23	13	0	1		8	109	109	1
10	50	53	-3	2	2120	1956	75	0	67	64	6	9	31	37	-9
				4	362	370	-15	2	72	70	3	10	68	64	6
-6	0	1		6	155	152	8	4							
				8	51	57	-8	0	75	65	19	-7	1	1	
2	289	282	15	10	96	78	28	0	75	65	19				
4	91	86	12					0							
6	32	22	10	0	447	447	0								
8	81	80	1	2	379	381	-4	1	-31	6	-25	1	56	57	-3
10	39	28	10	4	415	415	-1	2	53	66	-25	2	69	56	36
				6	62	71	-16	3	126	139	-31	3	172	175	-12
-5	0	1		8	65	68	-5	4	57	53	8	4	219	217	5
				10	71	78	-11	5	104	97	13	5	13	17	-4
2	370	362	17									6	299	294	13
4	333	328	10	0	447	447	0	-13	1	1		7	269	267	5
6	159	153	12	2	379	381	-4	1	33	15	18	8	32	17	16
8	100	87	23	4	415	415	-1	2	188	185	6	9	130	140	-29
10	158	153	8	6	62	71	-16	3	44	42	3	10	71	68	5
				8	65	68	-5	4	78	75	7				
-4	0	1		10	71	78	-11	5	74	67	15	-6	1	1	
									87	91	-9	1	80	77	13
2	130	137	-22	0	209	211	-9								
4	696	691	6	2	958	941	16								
6	391	388	5	4	18	23	-4								
				6	68	70	-2								
				8	75	81	-9								

Supplementary material,  
page 54

Azo-1 Crown-5-Cyanine

2	19	33	-26	11	84	91	-17	3	215	216	-3	12	1	1
3	355	347	21					4	177	173	10			
4	269	263	16		0	1		5	46	50	-9	0	28	31
5	151	150	4					6	47	39	15	1	117	118
6	137	139	-5		1	136	139	-16	7	174	184	-28	2	-25
7	408	404	8		2	644	663	-33	8	52	41	18	3	44
8	31	19	15		3	277	276	2	9	-8	1	-1	4	43
9	129	126	9		4	339	342	-6	10	-30	12	-24		
10	96	88	17		5	18	21	-3					13	1
11	27	33	-7		6	32	35	-5	6	1	1			
					7	166	169	-9					0	30
	-5	1	1		8	13	5	4	0	68	70	-10	1	12
					9	79	80	0	1	109	118	-33	2	16
1	235	233	7		10	13	7	2	2	53	49	10	3	37
2	239	239	0		11	125	110	33	3	94	86	26		
3	393	378	36						4	105	102	7	14	1
4	382	374	20		1	1	1		5	106	99	17		
5	512	513	-3						6	133	134	-1	0	13
6	94	86	23		0	294	303	-36	7	-5	19	-10	1	27
7	11	13	-1		1	328	333	-18	8	60	46	25		
8	103	100	6		2	459	463	-9	9	-16	9	-8	-14	2
9	32	16	16		3	364	359	14						
10	169	164	11		4	136	138	-10	7	1	1		1	49
11	30	28	3		5	44	43	2	0	312	301	37	2	102
					6	120	124	-12	1	28	24	6	3	82
	-4	1	1		7	117	113	12	2	449	451	-3	4	120
					8	28	21	8	3	84	88	-13	5	42
1	328	331	-8		9	80	81	-4	4	60	54	14		
2	509	510	-1		10	40	30	13	5	2	4	0	-13	2
3	51	51	1		11	136	127	19	6	126	127	-4	1	173
4	120	124	-12						7	74	80	-14	2	138
5	186	187	-4		2	1	1		8	-9	7	-3	3	12
6	27	17	13						9	13	20	-4	4	74
7	18	27	-11		0	131	131	2	8	1	1		5	41
8	111	111	1		1	517	504	27	9				6	14
9	325	317	17		2	1207	1219	-11						
10	34	0	24		3	216	218	-5	8	1	1		1	30
11	35	41	-8		4	103	102	5	0	300	296	12	-12	2
					5	100	104	-13	1	129	127	6		
	-3	1	1		6	60	54	15	2	174	165	26	1	22
					7	30	33	-5	3	66	61	14	2	33
1	743	750	-10		8	61	53	17	4	9	3	1	3	21
2	23	29	-12		9	-11	10	-6	5	178	176	4	4	23
3	146	152	-26		10	68	64	9	6	-12	7	-5	5	19
4	318	320	-7						7	47	45	4	6	28
5	78	82	-12		3	1	1		8	24	1	12	7	7
6	20	18	3										8	121
7	328	326	7		0	379	388	-27	9	1	1			
8	32	13	22		1	260	259	2					-11	2
9	109	106	7		2	545	530	35	0	18	21	-5	1	109
10	30	13	14		3	207	199	27	1	-9	19	-14	2	188
11	50	46	7		4	219	214	17	2	76	79	-8	3	289
					5	138	127	36	3	47	49	-3	4	289
	-2	1	1		6	73	66	20	4	17	19	-1	5	93
					7	48	44	7	5	54	60	-12	6	30
1	347	352	-16		8	85	75	24	6	-18	18	-16	7	39
2	656	657	-2		9	111	109	4	7	23	31	-9	8	7
3	-9	6	-5		10	22	7	9						
4	86	92	-21						10	1	1		8	80
5	15	8	6		4	1	1							
6	105	108	-9										-10	2
7	19	10	7		0	559	555	9	0	-9	7	-6		
8	-25	4	-21		1	80	84	-16	1	32	42	-18	1	114
9	36	36	0		2	537	535	4	2	-12	8	-6	2	31
10	30	20	10		3	241	241	0	3	28	41	-20	3	46
11	94	82	24		4	809	799	12	4	6	31	-23	4	52
					5	37	45	-17	5	121	120	3	5	62
	-1	1	1		6	35	40	-10	6	42	53	-20	6	-16
					7	68	66	5					7	85
1	42	49	-16		8	84	95	-28	11	1	1		8	76
3	392	399	-19		9	-24	4	-15					9	71
4	207	211	-11		10	24	34	-11						
5	106	107	-2						0	45	34	26		
6	59	61	-4		5	1	1		1	111	114	-7	-9	2
7	10	3	3						2	54	59	-10		
8	39	34	9						3	50	57	-14	1	72
9	175	172	7		0	175	177	-6	4	39	43	-6	2	160
10	31	33	-2		1	28	23	8	5	95	94	3	3	28
					2	453	446	16	6	34	31	3	4	93
													5	292

Supplementary material, page 55

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Azo-15-Crown-5-Cyanine

6	78	76	4	3	71	71	0	8	46	44	3	5	29	32	-3	
7	49	42	11	4	125	122	13	9	75	71	8	6	59	64	-10	
8	120	111	20	5	299	301	-4	10	37	23	16	7	12	22	-8	
9	33	50	-28	6	91	95	-13					8	135	130	12	
10	67	66	0	7	250	253	-6		3	2	1					
	-8	2	1	8	19	21	-2						9	2	1	
				9	113	117	-12	0	814	808	8					
1	81	85	-11	10	143	142	-3	1	213	216	-10	0	349	348	1	
2	193	195	-7	11	34	38	-4	2	105	110	-21	1	90	91	-3	
3	82	88	-18					3	46	41	11	2	158	154	12	
4	252	252	0		-2	2	1	4	56	52	9	3	171	175	-9	
5	52	49	6	1	635	638	-5	5	291	282	25	4	13	0	4	
6	52	40	23	2	414	415	-2	6	25	25	1	5	37	24	16	
7	31	25	6	3	248	246	7	7	51	49	3	6	35	47	-19	
8	129	129	-1	4	138	142	-18	8	9	5	1	7	139	135	10	
9	80	85	-10	5	35	33	3	9	134	123	25					
10	102	101	1	6	89	91	-9	10	30	28	2	10	2	1		
	-7	2	1	7	141	138	8		4	2	1		0	156	158	-9
				8	70	64	15						1	57	60	-8
1	16	15	1	9	-20	5	-12	0	569	557	24	2	209	208	1	
2	195	185	31	10	63	54	17	1	135	136	-3	3	44	39	8	
3	144	150	-20	11	65	69	-6	2	587	578	15	4	13	27	-13	
4	89	81	24					3	23	16	10	5	-29	2	-22	
5	275	272	8		-1	2	1	4	511	512	-3	6	22	13	6	
6	36	34	3	1	186	195	-44	5	321	319	5					
7	81	81	0	2	1419	1448	-23	6	203	201	4	11	2	1		
8	131	132	-3	3	13	8	4	7	3	28	-22					
9	191	189	3	4	158	155	9	8	22	16	5	0	174	168	23	
10	58	53	9	5	40	41	-3	9	71	60	22	1	164	164	0	
	-6	2	1	6	114	117	-8	10	31	16	13	2	49	59	-20	
				7	49	50	-1		5	2	1	3	-5	25	-16	
1	36	36	0	8	71	66	8					4	-23	0	-14	
2	250	251	-1	9	5	6	0	0	445	437	19	5	-5	8	-2	
3	48	51	-8	10	26	2	15	1	-12	13	-12					
4	246	242	10	11	58	41	27	2	505	505	0	12	2	1		
5	446	436	21					3	431	416	33	0	31	34	-7	
6	97	94	7		0	2	1	4	27	9	20	1	-17	9	-9	
7	33	20	18	0	293	294	-5	5	88	87	1	2	33	25	9	
8	34	26	11	1	252	258	-23	6	141	139	5	3	59	58	2	
9	22	9	9	2	604	623	-35	7	44	29	22	4	91	82	18	
10	10	11	0	3	30	29	0	8	41	14	29					
11	44	55	-18	4	241	243	-7	9	-18	15	-13	13	2	1		
	-5	2	1	5	87	87	0		6	2	1		0	50	55	-14
				6	-16	13	-16						1	41	38	4
1	282	276	17	7	143	148	-17	0	232	230	7	2	40	42	-2	
2	205	212	-23	8	-24	10	-21	1	19	13	6	3	25	25	0	
3	337	328	25	9	197	197	-1	2	217	224	-23					
4	203	200	9	10	22	7	9	3	173	175	-7	14	2	1		
5	92	86	21	11	18	6	6	4	333	327	15					
6	69	66	7					5	236	243	-19	0	58	69	-31	
7	143	145	-6	1	2	1		6	412	413	-3	1	-11	25	-16	
8	85	81	8					7	83	75	19					
9	32	9	21	0	123	122	6	8	27	18	9	-14	3	1		
10	43	25	24	1	299	310	-38	9	26	14	9					
11	109	104	10	2	670	672	-2						1	14	32	-17
	-4	2	1	3	408	416	-19		7	2	1		2	67	64	6
				4	468	473	-10						3	56	40	25
1	46	38	21	5	330	335	-11		0	176	165	47	4	24	6	11
2	716	711	8	6	129	131	-6		1	15	35	-37				
3	467	477	-23	7	45	41	7		2	15	23	-9	-13	3	1	
4	33	33	0	8	87	84	8		3	170	163	20				
5	113	110	9	9	29	8	18		4	136	133	8	1	184	186	-5
6	338	334	11	10	19	10	5		5	141	155	-40	2	21	17	3
7	62	62	0	11	36	23	14		6	57	70	-29	3	36	36	0
8	103	93	25						7	76	81	-11	4	34	22	13
9	189	187	3	2	2	1			8	98	92	14	5	18	8	5
10	39	42	-5						9	22	25	-2	6	37	32	6
11	24	29	-6	0	25	26	-2									
	-3	2	1	1	591	593	-4		8	2	1		-12	3	1	
				2	573	581	-15									
1	33	33	0	3	647	645	3		0	153	151	11	1	35	39	-7
2	397	396	3	4	355	348	18		1	245	241	10	2	82	84	-5
				5	161	156	17		2	93	92	3	3	143	141	3
				6	343	339	9		3	116	112	10	4	83	84	-4
				7	35	44	-18		4	13	36	-31	5	37	27	13

Supplementary material, page 56

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Azo-15-Crown-5-Cyanine

6	23	20	2						6	196	190	18							
7	41	28	16		-5	3	1		7	195	195	1	0	241	244	-11			
-11	3	1							8	99	95	12	1	221	218	9			
1	60	60	0		1	340	336	12	9	40	47	-12	2	121	120	1			
2	113	114	-3		2	227	204	74	10	77	70	16	3	72	69	10			
3	-21	15	-18		3	189	176	43	11	77	65	22	4	56	53	8			
4	63	63	0		4	159	157	7					5	22	14	8			
5	31	39	-12		5	484	477	13	1	3	1		6	71	72	-2			
6	32	37	-7		6	153	156	-10	0	525	545	-47	7	158	165	-18			
7	68	55	23		7	93	101	-24	1	50	53	-8	8	88	85	7			
8	19	17	1		8	22	26	-4	2	185	197	-50	9	66	60	11			
					9	105	96	22	3	54	56	-4							
					10	85	79	14	4	555	565	-18	7	3	1				
					11	58	69	-21	5	328	339	-28	0	210	202	34			
-10	3	1							6	98	98	-1	1	86	77	27			
					-4	3	1		7	301	312	-29	2	90	93	-10			
1	90	87	9		1	133	135	-11	8	81	83	-6	3	171	167	14			
2	154	150	10		2	-1	5	-1	9	203	197	17	4	112	120	-26			
3	240	239	1		3	62	75	-49	10	34	26	9	5	55	56	0			
4	114	121	-18		4	198	208	-33	11	34	16	16	6	60	67	-17			
5	84	95	-28		5	49	43	16					7	127	134	-18			
6	21	25	-4		6	-17	8	-13	2	3	1		8	-16	24	-19			
7	77	69	17		7	217	220	-8	0	620	630	-20							
8	96	89	14		8	32	34	-1	1	539	541	-2	8	3	1				
9	-30	2	-23		9	42	36	10	2	235	231	15	0	70	72	-9			
					10	19	6	7	3	258	258	0	1	23	23	0			
					11	70	59	19	4	146	148	-5	2	151	150	4			
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9	99	91	18																
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11	35	33	2																

Supplementary material,  
page 57

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J. Am. Chem. Soc. v. 115  
p. 2524 Marder

Azo-15-Crown-5-Cyanine

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Supplementary material, page 58  
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J. Am. Chem. Soc. v. 115  
p. 2524 Marder

Azo-15-Crown-5-Cyanine

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Supplementary material,  
page 59

©1993 Am. Chem. Soc.  
J. Am. Chem. Soc. v. 115  
p. 2524 Marder

Azo-15-Crown-5-Cyanine

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Supplementary material, page 60 ©1993 Am. Chem. Soc. J. Am. Chem. Soc. v. 115 p. 2524 Marder

Azo-15-Crown-5-Cyanine

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Supplementary material, page 61 ©1993 Am. Chem. Soc. J. Am. Chem. Soc. v. 115 p. 2524 Marder



Azo-15-Crown-5-Cyanine

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Supplementary material, page 63



Azo-15-Crown-5-Cyanine

Page 11

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Supplementary material, page 64





Azo-15-Crown-5-Cyanine

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Supplementary material, page 67

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## Azo-15-Crown-5-Cyanine

Page 15

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				3	16	1		4	82	75	13				
1	24	18	5	0	-13	24	-25					5	17	1	
2	52	64	-24	1	6	18	-6	-2	17	1					
3	-28	1	-20	2	-25	2	-16	1	33	23	11	0	45	55	-22
4	13	21	-6	3	19	17	1	2	60	64	-8	1	27	8	13
5	-9	12	-5	4	-12	17	-10	3	46	36	14	-3	18	1	
								4	72	71	2				
-2	16	1		4	16	1						1	9	17	-4
								-1	17	1					
1	70	74	-9	0	179	182	-8					-2	18	1	
2	-13	23	-17	1	85	79	11	1	79	68	22				
3	6	8	0	2	-13	0	-4	2	-14	27	-22	1	-28	21	-29
4	78	75	6	3	38	35	4	3	13	3	3	2	63	63	0
5	-6	10	-3	4	42	41	0	4	30	23	7				
-1	16	1		5	16	1		0	17	1		-1	18	1	
1	-28	2	-21	0	100	94	18	1	22	14	5	1	-21	12	-14
2	23	23	0	1	62	57	8	2	48	39	13	2	-10	14	-6
3	27	16	10	2	-7	5	-1	3	-8	6	-2	0	18	1	
4	62	56	11	3	-16	0	-5	4	-9	18	-9				
5	87	73	27												
0	16	1		6	16	1		1	17	1		0	31	19	11
												1	21	6	8
0	-12	2	-4	0	56	62	-17	0	23	20	3	2	81	77	8
1	-24	10	-17	1	14	13	0	1	68	73	-10				
2	-17	3	-7	2	48	58	-17	2	81	83	-2	1	18	1	
3	63	64	0					3	-5	2	0	0	44	41	6
4	53	58	-10	7	16	1		4	32	32	0	1	68	66	5
5	19	27	-7									2	38	43	-8
				0	22	31	-13	2	17	1					
1	16	1		1	16	17	0					2	18	1	
0	68	67	2	-5	17	1		0	-5	16	-9				
1	-5	21	-11					1	6	3	0	0	70	67	8
2	-11	1	-3	1	68	57	20	2	-23	3	-13	1	18	26	-7
3	41	39	2	2	80	78	5	3	28	35	-8	2	48	35	18
4	9	15	-3	3	39	50	-17	4	-29	13	-2				
5	-22	8	-13									3	18	1	
				-4	17	1		3	17	1					
												0	39	33	10
								0	13	14	0	1	22	3	9

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p. 2524 Marder

Supplementary material,  
page 68

Table 6. Observed and Calculated Structure Factors for  
2-Aza-2-Methyl-10,10-Dicyanodec-3,5,7,9-tetraene.

The columns contain, in order,  $k$ ,  $10F_{obs}$ ,  $10F_{calc}$  and  $10\left(\frac{F_{obs}^2 - F_{calc}^2}{\sigma F_{obs}^2}\right)$ . A minus sign preceding  $F_{obs}$  indicates that  $F_{obs}^2$  is negative.

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p. 2524 Marder

Supplementary material,  
page 69

2-Aza-2-Methyl-10,10-Dicyanodec-3,5,7,9-tetraene.

-10	k	1		6	81	81	-2	-8	k	2		1	10	1	12
				7	58	50	55					2	21	22	-6
1	17	7	25	8	32	20	54	0	52	57	-26	3	9	4	7
2	37	33	23	9	21	17	15	1	9	6	7	4	11	2	14
3	41	39	10	10	18	15	9	2	42	38	28	5	39	41	-13
4	32	33	-6					3	37	38	-9	6	31	29	10
5	42	42	-2	-9	k	3		4	22	18	18	7	48	48	-2
6	25	27	-12					5	33	33	-2				
7	12	12	-1	1	6	3	3	6	33	34	-11	-8	k	8	
				2	11	8	6	7	35	31	20				
				3	38	37	7	8	53	48	37	0	16	5	16
-10	k	2		4	47	42	30	9	61	58	20	1	35	36	-4
0	12	2	13	5	61	60	8	10	32	29	15	2	17	6	25
1	21	12	31	6	21	5	47	11	14	17	-8	3	37	34	17
2	16	1	29	7	50	43	42	12	8	6	3				
3	66	65	6	8	58	56	16	13	3	2	0	-7	k	1	
4	49	47	13	9	29	29	2								
5	31	19	51	10	15	6	20								
6	22	13	31					-8	k	3		1	10	13	-10
7	25	20	21					1	8	11	-9	2	57	56	3
				0	21	20	0	2	44	42	12	3	102	99	25
-10	k	3		1	8	4	5	3	43	44	-1	4	83	84	-7
1	14	1	23	2	28	29	-3	4	19	19	-3	5	53	55	-18
2	18	9	27	3	45	46	-8	5	27	28	-7	6	17	11	24
3	22	15	25	4	17	16	7	6	35	34	2	7	23	20	15
4	24	5	54	5	10	1	12	7	22	19	13	8	85	86	-8
5	72	68	24	6	16	12	13	8	14	11	10	9	70	71	-7
6	47	40	40	7	6	0	4	9	11	1	14	10	57	60	-25
7	32	23	40	8	30	27	12	10	8	2	8	11	9	1	10
				9	19	18	1	11	12	11	3	12	18	19	-5
				10	29	26	15	12	13	11	4	13	-8	0	-8
												14	-16	7	-42
-10	k	4		-9	k	5		-8	k	4		-7	k	2	
0	-6	4	-5					0	121	123	-11	0	54	46	49
1	26	26	0	1	10	11	-3	1	16	0	35	1	93	91	17
2	14	8	16	2	17	14	12	2	16	14	7	2	85	85	-1
3	20	15	18	3	4	2	1	3	15	10	16	3	67	66	8
4	31	28	11	4	-6	8	-13	4	-3	12	-24	4	23	27	-31
5	28	16	47	5	12	9	6	5	27	27	0	5	12	14	-7
6	30	22	37	6	4	2	1	6	-6	7	-12	6	-3	3	-3
7	28	13	51	7	-11	4	-18	7	18	17	6	7	44	44	0
				8	-2	0	0	8	13	18	-19	8	28	30	-13
-10	k	5		9	2	12	-15	9	9	10	-3	9	23	27	-21
1	11	1	13					10	23	28	-28	10	46	41	29
2	12	14	-6	-9	k	6		11	-8	11	-6	11	33	34	-10
3	16	17	0					12	-5	3	-4	12	41	43	-11
4	21	18	14	0	7	0	5					13	16	18	-10
5	11	8	6	1	7	1	6	-8	k	5		14	12	8	10
				2	10	8	3								
-10	k	6		3	7	11	-8	1	-5	3	-6	-7	k	3	
0	27	29	-4	4	-4	0	-2	2	0	9	-10				
1	23	25	15	5	7	8	-1	3	-4	1	-2	1	11	6	13
2	13	9	9	6	14	6	16	4	16	22	-24	2	23	16	36
				7	-7	6	-11	5	-7	4	-9	3	50	53	-24
								6	19	19	0	4	-5	1	-6
-9	k	1		-9	k	7		7	7	6	2	5	7	6	1
1	-5	5	-7	1	15	6	20	8	-9	1	-10	6	21	22	-5
2	10	9	3	2	14	5	17	9	8	5	4	7	11	13	-4
3	58	55	22	3	14	12	6	10	-11	1	-15	8	13	16	-13
4	44	41	19	4	19	22	-12	11	-5	2	-3	9	23	24	-6
5	26	15	46									10	13	14	-2
6	60	58	12	-8	k	1		-8	k	6		11	15	15	1
7	23	13	35					0	19	18	2	12	38	35	16
8	36	34	11	1	8	8	1	1	13	17	-14	13	19	24	-22
9	25	18	27	2	11	7	12	2	17	17	2	14	-8	5	-12
10	32	30	10	3	60	57	24	3	9	8	2				
				4	25	26	-8	4	19	21	-10				
				5	88	87	1	5	20	21	-6				
				6	80	75	39	6	18	22	-16	0	28	31	-13
				7	150	148	12	7	23	23	0	1	29	26	15
				8	30	26	19	8	31	33	-9	2	12	10	7
				9	24	19	23	9	27	23	15	3	3	4	-1
				10	18	9	25	10	16	8	19	4	22	22	-3
				11	0	6	-5					5	-15	2	-39
				12	14	8	13					6	30	30	-3
								-8	k	7		7	-4	8	-11
												8	22	23	-6

Supplementary material, page 70







2-Aza-2-Methyl-10,10-Dicyanodec-3,5,7,9-tetraene.

Page 4

12	6	5	0	11	49	42	54	6	43	46	-21	4	67	71	-38
13	-3	5	-4	12	95	97	-15	7	50	53	-27	5	107	95	96
14	-12	0	-17	13	105	106	-10	8	37	41	-30	6	82	85	-33
				14	92	92	3	9	34	34	-2	7	45	46	-8
	-3	k	7	15	92	94	-13	10	-9	11	-29	8	-5	10	-24
				16	-12	2	-20	11	-6	1	-5	9	47	49	-19
				17	18	11	23	12	-7	3	-8	10	176	177	-6
				18	8	7	1	13	-8	10	-23	11	122	124	-9
								14	16	17	-5	12	170	171	-8
					-2	k	3	15	-8	4	-11	13	35	28	43
												14	76	77	-2
				1	249	246	13		-2	k	7	15	31	32	-8
				2	381	386	-14					16	49	52	-24
				3	85	87	-24	1	34	40	-42	17	35	35	3
				4	136	131	30	2	21	25	-25	18	7	8	-1
				5	110	110	-2	3	27	32	-29				
				6	141	146	-36	4	36	35	2				
				7	42	46	-40	5	-10	11	-34		-1	k	3
				8	121	126	-40	6	-7	10	-24	1	10	10	1
				9	32	28	27	7	-13	9	-39	2	404	399	15
				10	99	102	-25	8	24	26	-13	3	156	160	-21
				11	31	31	0	9	17	18	-3	4	10	1	24
				12	78	76	16	10	11	8	5	5	145	145	-1
				13	162	161	0	11	7	11	-8	6	75	73	17
				14	54	51	19	12	32	28	18	7	9	11	-8
				15	16	11	16	13	17	11	16	8	213	215	-11
				16	-8	0	-10					9	148	146	17
				17	-8	3	-10		-2	k	8	10	86	83	23
				18	22	23	-2					11	14	14	0
								0	93	94	-4	12	48	49	-8
					-2	k	4	1	15	11	11	13	52	53	-9
								2	17	19	-9	14	10	2	13
				0	147	140	42	3	20	22	-9	15	78	76	14
				1	36	34	20	4	0	11	-17	16	77	75	9
				2	46	46	9	5	15	15	0	17	33	31	12
				3	2	6	-7	6	13	14	-4	18	21	21	2
				4	35	36	-7	7	-10	3	-14				
				5	203	207	-21	8	14	15	-1				
				6	3	1	2	9	15	15	1				
				7	11	15	-16	10	10	2	11				
				8	71	77	-52					0	197	188	38
				9	120	122	-9					1	200	204	-20
				10	115	117	-14		-2	k	9	2	80	81	-11
				11	25	25	-3	1	43	39	26	3	8	7	3
				12	9	8	3	2	23	21	9	4	58	52	49
				13	27	23	19	3	18	21	-12	5	215	214	7
				14	10	14	-11	4	14	1	20	6	117	108	65
				15	40	37	16	5	25	25	-3	7	30	34	-33
				16	23	23	1	6	31	28	17	8	32	30	12
				17	19	18	4	7	7	6	1	9	-8	2	-15
												10	-14	2	-39
					-2	k	5		-1	k	1	11	36	35	6
				1	50	43	62	1	77	74	37	12	49	46	17
				2	32	33	-6	2	50	58	-109	13	-8	7	-19
				3	124	123	5	3	72	70	29	14	-5	7	-10
				4	59	55	37	4	250	253	-12	15	25	25	0
				5	74	69	38	5	125	122	19	16	22	22	-1
				6	51	52	-4	6	105	96	70	17	4	6	-3
				7	102	101	2	7	116	110	44				
				8	61	61	5	8	71	69	19				
				9	-10	6	-24	9	13	16	-18	1	76	69	63
				10	14	17	-11	10	46	50	-31	2	4	12	-26
				11	-12	8	-36	11	52	53	-5	3	46	49	-30
				12	-9	8	-22	12	255	262	-27	4	35	39	-32
				13	36	33	15	13	110	106	26	5	49	45	38
				14	25	27	-11	14	27	14	60	6	23	26	-23
				15	-6	3	-6	15	9	5	6	7	9	14	-22
				16	6	5	0	16	30	34	-23	8	-13	11	-55
								17	-1	12	-18	9	-13	5	-36
					-2	k	6	18	13	8	13	10	-11	3	-21
												11	35	37	-10
				0	40	48	-50		-1	k	2	12	-8	8	-20
				1	-8	2	-14					13	-11	4	-19
				2	37	37	6	0	232	251	-81	14	-1	2	0
				3	13	16	-14	1	415	424	-25	15	-14	0	-27
				4	26	28	-10	2	849	841	10	16	31	32	-1
				5	13	9	11	3	589	611	-44				
													-1	k	6

Supplementary material, page 73

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2-Aza-2-Methyl-10,10-Dicyanodec-3,5,7,9-tetraene.

0	19	28	-46	9	138	143	-41	1	68	74	-72	5	223	227	-22
1	71	67	33	10	23	22	10	2	90	93	-37	6	136	132	30
2	105	103	17	11	74	75	-10	3	-7	1	-15	7	17	19	-18
3	14	12	6	12	14	10	20	4	100	103	-26	8	20	21	-6
4	63	58	46	13	162	158	29	5	60	58	30	9	139	139	0
5	33	35	-16	14	148	147	5	6	11	7	19	10	298	301	-9
6	12	17	-21	15	86	85	10	7	45	44	7	11	103	99	26
7	21	18	14	16	17	16	7	8	56	59	-38	12	67	68	-4
8	-12	2	-26	17	21	21	0	9	-9	0	-18	13	115	116	-5
9	11	14	-11	18	20	21	-5	10	19	21	-11	14	71	69	17
10	30	31	-2	19	5	14	-26	11	52	53	-10	15	60	58	9
11	-7	3	-9					12	11	4	-30	16	12	15	-11
12	16	17	-6	0	k	2		13	59	57	19	17	19	27	-38
13	-2	6	-6	0				14	35	35	0	18	42	38	22
14	8	9	-2	0	197	198	-6	15	7	12	-18	19	5	0	3
				1	205	224	-121	16	10	1	-17				
				2	130	140	-95					1	k	1	
-1	k	7		3	82	85	-31	0	k	6					
				4	374	371	9					1	343	346	-12
1	59	64	-43	5	134	138	-34	0	159	151	46	2	229	226	16
2	43	45	-15	6	175	171	23	1	47	43	43	3	593	609	-33
3	56	56	0	7	74	69	0	2	62	61	3	4	117	119	-18
4	15	20	-21	8	235	230	26	3	12	15	-18	5	79	72	67
5	-12	0	-22	9	150	147	22	4	11	15	-24	6	-5	2	-8
6	46	44	12	10	-5	0	-7	5	18	18	-3	7	300	291	33
7	10	9	0	11	89	93	-38	6	36	35	9	8	329	318	35
8	14	16	-9	12	13	12	7	7	43	42	11	9	38	39	-12
9	17	15	6	13	27	25	22	8	26	27	-7	10	-8	2	-14
10	11	10	4	14	32	24	58	9	-10	7	-34	11	47	49	-13
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12	25	25	-1	16	24	27	-27	11	41	39	11	13	91	94	-19
13	20	20	0	17	43	45	-19	12	57	56	15	14	4	3	1
				18	24	21	14	13	43	44	-9	15	5	0	4
								14	33	33	0	16	74	72	17
				0	k	s						17	56	54	18
				1	-9	1	-33	0	k	7		18	40	39	2
				2	170	169	11	1	57	60	-38				
				3	146	154	-63	2	40	42	-12	1	k	2	
				4	109	106	34	3	60	60	-7	0	558	587	-51
				5	265	253	55	4	45	50	-46	1	173	163	61
				6	65	65	9	5	13	12	3	2	214	214	-3
				7	148	139	65	6	47	48	-5	3	34	33	5
				8	23	27	-51	7	54	54	0	4	105	97	72
				9	13	18	-36	8	13	9	16	5	139	135	24
				10	32	36	-51	9	53	51	18	6	316	309	25
				11	24	22	15	10	66	62	42	7	196	185	58
				12	28	29	-5	11	64	60	31	8	61	59	21
				13	-9	3	-22	12	12	13	-3	9	9	14	-18
				14	57	56	17					10	21	22	-10
				15	12	19	-36	0	k	8		11	6	17	-46
				16	-7	2	-12	0	15	16	-3	12	68	70	-14
				17	7	14	-25	1	26	25	7	13	30	31	-5
				18	-9	6	-22	2	12	10	6	14	13	16	-12
								3	28	26	18	15	-8	11	-27
				0	k	4		4	60	56	37	16	38	38	11
				0	69	67	17	5	52	49	20	17	26	27	-6
				1	110	115	-42	6	30	23	43	18	-12	4	-19
				2	31	37	-77	7	25	13	60				
				3	127	129	-14	8	19	7	45	1	k	3	
				4	-6	0	-11	9	13	11	7				
				5	21	24	-40					1	56	56	0
				6	12	11	2					2	194	183	55
				7	73	69	47	0	k	9		3	22	17	30
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				9	108	108	0	2	31	28	21	5	86	83	30
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				12	16	19	-18	5	42	38	30	8	46	47	-11
				13	-2	14	-38					9	13	11	10
				14	29	32	-20	1	k	0		10	52	51	7
				15	11	13	-6					11	-12	4	-32
				16	-9	4	-18	0	36	20	136	12	42	46	-37
				17	16	20	-23	1	191	175	90	13	-13	7	-34
								2	355	357	-6	14	-6	16	-39
				0	k	5		3	801	804	-4	15	31	34	-21
								4	509	520	-26	16	45	48	-14
												17	-9	1	-9

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2-Aza-2-Methyl-10,10-Dicyanodec-3,5,7,9-tetraene.

1	k	4		4	38	35	19	1	48	47	7	4	33	32	3
0	214	190	97	5	13	11	6	2	152	140	74	5	21	19	9
1	206	203	14	6	80	78	16	3	207	211	-23	6	30	23	36
2	120	122	-19	7	26	25	4	4	-6	4	-12	7	13	4	17
3	44	39	42	8	39	38	6	5	73	76	-25	8	47	42	30
4	168	159	53	1	k	9		6	146	145	5	9	19	17	6
5	55	53	22					7	46	51	-45	10	37	36	3
6	1	10	-21	1	9	7	4	8	10	18	-38	11	14	13	4
7	20	23	-19	2	5	0	3	9	61	63	-13				
8	56	54	15					10	51	50	12	2	k	8	
9	47	49	-19	2	k	0		11	14	17	-13				
10	-10	6	-23	0	239	252	-55	12	79	85	-50	0	7	3	3
11	22	26	-19	1	379	371	24	13	49	51	-16	1	42	42	-1
12	37	39	-14	2	-4	6	-14	14	-9	2	-12	2	-5	1	-4
13	13	14	-1	3	116	116	-1	15	12	14	-4	3	26	26	0
14	38	44	-41	4	366	367	-5	16	-15	2	-30	4	36	37	-4
15	28	28	-7	5	347	335	38	17	-13	1	-21	5	15	11	11
16	11	11	1	6	123	110	98	2	k	4		6	31	31	0
				7	138	128	73					7	-3	4	-3
				8	182	176	31	0	85	83	7				
1	k	5		9	39	45	-68	1	116	115	9	3	k	0	
1	155	160	-32	10	84	87	-25	2	123	120	22	0	6	1	5
2	69	66	27	11	48	54	-50	3	56	59	-25	1	420	409	-28
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6	-7	8	-23	15	10	16	-18	7	94	96	-9	5	120	120	3
7	47	46	6	16	20	24	-21	8	17	15	8	6	147	145	9
8	-14	2	-34	17	27	32	-25	9	17	13	18	7	219	216	13
9	-12	4	-26	18	36	38	-10	10	70	70	0	8	121	119	19
10	12	15	-11					11	79	81	-15	9	82	79	25
11	23	23	-2	2	k	1		12	74	74	3	10	25	25	0
12	1	8	-8	1	260	261	-5	13	43	46	-17	11	48	50	-17
13	55	54	6	2	153	159	-42	14	-13	0	-25	12	-5	1	-4
14	6	10	-7	3	-12	1	-34	15	14	13	3	13	33	39	-40
15	13	13	-1	4	22	26	-32	16	36	36	0	14	38	42	-23
				5	337	331	21					15	13	13	1
				6	12	1	30	2	k	5		16	12	11	2
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1	51	55	-34	8	72	51	169	2	47	49	-14	18	24	22	8
2	76	72	32	9	3	11	-22	3	69	67	12				
3	28	24	23	10	-9	11	-43	4	94	93	8	3	k	1	
4	44	49	-41	11	37	36	10	5	84	84	-5	1	109	96	99
5	67	65	12	12	35	34	2	6	24	27	-19	2	115	109	42
6	9	7	5	13	44	41	21	7	52	54	-14	3	85	84	9
7	19	18	4	14	21	23	-10	8	124	124	3	4	40	34	57
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11	24	18	25	18	12	10	4	12	19	23	-18	8	47	45	19
12	-8	6	-12					13	3	4	-1	9	28	29	-8
13	-8	15	-37	2	k	2		14	-12	8	-26	10	0	11	-20
14	-15	2	-28	0	71	69	13	15	12	15	-10	11	59	62	-20
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				2	347	332	48	2	k	6		13	40	47	-53
1	33	31	12	3	45	44	6	0	73	74	-7	14	39	44	-39
2	38	37	4	4	31	27	31	1	12	11	-2	15	38	45	-44
3	57	55	13	5	48	51	-26	2	19	21	-13	16	7	17	-30
4	48	47	7	6	57	58	-14	3	17	17	-2	17	-10	8	-22
5	22	12	35	7	82	88	-56	4	53	50	22	18	5	10	-9
6	27	16	48	8	-9	11	-45	5	142	141	4				
7	165	158	39	9	35	33	19	6	69	64	34	3	k	2	
8	57	52	29	10	145	133	75	7	30	19	51	0	576	547	48
9	18	8	27	11	15	14	4	8	14	3	24	1	93	91	11
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11	-6	3	-6	13	52	54	-20	10	25	22	12	3	118	118	-1
12	6	6	0	14	-10	9	-28	11	21	23	-10	4	69	67	23
				15	13	15	-9	12	10	9	1	5	170	164	35
				16	8	13	-13	13	-11	1	-16	6	71	74	-23
0	-8	10	-16	17	-9	2	-10					7	59	58	11
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2	45	39	36									9	-5	3	-8
3	21	17	18	2	k	3		1	9	8	2	10	40	43	-29
								2	23	26	-14	11	42	42	0
								3	68	67	4	12	43	46	-28

Supplementary material, page 75  
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 J. Am. Chem. Soc. v. 115  
 p. 2524 Marder

2-Aza-2-Methyl-10,10-Dicyanodec-3,5,7,9-tetraene.

13	20	31	-69					16	-7	7	-14		5	k	0		
14	55	62	-50	1	-10	3	-17										
15	1	7	-6	2	30	26	25	4	k	3			0	382	352	72	
16	-9	0	-11	3	28	29	-7						1	126	127	-9	
17	21	22	-8	4	25	26	-4	1	94	95	-8		2	120	116	30	
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	3	k	3	6	11	10	1	3	52	53	-11		4	84	88	-34	
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2	199	199	2	9	14	12	5	6	69	67	15		7	92	95	-27	
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12	30	31	-4	4	k	0											
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16	28	22	27	2	270	253	70	1	48	52	-33		2	153	141	72	
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	3	k	4	4	101	103	-21	3	26	28	-13		4	69	74	-52	
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4	74	73	5	10	69	65	37	9	9	3	10		10	95	96	-9	
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14	-8	8	-16					2	22	26	-26		0	28	20	36	
15	-5	11	-17	1	134	117	116	3	93	93	0		1	87	86	14	
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12	-4	3	-4	16	-15	9	-41	1	23	28	-25						
13	-16	3	-39	17	-7	2	-7	2	8	7	0						
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	3	k	6					5	9	11	-4		2	12	14	-6	
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				15	9	17	-24						0	120	125	-28	

2-Aza-2-Methyl-10,10-Dicyanodec-3,5,7,9-tetraene.

Page 8

1	18	13	20	12	-6	3	-6	1	20	18	19	3	18	19	-6
2	35	40	-38	13	11	14	-8	2	82	84	-15	4	17	20	-12
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				8	87	88	-4	7	k	1		9	83	84	-6
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2	39	43	-27	10	17	21	-15	1	10	9	5	11	15	10	12
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8	21	25	-19	6	k	3		7	45	41	27	2	14	5	22
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5	71	73	-16					5	-12	5	-26	4	7	11	-10
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9	80	76	25	2	9	15	-19	9	20	25	-22	8	4	1	1
10	103	104	-5	3	-9	7	-16	10	32	31	6				
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12	9	8	1	5	-13	1	-22								
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								3	7	10	-5	5	9	14	-11
				6	k	6		4	16	19	-12				
1	23	26	-15					5	7	7	-7	9	k	0	
2	85	85	4	0	13	14	-1	6	-9	7	-17				
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8	124	126	-13									5	17	11	18
9	16	9	22	7	k	0		1	-11	5	-19	6	15	5	22
10	18	15	10					2	-12	3	-20	7	17	19	-8
11	32	31	9	0	33	35	-11								

Supplementary material, page 77

2-Aza-2-Methyl-10,10-Dicyanodec-3,5,7,9-tetraene.

										Page	9				
8	14	10	9	7	14	15	-2	7	9	8	1	2	40	39	5
9	12	5	13	8	4	10	-10					3	21	19	9
10	19	19	0					9	k	3		4	-4	4	-4
	9	k	1		9	k	2					5	-8	4	-10
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Table 5. Observed and Calculated Structure Factors for  
Me<sub>2</sub>N - III - CHO

The columns contain, in order,  $\ell$ ,  $10F_{obs}$ ,  $10F_{calc}$  and  $10\left(\frac{F_{obs}^2 - F_{calc}^2}{\sigma F_{obs}^2}\right)$ . A minus sign preceding  $F_{obs}$  indicates that  $F_{obs}^2$  is negative.



				21	-28	15	-23		1	1	1	6	152	148	16	
	0	0	1	22	131	141	-30					7	54	48	17	
				23	142	146	-13		1	20	34	-24	8	112	110	7
4	565	584	-38	24	164	160	9	2	368	373	-14	9	62	65	-7	
6	695	707	-19	25	61	66	-9	3	45	39	16	10	27	18	12	
8	504	511	-16	26	75	75	1	4	478	494	-37	11	175	179	-14	
10	321	317	12	27	29	36	-7	5	23	7	14	12	130	125	18	
12	43	50	-23	28	-25	25	-22	6	541	556	-30	13	210	204	22	
14	236	238	-6	29	32	16	13	7	57	60	-11	14	70	66	11	
16	3	8	-2	30	18	16	1	8	431	436	-11	15	141	138	9	
18	95	97	-10					9	134	134	1	16	24	30	-8	
20	97	97	-1		0	6	1	10	140	138	8	17	59	65	-15	
22	287	295	-26					11	184	180	18	18	24	15	9	
24	389	392	-8	0	218	217	1	12	51	51	1	19	-17	0	-8	
26	-21	6	-11	1	299	297	5	13	130	125	24	20	37	22	22	
28	34	41	-10	2	80	81	-1	14	240	243	-10	21	21	14	5	
30	-10	13	-5	3	81	89	-23	15	125	118	29	22	45	43	2	
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7	22	17	5	15	137	139	-6	27	5	5	0					
8	59	70	-38	16	137	134	9	28	63	61	5	1	190	192	-10	
9	164	167	-10	17	64	71	-14	29	24	0	8	2	-11	7	-5	
10	307	308	0	18	38	39	-2	30	85	84	2	3	35	42	-16	
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13	317	317	1	21	55	53	3	33	18	7	4	6	16	12	3	
14	136	125	42	22	73	65	15					7	134	137	-12	
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17	22	28	-9	25	20	27	-6					10	143	138	18	
18	204	209	-20					1	213	223	-45	11	143	147	-13	
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21	100	100	0	0	45	35	9	4	312	307	16	14	27	20	8	
22	196	201	-17	1	29	52	-32	5	15	10	3	15	15	13	1	
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												17	42	49	-12	

Supplementary material, page 80

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Supplementary material, page 81

©1993 Am. Chem. Soc. J. Am. Chem. Soc. v. 115 p. 2524 Marder

14	125	118	18					12	42	49	-12	6	4	23	-9
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Supplementary material, page 82

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29	48	32	23	8	75	77	-5	4	46	42	5	5	30	19	13
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Supplementary material, page 83

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Supplementary material, page 84

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J. Am. Chem. Soc. v. 115  
p. 2524 Marder

Supplementary material,  
page 85