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(±)4α, 8α, 14β-trimethyl-18-nor-5α, 13β-androst-9(11)-en-3, 17-dione, A SYNTHETIC PRECURSER TO FUSIDIC ACID

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(±)4α,8α,14β-trimethyl-18-nor-5α,13β-androst-9(11)-en-3,17-dione, a Synthetic Precurser to Fusidic Acid.*

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Abstract. Monoclinic, C2/c, a = 19.562(6)Å, b = 11.915(4)Å, c = 15.623(4)Å, β = 107.84(4)°, 24°C, $C_{21}H_{30}O_2$, M = 314.47, Z = 8, D_x = 1.208 g.cm^{-3}, racemic material prepared by W. G. Dauben, et al. (1972) and crystallized from a cyclohexane-methanol solution. Unusual stereochemistry is exhibited by the 8α configuration and by the 13β,14β cis C/D ring junction.

Introduction. Fusidic acid has been shown to be effective in combatting infections caused by staphylococci. The total synthesis of the tetracyclic nucleus of fusidic acid has been accomplished by Dauben, et al. (1972) yielding a (±) material whose NMR spectrum is essentially identical with that of the (+) material obtained from fusidic acid. The crystal and molecular structure determination of the synthetic (±) material, 4α,8α,14β-trimethyl-18-nor-5α,13β-androst-9(11)-en-3,17-dione, $C_{21}H_{30}O_2$, was undertaken to establish its structure and stereochemistry. The structural formula is shown in Figure 1.

* Work performed under the auspices of the U. S. Atomic Energy Commission.

Experimental. A crystal of approximate dimensions 0.30 x 0.16 x 0.13 mm ($\mu_{MoK\alpha}$ = 0.81 cm^{-1}) was used. Weissenberg photographs revealed the diffraction conditions to be $hk\ell$: $h + k = 2n$ and $h0\ell$: $\ell = 2n$ ($h = 2n$) indicative of the space groups C2/c and Cc. Diffraction data were measured at 24°C with a Picker FACS-I automatic diffractometer using graphite monochromatized MoKα radiation. The cell parameters were determined by a least-squares fit to the angular settings of 12 reflections in the range $35° < 2\theta < 39°$. Intensities for the hemisphere with k positive were collected for $2\theta < 40°$ using the θ-2θ scan method. Assuming 2/m symmetry, equivalent reflections were averaged to give 1622 unique reflections of which 495, with $I < 3\sigma(I)$, were given zero weight; 1127 reflections were used in the least-squares refinement.

The crystal structure was solved using the program MULTAN (Germain, Main, and Woolfson (1971)). It was refined by full-matrix least-squares to $R_1 = \Sigma|\Delta F|/\Sigma|F_o| = 0.0336$ and $R_2 = \{\Sigma w(\Delta F)^2/\Sigma w(F_o)^2\}^{\frac{1}{2}} = 0.0412$; $R_1 = 0.0539$ including zero-weighted data. The scattering factors of Doyle and Turner (1968) were used for oxygen and carbon, those of Stewart, Davidson and Simpson (1965) for hydrogen, and the anomalous scattering factors of Cromer and Liberman (1970) for all atoms. Three additional cycles of full-matrix least-squares refinement using the polar complex hydrogen scattering factors as described by Templeton, Olson, Zalkin and Templeton (1972) led to $R_1 = 0.0338$, $R_2 = 0.0409$, R_1 (including zero-weighted data) = 0.0538, and the parameters

listed in Table 1. The structure factors are listed in Table 4.

Discussion. The structure is closely related to that of fusidic acid reported as the methyl ester 3-p-bromobenzoate by Cooper and Hodgkin (1968). A major difference between the stereochemistry of the tetracyclic nucleus in the two structures is the 13β-hydrogen in the present compound leading to a cis C/D ring junction; this is apparently of no consequence in establishing a chemical relationship between the two compounds as the configuration at C(13) can be inverted by the enol-keto equilibrium at C(17) during the anticipated synthesis of fusidic acid from the present compound.

Bond lengths are listed in Table 2 and bond angles in Table 3; these values have not been corrected for thermal motion. The C-H bond lengths before the refinement with the polar complex hydrogen scattering factors averaged approximately 0.09A shorter than the final values listed in Table 2. The observed bond lengths do not appear to differ significantly from the typical values for steroid structures. Angle distortion in the 5-member D ring appears to be a real effect of strains in the molecule resulting from the >C=O entity at C(17), the 9(11) >C=C< bond, the cis C/D ring junction, and the methyl groups substituted at C(8) and C(14). Similar effects were reported for fusidic acid by Cooper and Hodgkin (1968).

TABLE 1. Atomic Parameters

Atom	X	Y	Z	B
O (1)	.3904(2)	.3918(3)	-.0399(2)	
O (2)	-.0474(2)	.4822(3)	.1085(2)	
C (1)	.1241(2)	.3548(3)	.1487(3)	
C (2)	.0550(2)	.3693(4)	.1743(4)	
C (3)	.0174(2)	.4775(3)	.1424(2)	
C (4)	.0639(2)	.5810(3)	.1586(3)	
C (5)	.1325(2)	.5610(3)	.1307(2)	
C (6)	.1789(2)	.6675(3)	.1453(3)	
C (7)	.2595(2)	.6466(3)	.1641(3)	
C (8)	.2775(2)	.5419(2)	.1182(2)	
C (9)	.2394(1)	.4391(3)	.1397(2)	
C(10)	.1747(2)	.4558(3)	.1748(2)	
C(11)	.2632(2)	.3385(3)	.1272(2)	
C(12)	.3282(2)	.3142(3)	.0982(3)	
C(13)	.3794(2)	.4132(3)	.1078(2)	
C(14)	.3613(2)	.5212(2)	.1515(2)	
C(15)	.4042(2)	.6129(3)	.1189(3)	
C(16)	.4178(3)	.5701(4)	.0337(4)	
C(17)	.3952(2)	.4498(4)	.0251(3)	
C(19)	.2025(2)	.4656(4)	.2785(2)	
C(30)	.0214(3)	.6836(4)	.1128(4)	
C(31)	.2502(2)	.5605(4)	.0157(2)	
C(32)	.3885(2)	.5101(4)	.2537(3)	
H (1)	.111(1)	.345(2)	.076(2)	2.7(7)
H (2)	.152(2)	.280(3)	.184(2)	6.2(10)
H (3)	.018(2)	.304(3)	.139(2)	5.7(10)
H (4)	.070(2)	.366(3)	.250(3)	6.2(11)
H (5)	.081(2)	.596(2)	.232(2)	3.4(7)
H (6)	.112(2)	.545(2)	.055(2)	3.8(7)
H (7)	.159(2)	.726(3)	.088(2)	5.5(10)
H (8)	.168(2)	.710(3)	.205(2)	5.3(9)
H (9)	.283(2)	.638(3)	.235(2)	3.7(9)
H(10)	.279(2)	.718(3)	.134(2)	4.7(9)
H(11)	.237(1)	.270(2)	.138(2)	1.7(6)
H(12)	.310(2)	.289(3)	.025(2)	5.3(9)
H(13)	.363(2)	.242(4)	.147(3)	7.3(10)
H(14)	.433(2)	.387(2)	.150(2)	3.4(7)
H(15)	.373(2)	.694(3)	.103(2)	4.6(8)
H(16)	.454(2)	.627(3)	.169(2)	5.2(10)
H(17)	.384(2)	.612(3)	-.032(2)	5.2(10)
H(18)	.471(2)	.579(3)	.038(3)	6.9(12)
H(19)	-.028(3)	.693(4)	.131(3)	8.4(13)
H(20)	.013(3)	.676(4)	.037(4)	10.6(17)
H(21)	.053(2)	.763(4)	.143(3)	6.9(11)
H(22)	.231(2)	.537(3)	.301(2)	5.2(11)
H(23)	.159(2)	.470(3)	.312(2)	5.3(8)
H(24)	.241(2)	.391(3)	.310(2)	6.9(10)
H(25)	.192(2)	.573(2)	-.004(2)	3.0(7)
H(26)	.278(2)	.637(3)	-.001(2)	5.8(9)
H(27)	.260(2)	.484(3)	-.021(2)	4.7(9)
H(28)	.442(2)	.475(3)	.275(2)	5.4(9)
H(29)	.357(2)	.443(3)	.281(2)	5.5(9)
H(30)	.389(2)	.586(3)	.289(3)	6.6(11)

TABLE 1. (Continued)

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
O (1)	11.7(2)	6.9(2)	6.5(2)	-.1(2)	6.0(2)	-.9(2)
O (2)	2.8(1)	9.2(2)	8.2(2)	-.2(1)	1.1(1)	.2(1)
C (1)	3.6(2)	3.6(2)	4.6(2)	-.4(2)	1.7(2)	-.4(2)
C (2)	3.6(2)	4.8(2)	6.6(3)	-.5(2)	2.3(2)	-.2(2)
C (3)	3.1(2)	5.5(2)	4.2(2)	-.1(2)	1.7(1)	-.0(2)
C (4)	3.3(2)	4.3(2)	4.7(2)	.7(2)	1.5(2)	.3(2)
C (5)	2.8(2)	3.3(2)	3.6(2)	.5(1)	1.1(1)	.3(1)
C (6)	4.1(2)	3.1(2)	5.6(2)	.5(2)	2.0(2)	-.0(2)
C (7)	3.5(2)	2.6(2)	5.0(2)	.0(1)	1.7(2)	-.5(2)
C (8)	2.9(2)	2.5(1)	2.7(2)	.0(1)	.9(1)	.1(1)
C (9)	2.6(1)	2.3(2)	2.3(1)	.1(1)	.3(1)	-.2(1)
C(10)	2.9(2)	2.6(1)	2.8(2)	.2(1)	1.0(1)	.1(1)
C(11)	3.4(2)	2.6(2)	4.1(2)	-.6(2)	1.5(1)	.0(1)
C(12)	4.0(2)	3.5(2)	5.4(2)	-.1(2)	2.4(2)	-.5(2)
C(13)	3.0(2)	3.0(2)	3.7(2)	.2(1)	1.4(1)	.0(1)
C(14)	2.7(2)	3.0(2)	3.4(2)	-.0(1)	.9(1)	-.3(1)
C(15)	4.0(2)	3.5(2)	6.8(3)	-.3(2)	2.5(2)	-.3(2)
C(16)	6.1(3)	4.7(3)	8.3(3)	.3(2)	5.0(3)	.7(2)
C(17)	5.0(2)	4.6(2)	5.2(2)	.4(2)	3.0(2)	-.2(2)
C(19)	4.1(2)	5.0(2)	2.9(2)	.4(2)	1.5(2)	-.0(2)
C(30)	4.3(2)	5.7(3)	10.2(4)	2.2(2)	2.9(3)	1.3(3)
C(31)	3.8(2)	4.5(2)	3.4(2)	.5(2)	1.1(1)	1.1(2)
C(32)	3.2(2)	5.5(2)	4.1(2)	.2(2)	.2(2)	-.9(2)

Thermal parameters are in units of $Å^2$.

The anisotropic temperature factor has the form:

$$\exp\{-\frac{1}{4}\Sigma_i\Sigma_j(a_i^* a_j^* h_i h_j B_{ij})\}$$

where a_i^* is a reciprocal cell edge and h_i is one of the Miller indices.

TABLE 2. Bond Lengths

Bond	length	Bond	length
O(1)--C(17)	1.208(4) A	C(1)—H(1)	1.09(3) A
O(2)—C(3)	1.216(4)	C(1)--H(2)	1.10(4)
C(1)--C(2)	1.532(5)	C(2)--H(3)	1.09(4)
C(1)—C(10)	1.532(4)	C(2)--H(4)	1.13(4)
C(2)—C(3)	1.492(5)	C(4)—H(5)	1.11(3)
C(3)—C(4)	1.507(5)	C(5)—H(6)	1.15(3)
C(4)—C(5)	1.552(5)	C(6)—H(7)	1.10(4)
C(4)—C(30)	1.528(5)	C(6)--H(8)	1.14(4)
C(5)—C(6)	1.536(5)	C(7)—H(9)	1.06(3)
C(5)—C(10)	1.541(4)	C(7)--H(10)	1.10(4)
C(6)—C(7)	1.532(5)	C(11)-H(11)	1.00(3)
C(7)—C(8)	1.534(4)	C(12)-H(12)	1.13(4)
C(8)—C(9)	1.522(4)	C(12)-H(13)	1.21(5)
C(8)—C(14)	1.579(4)	C(13)-H(14)	1.10(3)
C(8)—C(31)	1.542(5)	C(15)-H(15)	1.13(4)
C(9)—C(10)	1.540(4)	C(15)-H(16)	1.06(4)
C(9)—C(11)	1.322(4)	C(16)-H(17)	1.15(4)
C(10)-C(19)	1.548(4)	C(16)-H(18)	1.02(4)
C(11)-C(12)	1.502(5)	C(19)-H(22)	1.02(4)
C(12)-C(13)	1.525(5)	C(19)-H(23)	1.13(4)
C(13)-C(14)	1.548(4)	C(19)-H(24)	1.18(4)
C(13)-C(17)	1.483(5)	C(30)-H(19)	1.09(5)
C(14)-C(15)	1.555(5)	C(30)-H(20)	1.15(6)
C(14)-C(32)	1.526(5)	C(30)-H(21)	1.15(4)
C(15)-C(16)	1.524(6)	C(31)-H(25)	1.10(3)
C(16)-C(17)	1.494(6)	C(31)-H(26)	1.13(4)
		C(31)-H(27)	1.12(4)
		C(32)-H(28)	1.08(4)
		C(32)-H(29)	1.17(4)
		C(32)-H(30)	1.06(4)

TABLE 3. Bond Angles

Atoms	angle	Atoms	angle
C(2)—C(1)—C(10)	113.1(3)	C(12)-C(13)-C(14)	117.0(3)
C(1)—C(2)—C(3)	113.2(3)	C(12)-C(13)-C(17)	116.6(3)
C(2)—C(3)—O(2)	121.8(3)	C(14)-C(13)-C(17)	106.1(3)
C(4)—C(3)—O(2)	122.0(3)	C(8)—C(14)-C(13)	109.8(2)
C(2)—C(3)—C(4)	116.2(3)	C(8)—C(14)-C(15)	113.1(3)
C(3)—C(4)—C(5)	110.9(3)	C(8)—C(14)-C(32)	110.6(3)
C(3)—C(4)—C(30)	111.3(4)	C(13)-C(14)-C(15)	102.7(3)
C(5)—C(4)—C(30)	112.6(3)	C(13)-C(14)-C(32)	109.6(3)
C(4)—C(5)—C(6)	110.8(3)	C(15)-C(14)-C(32)	110.7(4)
C(4)—C(5)—C(10)	113.0(3)	C(14)-C(15)-C(16)	107.9(3)
C(6)—C(5)—C(10)	113.2(3)	C(15)-C(16)-C(17)	105.8(3)
C(5)—C(6)—C(7)	114.9(3)	C(13)-C(17)-O(1)	125.5(3)
C(6)—C(7)—C(8)	114.4(3)	C(16)-C(17)-O(1)	124.6(3)
C(7)—C(8)—C(9)	110.7(3)	C(13)-C(17)-C(16)	109.8(3)
C(7)—C(8)—C(14)	109.7(3)	C(2)—C(1)—H(1)	110.(1)
C(7)—C(8)—C(31)	108.2(3)	C(2)—C(1)—H(2)	108.(2)
C(9)—C(8)—C(14)	109.3(2)	C(10)-C(1)—H(1)	107.(1)
C(9)—C(8)—C(31)	107.9(3)	C(10)-C(1)—H(2)	108.(2)
C(14)-C(8)—C(31)	111.1(3)	H(1)—C(1)—H(2)	110.(3)
C(8)—C(9)—C(10)	119.1(2)	C(1)—C(2)—H(3)	107.(2)
C(8)—C(9)—C(11)	118.6(3)	C(1)—C(2)—H(4)	108.(2)
C(10)-C(9)—C(11)	122.3(3)	C(3)—C(2)—H(3)	105.(2)
C(1)—C(10)-C(5)	107.8(3)	C(3)—C(2)—H(4)	109.(2)
C(1)—C(10)-C(9)	109.8(3)	H(3)—C(2)—H(4)	115.(4)
C(1)—C(10)-C(19)	109.2(3)	C(3)—C(4)—H(5)	106.(1)
C(5)—C(10)-C(9)	109.4(2)	C(5)—C(4)—H(5)	108.(1)
C(5)—C(10)-C(19)	112.0(3)	C(30)-C(4)—H(5)	108.(1)
C(9)—C(10)-C(19)	108.6(2)	C(4)—C(5)—H(6)	105.(1)
C(9)—C(11)-C(12)	126.0(3)	C(6)—C(5)—H(6)	107.(1)
C(11)-C(12)-C(13)	114.3(3)	C(10)-C(5)—H(6)	107.(1)

TABLE 3. (Continued)

Atoms	angle	Atoms	angle
C(5)—C(6)—H(7)	110.(2)	C(4)—C(30)-H(19)	111.(2)
C(5)—C(6)—H(8)	104.(2)	C(4)—C(30)-H(20)	108.(2)
C(7)—C(6)—H(7)	111.(2)	C(4)—C(30)-H(21)	109.(2)
C(7)—C(6)—H(8)	111.(2)	H(19)-C(30)-H(20)	114.(5)
H(7)—C(6)—H(8)	106.(3)	H(19)-C(30)-H(21)	102.(4)
C(6)—C(7)—H(9)	108.(2)	H(20)-C(30)-H(21)	113.(5)
C(6)—C(7)—H(10)	105.(2)	C(10)-C(19)-H(22)	114.(2)
C(8)—C(7)—H(9)	109.(2)	C(10)-C(19)-H(23)	115.(2)
C(8)—C(7)—H(10)	105.(2)	C(10)-C(19)-H(24)	110.(2)
H(9)—C(7)—H(10)	115.(3)	H(22)-C(19)-H(23)	102.(4)
C(9)—C(11)-H(11)	119.(1)	H(22)-C(19)-H(24)	106.(4)
C(12)-C(11)-H(11)	115.(1)	H(23)-C(19)-H(24)	109.(3)
C(11)-C(12)-H(12)	109.(2)	C(8)—C(31)-H(25)	108.(1)
C(11)-C(12)-H(13)	108.(2)	C(8)—C(31)-H(26)	109.(2)
C(13)-C(12)-H(12)	108.(2)	C(8)—C(31)-H(27)	111.(2)
C(13)-C(12)-H(13)	106.(2)	H(25)-C(31)-H(26)	111.(3)
H(12)-C(12)-H(13)	113.(3)	H(25)-C(31)-H(27)	107.(3)
C(12)-C(13)-H(14)	108.(2)	H(26)-C(31)-H(27)	112.(3)
C(14)-C(13)-H(14)	106.(1)	C(14)-C(32)-H(28)	111.(2)
C(17)-C(13)-H(14)	101.(1)	C(14)-C(32)-H(29)	113.(2)
C(14)-C(15)-H(15)	112.(2)	C(14)-C(32)-H(30)	114.(2)
C(14)-C(15)-H(16)	110.(2)	H(28)-C(32)-H(29)	101.(3)
C(16)-C(15)-H(15)	108.(2)	H(28)-C(32)-H(30)	108.(4)
C(16)-C(15)-H(16)	109.(2)	H(29)-C(32)-H(30)	109.(4)
H(15)-C(15)-H(16)	109.(3)		
C(15)-C(16)-H(17)	115.(2)		
C(15)-C(16)-H(18)	110.(2)		
C(17)-C(16)-H(17)	105.(2)		
C(17)-C(16)-H(18)	112.(2)		
H(17)-C(16)-H(18)	108.(4)		

An ORTEP drawing (Johnson (1965)) of the molecule is shown in Figure 2. This particular view of the molecule emphasises the distortion of the tetracyclic nucleus from the relatively planar form found when there are all trans ring junctions and when there is no unsaturation in or adjacent to the rings (see, for example, Geise and Romers (1966)).

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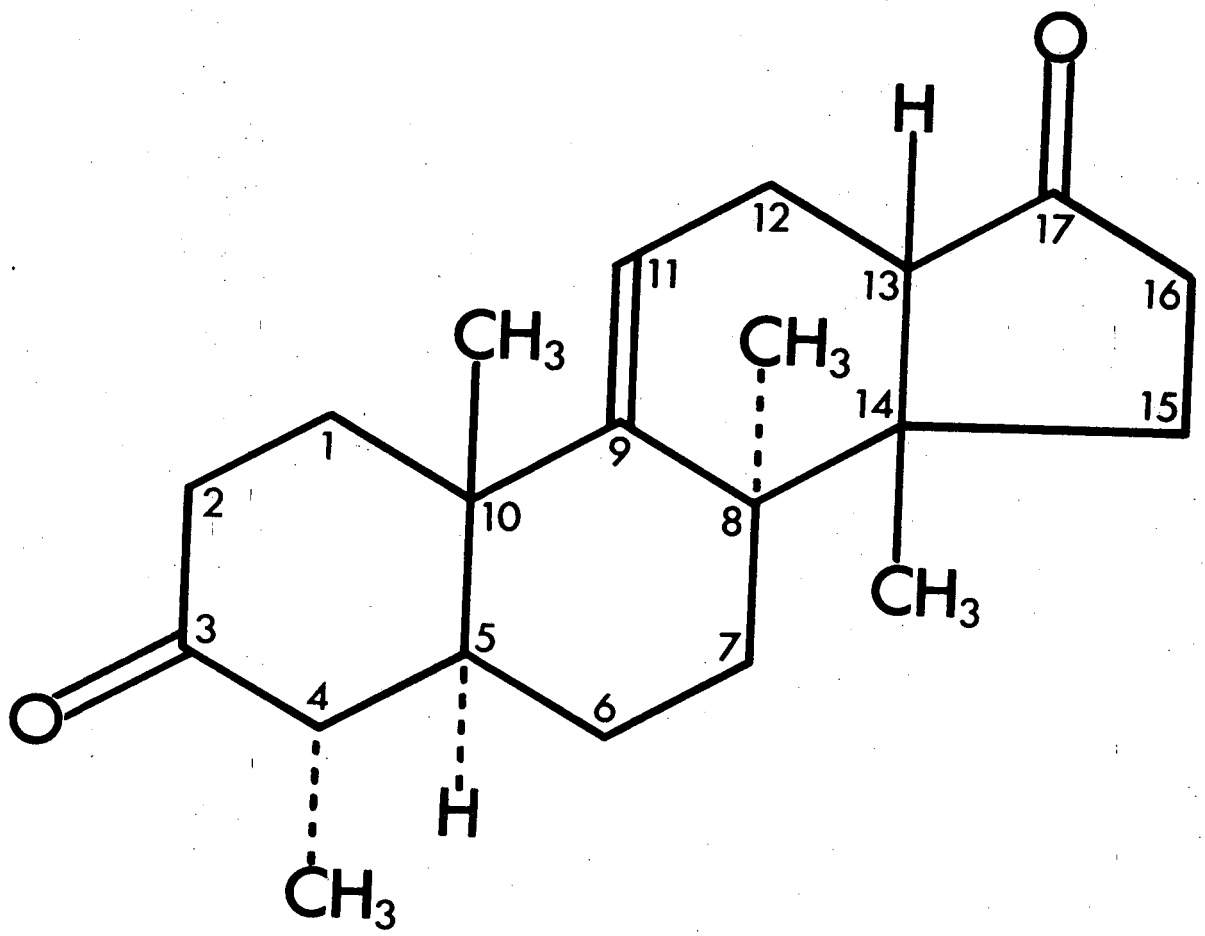
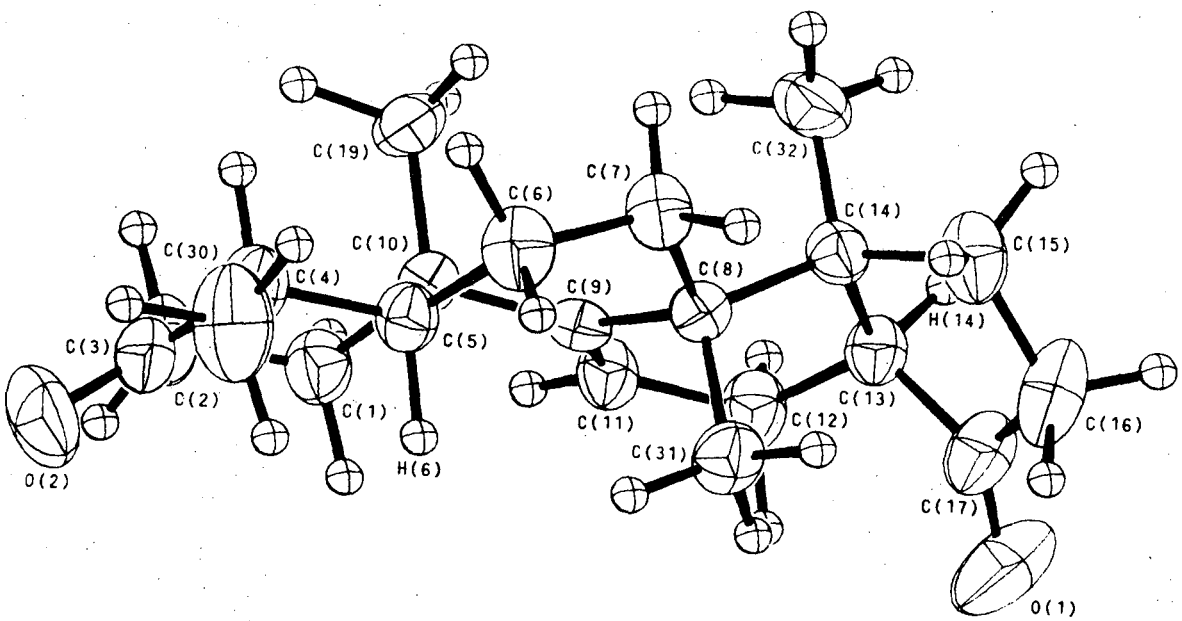


XBL 7212-7483

FIGURE 1.

Structural Formula.



XBL 7212-7482

FIGURE 2.

Molecular Structure.

The thermal ellipsoids were drawn at the 50% probability level and the hydrogens were given arbitrary temperature factors of 1.0Å^2.

Table 4.

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (X 1.0) FOR
D-L DIASSA C21.H30.O2 D.L.WARD,A.ZALKIN,D.H.TEMPLETON 25 F(0,0,0) = 1376

FOB AND FCA ARE THE OBSERVED AND CALCULATED STRUCTURE FACTORS.
SG = ESTIMATED STANDARD DEVIATION OF FOB. DEL = /FOB/ - /FCA/.
* INDICATES ZERO WEIGHTED DATA.

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=		0,	0	H,K=		0,	8	-13	0	6	-4*	12	20	1	-1	H,K=		2,	0
2	28	1	-1	0	48	1	1	-12	3	7	1*	H,K=		1,	7	-14	18	1	-1
4	290	7	-5	1	20	2	-2	-11	3	4	0*	-11	29	1	-0	-12	31	1	1
6	130	3	1	2	34	1	0	-10	17	1	-1	-10	13	1	-1	-10	48	1	1
8	140	4	-0	3	4	5	0*	-9	41	1	-2	-9	8	2	-3*	-8	45	1	-1
10	50	1	1	4	23	1	0	-8	34	1	1	-8	4	5	4*	-6	10	1	3
12	19	1	1	5	8	3	-1*	-7	30	1	-0	-7	6	3	2*	-4	126	3	-2
14	9	3	4*	6	8	3	-0*	-6	6	2	-1*	-6	4	5	-1*	-2	45	1	-1
H,K=		0,	2	7	19	1	-1	-5	26	1	0	-5	20	1	0	0	82	2	-5
0	340	9	-5	8	22	1	0	-4	3	4	2*	-4	36	1	1	2	28	1	-1
1	5	5	3*	9	0	6	-4*	-3	39	2	1	-3	27	1	1	4	93	2	-0
2	22	1	-0	10	11	4	1*	-2	62	2	2	-2	15	1	0	6	82	2	4
3	49	1	0	H,K=		0,	10	-1	98	7	-6	-1	25	1	1	8	89	2	3
4	32	1	-0	0	42	1	2	0	28	1	1	0	22	1	-0	10	21	1	-0
5	39	1	0	1	8	2	1*	1	24	1	0	1	5	2	1*	12	37	1	1
6	36	1	2	2	7	2	0*	2	145	4	0	2	42	1	2	H,K=		2,	2
7	36	1	-1	3	11	1	1	3	30	1	-0	3	18	1	0	-14	10	4	0*
8	58	2	3	4	14	2	-1	4	82	2	-1	4	23	1	-0	-13	4	8	-0*
9	37	1	1	5	2	5	1*	5	8	1	6	5	24	1	1	-12	4	5	4*
10	21	1	1	6	40	1	2	6	39	1	-3	6	6	2	2*	-11	22	1	1
11	3	5	2*	7	24	1	-0	7	7	1	0	7	6	7	-1*	-10	41	1	2
12	9	1	2	H,K=		1,	1	8	30	1	0	8	8	2	0*	-9	18	1	-1
13	5	6	4*	-14	19	1	-1	9	25	1	2	9	13	1	-0	-8	6	3	-0*
14	0	5	-0*	-13	10	2	1*	10	24	1	-0	10	32	1	1	-7	13	1	-0
H,K=		0,	4	-12	17	2	1	11	3	4	1*	11	2	8	-0*	-6	13	1	0
0	47	1	1	-11	9	3	1*	12	26	1	0	H,K=		1,	9	-5	43	1	-1
1	16	1	-1	-10	18	1	-1	13	6	7	1*	-9	24	1	1	-4	69	2	-1
2	48	1	2	-9	1	6	-5*	H,K=		1,	5	-8	36	1	1	-3	0	5	-2*
3	46	1	-0	-8	84	2	2	-13	10	1	4	-7	17	2	-0	-2	32	1	-1
4	32	1	-0	-7	55	1	1	-12	24	1	-1	-6	19	1	1	-1	38	1	-6
5	25	1	-1	-6	92	2	3	-11	16	1	-1	-5	52	2	-2	0	6	3	1*
6	41	1	-0	-5	59	2	-1	-10	4	4	1*	-4	17	1	-1	1	73	2	-6
7	4	2	2*	-4	196	5	-0	-9	38	1	-0	-3	2	4	1*	2	58	2	1
8	23	1	-2	-3	41	1	-3	-8	23	2	-0	-2	47	1	1	3	75	2	-4
9	23	1	0	-2	192	5	-4	-7	19	1	0	-1	62	2	-1	4	33	1	1
10	8	1	0	-1	0	12	-8*	-6	17	1	1	0	24	2	-1	5	15	1	-1
11	9	6	1*	0	29	3	-0	-5	13	1	0	1	41	1	-0	6	22	1	2
12	4	5	1*	1	23	2	-1	-4	25	2	0	2	69	2	3	7	36	1	-1
13	5	4	5*	2	384	10	-22	-3	18	1	0	3	32	1	-0	8	2	4	-0*
H,K=		0,	6	3	25	1	-1	-2	84	2	5	4	15	2	-1	9	24	1	0
0	33	1	-0	4	108	3	-2	-1	40	2	1	5	20	1	-0	10	4	6	1*
1	16	1	-3	5	27	1	1	0	76	2	1	6	17	2	-1	11	2	5	-2*
2	65	2	0	6	171	4	6	1	45	1	-1	7	4	7	-1*	12	10	5	3*
3	3	7	-1*	7	30	1	-1	2	51	1	0	8	18	1	1	13	21	1	0
4	49	1	-1	8	91	2	6	3	14	1	0	H,K=		1,	11	H,K=		2,	4
5	20	1	0	9	3	7	-2*	4	49	1	-1	-4	19	1	2	-13	5	2	-1*
6	14	1	0	10	15	2	-2	5	29	1	2	-3	5	7	-2*	-12	16	1	0
7	17	1	-1	11	7	2	-1*	6	11	2	2	-2	3	6	-5*	-11	29	1	1
8	14	2	1	12	1	4	1*	7	13	1	0	-1	24	1	0	-10	14	1	1
9	8	1	-1	13	9	2	-0*	8	4	4	3*	0	13	3	-0*	-9	14	1	-0
10	10	2	1*	14	17	1	1	9	45	2	0	1	23	1	2	-8	27	1	1
11	4	5	3*	H,K=		1,	3	10	23	1	0	2	22	1	-0	-7	58	2	2
12	13	2	-2	-14	5	5	-2*	11	12	1	-1	3	26	1	-1	-6	27	1	1

OBSERVED STRUCTURES FACTORS (CONT) FOR
D-L DIASSA C21.H30.O2 D.L.WARD,A.ZALKIN,D.H.TEMPLETON 25 PAGE 2

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-5	19	1	-1	3	6	2	-4*	-9	13	1	0	-3	20	1	-0	-13	38	1	1
-4	24	1	-1	4	49	1	-0	-8	71	2	1	-2	31	1	1	-12	39	1	0
-3	85	3	-4	5	22	1	0	-7	9	1	0	-1	6	2	2*	-11	2	4	-1*
-2	47	1	-1	6	19	1	2	-6	78	2	1	0	20	1	1	-10	35	1	0
-1	6	3	3*	7	19	1	1	-5	46	1	-2	1	22	1	-1	-9	17	1	0
0	5	5	2*	8	24	1	1	-4	36	1	-1	2	1	4	-1*	-8	0	4	-3*
1	40	2	1	9	5	3	2*	-3	38	1	-2	3	34	1	-0	-7	4	5	3*
2	57	1	1	H,K=		2,	10	-2	39	1	1	4	9	1	-2	-6	28	1	-0
3	65	2	1	-7	29	2	0	-1	64	2	-6	5	15	1	-1	-5	16	1	-1
4	42	1	-1	-6	45	1	-1	0	6	4	1*	6	5	2	-3*	-4	91	2	-1
5	9	1	-1	-5	5	6	0*	1	0	5	-3*	7	5	6	2*	-3	24	1	-3
6	14	1	1	-4	14	1	0	2	4	5	4*	8	6	2	2*	-2	23	1	-0
7	48	1	2	-3	66	2	0	3	84	2	-1	9	17	1	-0	-1	20	1	-1
8	54	1	1	-2	37	1	-1	4	26	1	2	10	0	5	-6*	0	52	1	-1
9	10	2	2*	-1	3	5	1*	5	30	1	-1	H,K=		3,	9	1	33	1	0
10	9	2	3*	0	52	1	1	6	8	1	-0	-9	12	1	1	2	62	2	2
11	44	1	0	1	44	1	-3	7	37	1	1	-8	6	2	3*	3	4	5	-3*
12	8	2	-3*	2	20	1	1	8	5	2	2*	-7	5	4	-1*	4	38	1	-0
H,K=		2,	6	3	21	1	1	9	19	2	0	-6	17	2	-0	5	6	1	-3*
-12	6	7	0*	4	39	1	1	10	35	1	0	-5	12	1	1	6	5	2	-2*
-11	18	2	-1	5	36	1	-1	11	25	1	-1	-4	30	1	-2	7	13	1	-0
-10	17	1	-0	6	9	2	-0*	12	14	2	-0	-3	20	1	1	8	2	4	0*
-9	38	1	-2	H,K=		3,	1	H,K=		3,	5	-2	13	1	-2	9	31	1	-1
-8	9	3	0*	-14	6	6	4*	-13	12	1	-2	-1	42	1	2	10	11	1	1
-7	18	1	-1	-13	4	6	1*	-12	6	4	1*	0	32	1	-0	11	4	6	-3*
-6	15	1	0	-12	9	2	-1*	-11	3	6	-1*	1	6	7	0*	12	17	1	1
-5	13	1	1	-11	7	3	2*	-10	7	2	-0*	2	44	1	1	H,K=		4,	4
-4	13	1	-1	-10	14	1	0	-9	47	1	-0	3	25	1	-0	-14	2	5	1*
-3	18	1	1	-9	20	1	0	-8	51	1	-0	4	5	3	-1*	-13	27	1	-1
-2	5	2	-2*	-8	64	2	3	-7	6	2	1*	5	18	1	-0	-12	47	1	-0
-1	6	1	2	-7	14	1	0	-6	41	1	2	6	47	1	-1	-11	21	1	-1
0	18	1	1	-6	13	1	-0	-5	36	1	-0	7	17	2	-0	-10	32	1	-1
1	51	1	-1	-5	79	2	-4	-4	35	1	2	H,K=		3,	11	-9	7	2	2*
2	17	1	1	-4	115	3	4	-3	38	1	-0	-4	16	1	0	-8	5	3	-1*
3	45	1	0	-3	10	1	-2	-2	62	2	3	-3	5	5	3*	-7	30	1	1
4	5	6	5*	-2	100	3	-3	-1	16	1	1	-2	6	4	-2*	-6	34	1	0
5	24	1	0	-1	11	1	-2	0	41	1	2	-1	14	1	0	-5	73	2	0
6	9	2	0*	0	126	3	-3	1	50	2	1	0	26	1	1	-4	38	1	-3
7	21	1	-0	1	17	1	-4	2	66	2	-2	1	10	2	2*	-3	62	2	0
8	11	1	0	2	20	1	1	3	104	3	1	2	19	1	-0	-2	47	1	0
9	11	1	2	3	36	1	-1	4	54	1	1	H,K=		4,	0	-1	126	3	-3
10	6	6	5*	4	21	1	-0	5	4	4	0*	-14	33	1	-2	0	39	1	1
11	22	2	-0	5	50	1	-1	6	51	1	-1	-12	19	1	-3	1	2	4	-1*
H,K=		2,	8	6	47	1	1	7	32	1	0	-10	34	2	3	2	64	2	-2
-10	7	4	0*	7	22	1	1	8	11	1	-1	-8	1	4	-1*	3	80	2	0
-9	28	1	-0	8	25	1	1	9	54	1	-1	-6	70	2	1	4	37	1	2
-8	18	1	1	9	20	1	0	10	0	5	-2*	-4	121	3	-2	5	13	1	0
-7	4	5	0*	10	9	1	0	11	14	1	-1	-2	12	1	-1	6	4	5	1*
-6	40	1	-1	11	18	1	1	H,K=		3,	7	0	58	1	-1	7	31	1	-0
-5	25	1	1	12	8	1	1	-11	0	5	-1*	2	44	1	-0	8	19	1	-1
-4	6	8	-1*	13	8	3	2*	-10	12	1	-0	4	3	4	2*	9	25	1	-1
-3	51	1	0	H,K=		3,	3	-9	1	6	1*	6	20	1	0	10	9	2	1*
-2	14	1	-0	-14	19	1	-1	-8	6	6	1*	8	31	1	-1	11	36	1	-0
-1	6	5	3*	-13	7	2	-1*	-7	7	4	-2*	10	13	1	1	12	3	5	-2*
0	47	1	1	-12	6	3	-3*	-6	7	2	1*	12	7	2	3*	H,K=		4,	6
1	38	1	-2	-11	2	5	1*	-5	7	2	-1*	H,K=		4,	2	-12	18	1	0
2	10	1	0	-10	30	1	1	-4	14	1	1	-14	20	1	1	-11	21	1	-0

OBSERVED STRUCTURES FACTORS (CONT) FOR
D-L DIASSA C21.H30.O2 D.L.WARD,A.ZALKIN,D.H.TEMPLETON 25 PAGE 3

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-10	24	1	1	-13	5	5	2*	-11	37	1	-1	2	8	1	2	-9	2	4	-5*
-9	2	6	1*	-12	19	1	1	-10	7	2	-2*	3	5	5	1*	-8	54	1	-1
-8	4	5	1*	-11	14	1	1	-9	46	1	0	4	11	1	1	-7	9	1	1
-7	13	1	-2	-10	6	5	1*	-8	18	1	1	5	8	9	4*	-6	69	2	3
-6	5	6	4*	-9	19	1	0	-7	21	1	2	6	24	1	1	-5	51	1	1
-5	62	2	-1	-8	74	2	0	-6	5	6	1*	H,K=		5,	11	-4	49	1	2
-4	25	1	0	-7	3	4	0*	-5	37	1	1	-2	11	1	-1	-3	29	1	-0
-3	66	2	3	-6	51	1	2	-4	15	2	0	-1	5	7	4*	-2	26	1	-0
-2	37	1	1	-5	3	4	1*	-3	88	2	-1	0	9	4	-1*	-1	31	1	1
-1	56	1	2	-4	47	1	-0	-2	139	4	4	H,K=		6,	0	0	94	2	5
0	51	2	0	-3	59	2	-7	-1	125	3	2	-14	27	1	-2	1	119	3	0
1	6	1	-3*	-2	6	6	-2*	0	2	6	2*	-12	33	1	0	2	13	1	3
2	14	1	1	-1	16	1	-1	1	68	2	-2	-10	23	1	-1	3	12	1	-1
3	27	1	0	0	210	5	-4	2	17	1	-0	-8	3	5	2*	4	31	1	1
4	47	1	0	1	89	2	-7	3	31	1	1	-6	82	2	2	5	41	1	-1
5	29	1	2	2	1	5	-0*	4	5	2	3*	-4	121	3	4	6	26	1	1
6	13	3	1*	3	69	2	-0	5	52	1	-1	-2	86	2	2	7	42	1	1
7	26	1	-1	4	61	2	3	6	21	1	0	0	140	4	-5	8	47	1	-1
8	14	1	1	5	2	5	-1*	7	0	5	-5*	2	39	1	-0	9	20	1	-0
9	21	1	-3	6	20	1	-0	8	21	1	-0	4	6	2	2*	10	0	5	-2*
10	7	3	-0*	7	12	1	-1	9	7	3	1*	6	6	1	0*	11	5	3	2*
H,K=		4,	8	8	19	1	1	10	27	1	-0	8	68	2	1	H,K=		6,	6
-10	2	7	-4*	9	11	1	5	11	6	3	0*	10	34	1	-1	-12	13	1	-1
-9	7	2	0*	10	23	1	0	H,K=		5,	7	12	0	6	-4*	-11	10	1	-1
-8	12	2	1	11	14	1	-1	-11	44	1	-0	H,K=		6,	2	-10	16	1	1
-7	26	1	-0	12	6	2	0*	-10	19	1	0	-14	23	2	-1	-9	22	1	-1
-6	27	1	2	H,K=		5,	3	-9	23	1	-0	-13	52	1	-3	-8	30	1	2
-5	18	2	-0	-14	6	8	-1*	-8	9	4	-1*	-12	4	7	-1*	-7	29	1	1
-4	16	1	1	-13	2	5	-1*	-7	2	5	1*	-11	5	6	1*	-6	38	1	-1
-3	9	1	-1	-12	16	1	-1	-6	14	1	-0	-10	44	1	-1	-5	29	1	-2
-2	0	4	-2*	-11	29	1	-1	-5	15	2	1	-9	7	1	-1	-4	20	1	2
-1	10	1	1	-10	7	1	1	-4	16	1	0	-8	29	1	1	-3	7	1	-0
0	21	1	1	-9	6	1	1*	-3	19	1	-1	-7	51	1	-0	-2	4	3	1*
1	2	5	-0*	-8	12	1	1	-2	24	1	-1	-6	32	1	2	-1	3	5	-3*
2	0	4	-3*	-7	37	1	-1	-1	13	1	0	-5	20	1	-0	0	65	2	2
3	9	1	-0	-6	23	1	1	0	15	1	1	-4	57	1	1	1	16	1	1
4	20	1	0	-5	18	2	-1	1	13	1	0	-3	24	1	1	2	47	1	0
5	1	5	0*	-4	88	2	4	2	13	1	-1	-2	102	3	2	3	16	1	1
6	20	1	0	-3	49	1	-2	3	15	1	-1	-1	12	1	0	4	19	1	-1
7	21	1	-1	-2	138	4	0	4	9	3	1*	0	101	3	2	5	11	2	-3
8	41	2	0	-1	112	3	-6	5	4	4	1*	1	45	1	-0	6	3	6	1*
H,K=		4,	10	0	78	2	-3	6	14	2	1	2	38	1	0	7	28	1	0
-7	2	7	1*	1	10	1	2	7	28	1	-1	3	22	1	-1	8	4	6	-0*
-6	13	1	2	2	3	4	2*	8	24	1	1	4	5	1	4*	9	8	5	2*
-5	2	5	1*	3	23	1	-0	9	4	5	3*	5	34	1	-1	H,K=		6,	8
-4	8	1	-2	4	6	1	-2*	H,K=		5,	9	6	18	1	2	-10	9	3	-1*
-3	12	1	0	5	54	1	3	-9	4	5	-0*	7	19	1	-1	-9	11	2	-0
-2	7	2	-2*	6	3	4	3*	-8	8	5	-5*	8	68	2	1	-8	3	5	2*
-1	20	1	0	7	9	2	2*	-7	2	5	-3*	9	6	7	-3*	-7	4	4	1*
0	28	1	-1	8	11	2	-1	-6	10	2	2	10	14	2	2	-6	8	2	1*
1	8	2	4*	9	4	4	1*	-5	9	2	-4	11	4	5	-1*	-5	9	5	-4*
2	6	1	3*	10	21	1	-1	-4	25	1	-1	H,K=		6,	4	-4	12	2	1
3	5	6	3*	11	8	4	-1*	-3	6	4	3*	-14	4	6	4*	-3	30	1	1
4	11	3	-1*	12	18	1	1	-2	10	1	-1	-13	29	1	-0	-2	20	1	-0
5	20	1	2	H,K=		5,	5	-1	0	5	-5*	-12	20	1	-2	-1	14	1	1
H,K=		5,	1	-13	26	1	-1	0	11	1	-1	-11	23	1	0	0	14	2	0
-14	9	2	-1*	-12	20	1	1	1	17	1	-1	-10	23	1	0	1	17	1	1

OBSERVED STRUCTURES FACTORS (CONT) FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
2	22	1	-1	-2	14	1	-0	6	5	5	4*	10	20	1	-0	-2	24	1	0
3	9	2	1*	-1	15	1	-1	7	8	4	0*	H,K=		8,	4	-1	28	1	-1
4	17	1	-3	0	58	1	2	8	0	7	-3*	-13	6	7	4*	0	0	8	-1*
5	10	1	1	1	38	1	-1	H,K=		7,	9	-12	18	1	1	1	19	1	-2
6	19	1	1	2	53	2	1	-8	13	1	1	-11	14	1	2	2	5	5	2*
7	4	3	-1*	3	38	1	0	-7	10	1	-1	-10	11	2	-1*	3	5	2	5*
H,K=		6,	10	4	53	1	1	-6	11	1	1	-9	4	6	0*	4	10	2	1*
-6	18	1	-2	5	11	2	-1	-5	8	3	-1*	-8	11	1	1	5	10	2	-1*
-5	24	1	-2	6	2	4	2*	-4	24	1	-1	-7	11	1	-0	6	2	7	-0*
-4	14	1	-1	7	31	1	1	-3	39	1	-2	-6	61	2	2	H,K=		8,	10
-3	4	5	-1*	8	21	1	-1	-2	5	3	1*	-5	18	1	0	-5	1	8	-5*
-2	36	1	-2	9	12	1	1	-1	4	5	-1*	-4	28	1	-1	-4	21	1	-1
-1	17	1	1	10	22	2	-1	0	24	1	-2	-3	25	1	1	-3	3	6	-0*
0	19	1	2	11	6	3	-3*	1	3	4	-3*	-2	55	1	0	-2	25	1	0
1	14	1	-0	H,K=		7,	5	2	8	3	0*	-1	34	1	0	-1	36	1	-1
2	12	1	0	-13	23	1	1	3	7	2	0*	0	17	1	-1	0	18	1	0
3	5	5	-1*	-12	10	2	2	4	9	1	1	1	4	5	3*	1	20	1	1
H,K=		7,	1	-11	20	1	-1	5	2	6	-2*	2	6	6	2*	H,K=		9,	1
-14	6	4	-0*	-10	11	2	-1*	H,K=		8,	0	3	11	1	-0	-14	51	2	-1
-13	10	2	2	-9	14	1	0	-14	8	2	5*	4	13	1	0	-13	10	1	0
-12	37	1	-1	-8	17	1	-0	-12	17	2	-4	5	21	1	-0	-12	35	1	-0
-11	55	2	-3	-7	7	1	-0*	-10	5	4	4*	6	10	1	0	-11	14	1	-1
-10	66	2	0	-6	32	1	1	-8	104	3	6	7	13	1	-1	-10	26	1	1
-9	9	2	-0*	-5	7	1	-0	-6	7	1	-1*	8	6	6	3*	-9	19	1	-0
-8	46	1	-1	-4	16	1	1	-4	98	2	9	9	16	2	-2	-8	8	2	5*
-7	42	1	-0	-3	28	1	-0	-2	153	4	1	10	17	2	1	-7	23	1	-0
-6	78	2	2	-2	34	1	2	0	101	3	-1	H,K=		8,	6	-6	65	2	3
-5	30	1	-2	-1	22	1	-1	2	36	1	0	-12	2	5	0*	-5	6	3	1*
-4	78	2	1	0	7	3	1*	4	4	4	2*	-11	8	2	-0*	-4	23	1	-0
-3	40	1	-0	1	5	5	4*	6	27	1	0	-10	25	1	-0	-3	62	2	3
-2	16	1	2	2	37	1	1	8	45	1	-0	-9	16	1	-0	-2	66	2	6
-1	6	3	-0*	3	28	1	1	10	39	1	0	-8	4	5	0*	-1	30	1	-0
0	4	5	4*	4	12	1	1	H,K=		8,	2	-7	28	1	1	0	135	3	2
1	55	2	-2	5	0	6	-0*	-14	9	1	-1	-6	18	1	0	1	37	1	2
2	113	3	2	6	30	1	1	-13	23	1	0	-5	27	1	-1	2	54	1	2
3	7	2	0*	7	44	1	0	-12	9	2	1*	-4	16	1	0	3	5	2	0*
4	12	1	2	8	3	4	2*	-11	6	2	4*	-3	6	6	2*	4	41	1	0
5	12	1	-1	9	17	1	1	-10	0	4	-1*	-2	25	1	1	5	17	1	-1
6	33	1	0	10	6	7	-0*	-9	54	2	-2	-1	9	1	-3	6	26	1	-0
7	2	4	2*	H,K=		7,	7	-8,	42	1	-1	0	4	5	4*	7	5	6	-1*
8	6	3	-1*	-11	28	1	0	-7	10	1	1	1	30	1	-1	8	28	1	-1
9	6	2	5*	-10	21	1	-0	-6	32	1	-2	2	25	1	-0	9	11	5	1*
10	37	1	-2	-9	19	1	-1	-5	108	3	-0	3	7	1	1	10	25	1	-1
11	8	4	-0*	-8	18	1	2	-4	4	2	-1*	4	15	1	-1	H,K=		9,	3
H,K=		7,	3	-7	23	1	-1	-3	10	3	-1*	5	24	1	-1	-14	24	1	1
-14	19	1	0	-6	17	1	-1	-2	22	1	-0	6	16	2	-1	-13	23	1	0
-13	4	5	3*	-5	21	1	1	-1	24	1	-1	7	13	1	1	-12	43	1	2
-12	23	1	1	-4	4	6	4*	0	44	1	2	8	12	3	-1*	-11	3	6	-1*
-11	56	2	-1	-3	14	2	-0	1	27	1	-1	H,K=		8,	8	-10	10	2	1*
-10	16	2	1	-2	16	1	2	2	21	1	2	-10	29	1	1	-9	20	1	1
-9	6	2	4*	-1	5	4	-0*	3	34	1	-1	-9	19	1	1	-8	11	2	-1
-8	6	1	5*	0	4	5	2*	4	5	5	3*	-8	31	1	1	-7	11	1	-0
-7	11	2	3	1	4	4	3*	5	8	1	0	-7	8	2	1*	-6	42	1	0
-6	20	1	1	2	4	5	3*	6	9	6	2*	-6	10	1	1	-5	19	1	0
-5	37	1	0	3	8	3	2*	7	22	1	-1	-5	7	2	-1*	-4	13	1	-0
-4	34	1	0	4	22	1	-1	8	32	1	1	-4	3	5	2*	-3	7	2	-0*
-3	4	2	0*	5	6	6	0*	9	3	4	-0*	-3	11	1	-1	-2	18	1	0

OBSERVED STRUCTURES FACTORS (CONT) FOR
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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-1	3	5	-0*	-4	4	6	1*	-3	6	4	-1*	-6	36	1	1	6	20	2	-0
0	17	1	0	-3	3	5	-2*	-2	40	1	-2	-5	7	3	-3*	7	20	1	-0
1	15	1	-1	-2	21	1	-0	-1	44	1	1	-4	32	1	0	H,K=	11,		7
2	11	2	2	-1	8	3	1*	0	3	4	-2*	-3	18	1	-1	-10	16	1	-2
3	21	1	-1	0	6	2	3*	1	9	2	-2	-2	44	1	3	-9	6	7	4*
4	10	1	0	1	4	5	1*	2	32	1	1	-1	31	1	-1	-8	29	1	2
5	23	1	1	2	19	2	1	3	0	4	-1*	0	18	1	-1	-7	10	1	3
6	27	1	-0	3	4	5	-2*	4	27	1	-1	1	16	1	-0	-6	17	1	-1
7	9	2	0*	H,K=	10,		0	5	5	5	-0*	2	17	1	1	-5	5	6	-1*
8	11	2	-1	-14	22	1	-0	6	11	1	-0	3	8	3	2*	-4	12	4	-0*
9	21	1	-0	-12	46	1	-2	7	15	1	-0	4	23	1	-1	-3	53	2	0
H,K=		9,	5	-10	26	1	-0	8	2	5	-3*	5	26	1	0	-2	8	2	0*
-13	21	1	-1	-8	5	6	-3*	H,K=		10,	6	6	36	1	1	-1	6	7	5*
-12	22	1	1	-6	60	2	3	-12	22	1	-1	7	4	7	2*	0	21	1	-0
-11	4	5	1*	-4	172	4	2	-11	24	1	-1	8	4	6	0*	1	26	1	-0
-10	11	1	-1	-2	8	2	-2*	-10	22	1	1	H,K=		11,	3	2	6	2	5*
-9	8	1	-1	0	46	1	2	-9	2	5	1*	-13	12	1	1	3	11	3	-1*
-8	7	2	1*	2	30	1	1	-8	20	1	-1	-12	23	1	1	4	11	3	1*
-7	4	5	1*	4	30	1	0	-7	18	1	1	-11	10	3	-2*	5	19	1	0
-6	0	6	-0*	6	41	1	-1	-6	6	3	1*	-10	0	5	-2*	H,K=	11,		9
-5	17	1	0	8	0	8	-2*	-5	35	1	1	-9	10	1	1	-5	21	1	-1
-4	24	1	0	H,K=	10,		2	-4	21	1	-1	-8	4	6	1*	-4	6	7	-0*
-3	21	1	-2	-14	22	1	1	-3	7	2	-1*	-7	20	1	1	-3	6	3	-2*
-2	40	1	-1	-13	25	1	-2	-2	15	1	-1	-6	3	5	0*	-2	19	1	-1
-1	15	1	0	-12	35	1	-1	-1	8	1	-2	-5	5	6	2*	-1	13	3	-2*
0	23	1	0	-11	8	1	-1	0	6	2	-2*	-4	1	4	-2*	0	14	2	1
1	15	1	-1	-10	13	1	1	1	17	1	-1	-3	7	2	-4*	H,K=	12,		0
2	3	4	2*	-9	12	1	-1	2	5	4	-5*	-2	5	2	-2*	-14	16	1	1
3	11	1	-0	-8	22	1	1	3	2	5	-0*	-1	36	1	-1	-12	0	6	-0*
4	0	6	-3*	-7	12	1	-1	4	7	2	2*	0	4	5	-1*	-10	3	5	-1*
5	4	5	2*	-6	14	1	1	5	9	3	-5*	1	43	1	3	-8	3	5	3*
6	9	2	-1*	-5	2	4	1*	6	0	6	-0*	2	23	1	-1	-6	14	1	-1
7	33	1	-0	-4	51	1	-0	7	12	1	-0	3	17	1	1	-4	16	1	0
8	12	2	-0	-3	20	1	-0	H,K=		10,	8	4	2	4	0*	-2	68	2	1
H,K=		9,	7	-2	41	1	-0	-9	4	5	0*	5	7	2	0*	0	12	1	1
-11	14	1	0	-1	18	1	-1	-8	27	1	0	6	18	2	1	2	12	2	-3
-10	11	2	1*	0	4	5	0*	-7	2	6	-2*	7	6	7	-1*	4	14	1	-2
-9	0	7	-2*	1	18	1	0	-6	7	2	3*	8	18	1	0	6	45	1	-0
-8	9	8	-3*	2	5	2	4*	-5	21	1	0	H,K=		11,	5	8	16	1	0
-7	22	1	-1	3	45	1	-0	-4	11	1	-3	-12	14	1	-1	H,K=		12,	2
-6	18	1	-1	4	35	1	0	-3	5	3	-3*	-11	37	1	1	-13	19	1	-0
-5	23	1	1	5	11	1	-1	-2	3	5	0*	-10	28	1	-0	-12	9	1	-2
-4	16	1	1	6	19	1	1	-1	13	2	-2	-9	19	1	-1	-11	2	4	-3*
-3	9	1	1	7	31	1	-0	0	1	6	-6*	-8	47	2	-1	-10	27	1	-1
-2	16	1	-1	8	13	2	0	1	22	1	2	-7	26	1	0	-9	16	1	-0
-1	29	1	0	9	10	2	-1	2	6	3	1*	-6	49	1	1	-8	30	1	1
0	8	2	-2*	H,K=	10,		4	3	18	1	-1	-5	14	1	1	-7	23	1	-0
1	14	1	2	-13	0	12	-0*	4	5	2	2*	-4	21	1	1	-6	39	1	-1
2	8	2	2*	-12	16	1	2	H,K=		11,	1	-3	43	1	-1	-5	23	1	1
3	3	4	3*	-11	25	1	-0	-14	12	2	-1*	-2	6	2	2*	-4	32	1	1
4	13	1	1	-10	10	1	-2	-13	14	2	0	-1	8	3	2*	-3	3	4	3*
5	5	7	0*	-9	8	2	0*	-12	28	1	-0	0	27	1	1	-2	25	1	-1
6	6	5	4*	-8	18	1	-1	-11	25	1	-1	1	34	1	-2	-1	8	1	0
H,K=		9,	9	-7	4	5	2*	-10	4	6	3*	2	20	1	0	0	38	1	0
-7	8	4	-2*	-6	4	5	-2*	-9	33	1	-0	3	11	1	0	1	35	1	-0
-6	38	1	-2	-5	6	1	5*	-8	42	1	2	4	12	2	-0*	2	8	3	2*
-5	11	1	2	-4	16	1	1	-7	24	1	2	5	11	1	1	3	8	2	4*

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L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
4	24	1	-1	-9	7	2	0*	-7	13	2	4	H,K= 14,				6	-1	24	2	-1
5	9	3	1*	-8	8	1	-1	-6	41	1	-0	-9	11	1	1	0	14	2	1
6	30	1	-1	-7	12	1	-0	-5	3	8	0*	-8	0	6	-1*	1	22	1	0
7	6	2	-1*	-6	3	4	3*	-4	31	1	0	-7	25	1	-1	2	17	2	-2
H,K= 12,				-5	5	5	-1*	-3	41	1	1	-6	11	2	0*	H,K= 16,			
-12	4	8	-1*	-4	46	1	1	-2	11	2	-1*	-5	16	2	-2	-10	2	6	-2*
-11	53	1	0	-3	9	1	1	-1	25	1	-1	-4	24	1	2	-8	31	1	0
-10	8	2	-0*	-2	21	1	-1	0	23	1	-0	-3	2	6	-0*	-6	15	2	0
-9	29	1	-0	-1	4	4	0*	1	22	1	-2	-2	10	2	1	-4	10	2	1
-8	24	1	-0	0	21	1	3	2	0	7	-6*	-1	38	2	-1	-2	7	2	-4*
-7	10	1	-0	1	5	3	2*	H,K= 14,				0	0	15	1	1	0	40	1	-1
-6	15	2	1	2	22	1	-0	-12	12	1	-1	1	5	6	-1*	2	30	1	1
-5	45	2	-0	3	10	1	2	-10	3	5	-2*	2	12	2	-1	H,K= 16,			2
-4	9	3	1*	4	17	1	1	-8	50	2	-1	H,K= 15,				1	-11	27	1	1
-3	21	2	0	5	4	5	-4*	-6	9	2	-0	-12	21	1	-0	-10	12	2	2*
-2	38	1	-1	6	14	1	1	-4	15	1	1	-11	2	4	-3*	-9	7	5	-4*
-1	12	1	1	7	4	5	3*	-2	33	1	-0	-10	21	1	-1	-8	0	5	-2*
0	25	1	1	H,K= 13,				3	0	55	2	1	-9	5	6	0*	-7	20	1	1
1	12	1	-2	-12	16	1	2	2	8	1	1	-8	10	2	1	-6	16	1	1
2	17	1	1	-11	41	1	-0	4	10	1	1	-7	14	1	1	-5	3	4	-3*
3	28	1	1	-10	24	1	-1	6	5	6	5*	-6	17	1	1	-4	13	1	0
4	17	1	-1	-9	19	1	-1	H,K= 14,				2	-5	9	3	1*	-3	8	3	-2*
5	31	1	1	-8	25	1	1	-12	25	2	1	-4	31	1	2	-2	7	3	2*
6	25	1	1	-7	24	1	0	-11	10	2	2	-3	8	2	2*	-1	9	4	1*
H,K= 12,				-6	61	2	1	-10	7	2	0*	-2	4	6	-0*	0	14	1	2
-11	26	1	-1	-5	4	5	-0*	-9	3	6	-4*	-1	18	1	-1	1	15	2	-1
-10	28	1	1	-4	19	1	0	-8	5	5	4*	0	30	1	0	2	0	5	-1*
-9	35	1	-0	-3	54	1	-2	-7	2	5	-1*	1	15	2	-1	3	26	2	2
-8	23	1	0	-2	34	2	0	-6	20	1	1	2	4	5	0*	H,K= 16,			4
-7	5	6	3*	-1	13	2	1	-5	21	2	1	3	10	3	-0*	-9	6	2	4*
-6	53	2	1	0	15	1	0	-4	53	1	1	4	9	2	2*	-8	8	3	1*
-5	72	2	1	1	14	1	2	-3	13	1	-0	H,K= 15,				3	-7	9	3	-1*
-4	43	1	-0	2	3	5	2*	-2	19	1	1	-11	13	2	1	-6	17	1	1
-3	21	1	-1	3	10	1	-1	-1	26	1	-3	-10	11	2	2*	-5	6	7	-1*
-2	58	2	-2	4	6	2	-1*	0	4	6	4*	-9	11	2	0*	-4	33	1	0
-1	48	2	-0	5	10	1	3	1	0	4	-3*	-8	17	1	0	-3	24	1	1
0	4	5	1*	6	16	2	4	2	28	1	-1	-7	17	2	0	-2	0	5	-3*
1	18	1	-1	H,K= 13,				5	3	21	1	-0	-6	55	1	2	-1	0	5	-2*
2	45	2	-1	-11	38	1	-0	4	15	2	-1	-5	29	1	-0	0	18	2	-1
3	15	1	-0	-10	4	5	-2*	5	5	5	-1*	-4	23	1	-1	1	1	5	-1*
4	3	6	1*	-9	44	1	-2	H,K= 14,				4	-3	44	1	1	H,K= 16,			6
5	19	2	-1	-8	16	1	0	-11	25	1	-0	-2	46	1	-1	-5	6	4	1*
H,K= 12,				-7	42	2	-1	-10	7	5	1*	-1	13	1	-0	-4	9	3	-1*
-7	0	6	-0*	-6	12	1	1	-9	48	1	-1	0	26	1	1	-3	3	6	-2*
-6	3	6	-2*	-5	12	1	-1	-8	28	1	1	1	41	1	2	H,K= 17,			1
-5	4	5	1*	-4	28	1	1	-7	40	1	-2	2	29	1	-1	-10	9	2	-0*
-4	4	6	-1*	-3	112	3	-2	-6	5	6	0*	3	0	5	-3*	-9	11	2	1
-3	5	5	1*	-2	30	1	2	-5	79	2	1	4	31	1	0	-8	10	1	-0
-2	4	4	3*	-1	30	1	1	-4	48	1	1	H,K= 15,				5	-7	15	1	-3
-1	8	3	-2*	0	24	2	0	-3	23	2	-2	-9	15	3	-2*	-6	15	1	-0
0	21	1	-1	1	47	2	0	-2	50	1	-1	-8	5	6	4*	-5	5	6	1*
1	5	7	0*	2	31	1	-1	-1	84	2	-0	-7	16	1	0	-4	29	1	-1
H,K= 13,				3	31	1	-2	0	5	6	-3*	-6	43	1	-3	-3	9	4	-1*
-13	9	2	0*	4	27	1	-1	1	19	1	2	-5	39	2	-0	-2	34	1	-0
-12	20	1	0	5	16	1	-0	2	34	1	1	-4	8	2	-0*	-1	8	2	1*
-11	7	3	-2*	H,K= 13,				7	3	51	1	1	-3	24	1	-1	0	11	3	0*
-10	14	1	1	-8	16	2	-0	4	0	5	-1*	-2	23	1	-2	1	4	5	-3*

OBSERVED STRUCTURES FACTORS (CONT) FOR
D-L DIASSA C21.H30.O2 D.L.WARD,A.ZALKIN,D.H.TEMPLETON 25 PAGE 7

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=		17,	3																
-9	22	1	1																
-8	4	5	0*																
-7	15	1	-2																
-6	9	2	1*																
-5	23	1	1																
-4	22	1	-1																
-3	2	5	-1*																
-2	23	1	1																
-1	10	1	3																
0	8	2	-1*																
H,K=		18,	0																
-8	11	1	-2																
-6	38	1	2																
-4	26	1	2																
-2	30	1	-1																
H,K=		18,	2																
-7	11	5	-1*																
-6	22	1	-1																
-5	31	1	-0																
-4	11	3	0*																
-3	6	2	-1*																
-2	23	1	-1																
-1	17	1	-3																

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