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JM9605070

Crystal data for compound (+)-9

Crystal data:

$C_{11}H_{17}NO_3 . C_4H_6O_6 . nH_2O$

$P2_1$ Mo(k_α) λ=0.71073 Å
a=11.951(2) Å
b=7.237(1) Å ß=106.28(1)°
c=12.832(2) Å
V=1065.2(2) Å^3
Z=2

Data collection:

Nonius CAD-4 diffractometer
θ-2θ scans θmax=30.0°
3468 measured reflections
3326 independent reflections
1607 observed reflections (I>3σ(I))

Structure solution and refinement:

The data were processed and refined using the MolEN software package (Fair, 1995). The structure was solved using the SIR program(Altomare et al. 1993) and refined by full-matrix least-squares techniques. All calculation were carried out on a AlphaServer 400 computer.

Refinement on F $\Delta\rho_{max}$=0.81 e Å^{-3}
R = 0.089 $\Delta\rho_{min}$=-.38 e Å^{-3}
Rw = 0.138 $w=1/\sigma^2(F_o)$
$(\Delta/\sigma)_{max}$=0.59
1607 reflections 247 parameters

Description:

The asymmetric unit contains one substituted tropane ring system, a tartrate anion, two water molecules and an additional undetermined solvent molecule. Although the undetermined solvent molecule was not resolvable by difference Fourier techniques, the stereochemistry of the substituents on the tropane ring was clearly determined.

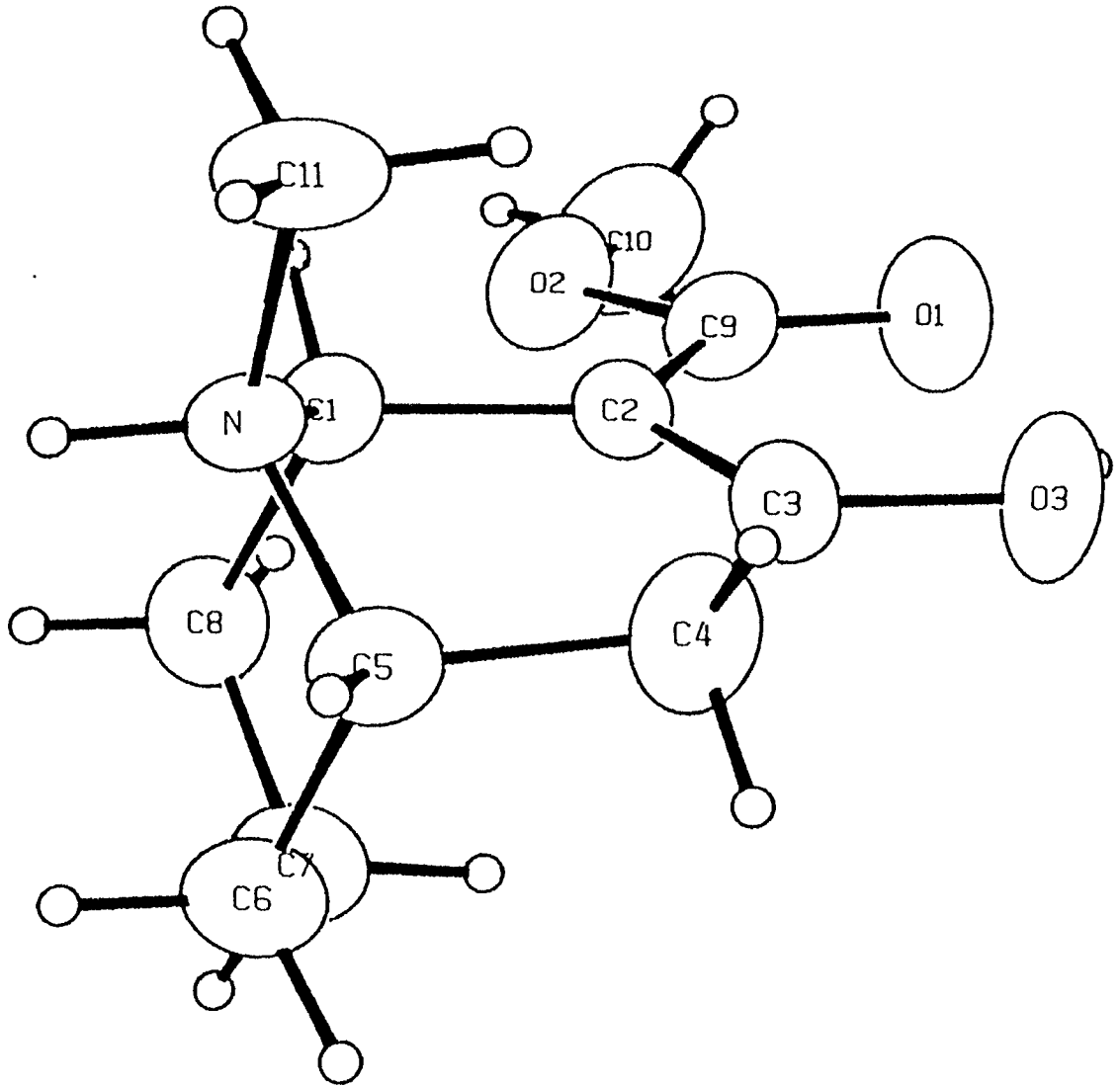
C11
C10
O2
C9
O1
N
C1
C2
C3
O3
C8
C5
C4
C7
C6

Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
O1	C9	1.21(1)	C1	C2	1.52(1)
O2	C9	1.32(1)	C1	C8	1.52(2)
O2	C10	1.45(1)	C2	C3	1.31(2)
O3	C3	1.36(1)	C2	C9	1.45(1)
O21A	C21	1.30(1)	C3	C4	1.51(1)
O21B	C21	1.21(1)	C4	C5	1.53(1)
O22	C22	1.40(1)	C5	C6	1.52(2)
O23	C23	1.43(1)	C6	C7	1.52(2)
O24A	C24	1.23(1)	C7	C8	1.50(2)
O24B	C24	1.23(1)	C21	C22	1.53(2)
N	C1	1.53(1)	C22	C23	1.52(1)
N	C5	1.51(2)	C23	C24	1.54(2)
N	C11	1.48(2)			

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Bond Angles in Degrees

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C9	O2	C10	117.5(9)	C6	C7	C8	112.(1)
C1	N	C5	110.5(9)	C1	C8	C7	111.(1)
C1	N	C11	114.1(8)	O1	C9	O2	123(1)
C5	N	C11	113(1)	O1	C9	C2	124.(1)
N	C1	C2	108.5(8)	O2	C9	C2	112.8(8)
N	C1	C8	107.4(8)	O21A	C21	O21B	125.(1)
C2	C1	C8	113(1)	O21A	C21	C22	113.8(7)
C1	C2	C3	122.2(9)	O21B	C21	C22	120.9(8)
C1	C2	C9	118.1(9)	O22	C22	C21	109.0(7)
C3	C2	C9	119.6(9)	O22	C22	C23	112.6(8)
O3	C3	C2	124.6(9)	C21	C22	C23	110.6(8)
O3	C3	C4	112(1)	O23	C23	C22	109.4(7)
C2	C3	C4	123.6(9)	O23	C23	C24	110.6(8)
C3	C4	C5	114.3(9)	C22	C23	C24	111.3(8)
N	C5	C4	108.0(8)	O24A	C24	O24B	128.(1)
N	C5	C6	107.0(9)	O24A	C24	C23	116.5(9)
C4	C5	C6	117.(1)	O24B	C24	C23	115.1(9)
C5	C6	C7	113(1)				

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Positional Parameters and Their Estimated Standard Deviations

Atom	x	y	z	B(A2)
O1	0.540	0.8235	0.5321(6)	4.6(2)
O2	0.3566(6)	0.766(1)	0.5306(5)	3.9(2)
O3	0.5821(6)	0.865(2)	0.3464(6)	4.5(2)
O21A	0.1854(6)	0.109(1)	-0.2238(6)	2.8(2)
O21B	0.3464(7)	0.106(1)	-0.0844(7)	4.0(2)
O22	0.3454(5)	0.469(1)	-0.0606(6)	2.8(2)
O23	0.1020(5)	0.395(1)	-0.0764(5)	2.9(1)
O24A	0.1806(6)	0.761(1)	-0.2274(6)	3.3(2)
O24B	0.0833(6)	0.749(1)	-0.1038(6)	4.0(2)
OW1	0.4632(6)	0.769(1)	-0.0907(6)	3.2(2)
OW2	-0.0304(5)	0.071(1)	-0.1021(6)	2.9(1)
N	0.2572(7)	0.660(1)	0.1989(7)	2.6(2)
C1	0.2713(8)	0.727(2)	0.3147(8)	2.7(2)
C2	0.3978(7)	0.779(2)	0.3649(8)	2.5(2)

Table of Positional Parameters and Their Estimated Standard Deviations (cont.)

Atom	x	y	z	B(A2)
C3	0.4671(8)	0.825(2)	0.3058(8)	3.0(2)
C4	0.4284(9)	0.836(2)	0.1837(8)	3.8(3)
C5	0.2975(8)	0.807(2)	0.1335(8)	3.0(2)
C6	0.219(1)	0.974(2)	0.129(1)	4.1(3)
C7	0.215(1)	1.042(2)	0.240(1)	4.4(3)
C8	0.1880(9)	0.888(2)	0.308(1)	3.9(3)
C9	0.4403(8)	0.788(2)	0.4825(9)	3.2(2)
C10	0.385(1)	0.801(3)	0.6460(9)	5.5(4)
C11	0.311(1)	0.477(2)	0.192(1)	4.3(3)
C21	0.2688(8)	0.187(2)	-0.1500(7)	2.1(2)
C22	0.2643(8)	0.400(2)	-0.1530(7)	2.3(2)
C23	0.1413(7)	0.467(1)	-0.1636(7)	2.0(2)
C24	0.1356(8)	0.681(2)	-0.1646(8)	2.2(2)
H1	0.263	0.631	0.365	4.2*

Table of Positional Parameters and Their Estimated Standard Deviations (cont.)

Atom	x	y	z	B(A2)
H4A	0.438	0.945	0.152	9.8*
H4B	0.467	0.748	0.148	3.6*
H5	0.292	0.767	0.055	1.7*
H8A	0.106	0.869	0.292	4.2*
H8B	0.204	0.913	0.422	4.8*
H22	0.267	0.438	-0.213	2.0*
H22A	0.413	0.465	0.947	8.7*
H23	0.098	0.414	-0.237	1.7*
H23A	0.050	0.275	0.936	10.2*
H3	0.399	0.389	0.582	7.7*
H6A	0.246	1.070	0.093	5.6*
H6B	0.142	0.939	0.090	5.6*
H7A	0.292	1.088	0.279	5.8*
H7B	0.161	1.135	0.234	5.8*

Table of Positional Parameters and Their Estimated Standard Deviations (cont.)

Atom	x	y	z	B(A2)
H10A	0.320	0.776	0.672	7.6*
H10B	0.413	0.919	0.663	7.6*
H10C	0.446	0.712	0.683	7.6*
H11A	0.287	0.386	0.235	6.3*
H11B	0.397	0.488	0.222	6.3*
H11C	0.296	0.435	0.120	6.3*
H	0.173(8)	0.64(2)	0.147(8)	6(3)*

Starred atoms were refined isotropically.
Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:
(4/3) * [a2*B(1,1) + b2*B(2,2) + c2*B(3,3) + ab(cos gamma)*B(1,2) + ac(cos beta)*B(1,3) + bc(cos alpha)*B(2,3)]

Table of General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
O1	0.045(4)	0.084(7)	0.041(4)	-0.012(5)	0.000(3)	-0.007(5)
O2	0.056(4)	0.063(6)	0.033(3)	-0.015(5)	0.017(3)	-0.005(4)
O3	0.032(3)	0.084(7)	0.052(4)	-0.018(4)	0.012(3)	-0.007(5)
O21A	0.044(3)	0.015(4)	0.045(4)	-0.001(3)	0.006(3)	-0.005(3)
O21B	0.049(4)	0.017(4)	0.068(5)	0.005(4)	-0.010(4)	0.004(4)
O22	0.030(3)	0.027(4)	0.047(4)	-0.002(3)	0.004(3)	-0.004(4)
O23	0.047(3)	0.017(4)	0.056(3)	-0.003(3)	0.033(2)	0.000(3)
O24A	0.059(4)	0.013(3)	0.060(4)	-0.002(4)	0.030(3)	-0.003(3)
O24B	0.076(4)	0.021(4)	0.070(4)	0.008(4)	0.047(3)	0.001(4)
OW1	0.042(3)	0.023(4)	0.054(4)	-0.006(4)	0.007(3)	-0.005(4)
OW2	0.032(3)	0.022(4)	0.056(4)	0.005(3)	0.014(3)	0.002(4)
N	0.035(4)	0.023(5)	0.038(4)	-0.001(4)	0.004(3)	-0.003(4)
C1	0.035(4)	0.039(7)	0.031(4)	-0.005(5)	0.010(3)	0.003(5)
C2	0.028(4)	0.032(6)	0.034(4)	0.001(5)	0.007(3)	0.001(5)

Table of General Anisotropic Displacement Parameter Expressions - U's (Cont)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C3	0.030(4)	0.042(7)	0.042(5)	-0.001(5)	0.007(4)	-0.001(6)
C4	0.042(5)	0.07(1)	0.035(5)	-0.009(6)	0.019(4)	0.003(6)
C5	0.043(5)	0.042(7)	0.030(4)	-0.001(6)	0.012(4)	0.005(5)
C6	0.052(6)	0.047(8)	0.051(6)	0.000(7)	0.007(5)	0.012(6)
C7	0.050(6)	0.033(7)	0.082(8)	0.011(6)	0.012(6)	-0.003(7)
C8	0.036(4)	0.046(8)	0.071(6)	0.006(6)	0.024(4)	-0.005(7)
C9	0.043(5)	0.038(7)	0.043(5)	-0.005(6)	0.012(4)	0.000(6)
C10	0.096(8)	0.08(1)	0.031(5)	-0.02(1)	0.020(5)	-0.010(7)
C11	0.074(7)	0.026(6)	0.059(7)	0.007(7)	0.009(6)	-0.006(6)
C21	0.030(4)	0.018(5)	0.036(4)	-0.002(4)	0.013(3)	-0.000(5)
C22	0.035(4)	0.020(5)	0.035(4)	-0.000(5)	0.015(3)	0.004(5)
C23	0.033(4)	0.011(4)	0.035(4)	-0.002(4)	0.014(3)	-0.005(4)
C24	0.028(4)	0.017(5)	0.039(4)	-0.001(4)	0.010(3)	-0.004(5)

The form of the anisotropic displacement parameter is:
exp [-2PI2{h2a2U(1,1) + k2b2U(2,2) + l2c2U(3,3) + 2hkabU(1,2) + 2hlacU(1,3) + 2klbcU(2,3)}] where a,b, and c are reciprocal lattice constants.

Crystal data for compound **12**

Crystal data:

$C_{17}H_{23}NO_2$	Mr=273.38
$P2_1/c$	Mo(k_α) λ=0.71073 Å
a=8.877(2) Å	
b=13.600(3) Å	ß=98.23(1)°
c=12.837(10) Å	
V=1533.9(5) Å^3	
Z=4	D_c=1.183 g/cm^3

Data collection:

Nonius CAD-4 diffractometer
θ-2θ scans — θmax=30.0°
4909 measured reflections
4705 independent reflections
2927 observed reflections (I>3σ(I))

Structure solution and refinement:

The data were processed and refined using the MolEN software package (Fair, 1995). The structure was solved using the SIR program(Altomare et al. 1994) and refined by full-matrix least-squares techniques. All calculation were carried out on a AlphaServer 400 computer.

Refinement on F	$\Delta\rho_{max}$=0.19 e Å^{-3}
R = 0.057	$\Delta\rho_{min}$=-.10 e Å^{-3}
Rw = 0.076	$w=1/\sigma^2(F_o)$
	$(\Delta/\sigma)_{max}$=0.20
2927 reflections	181 parameters

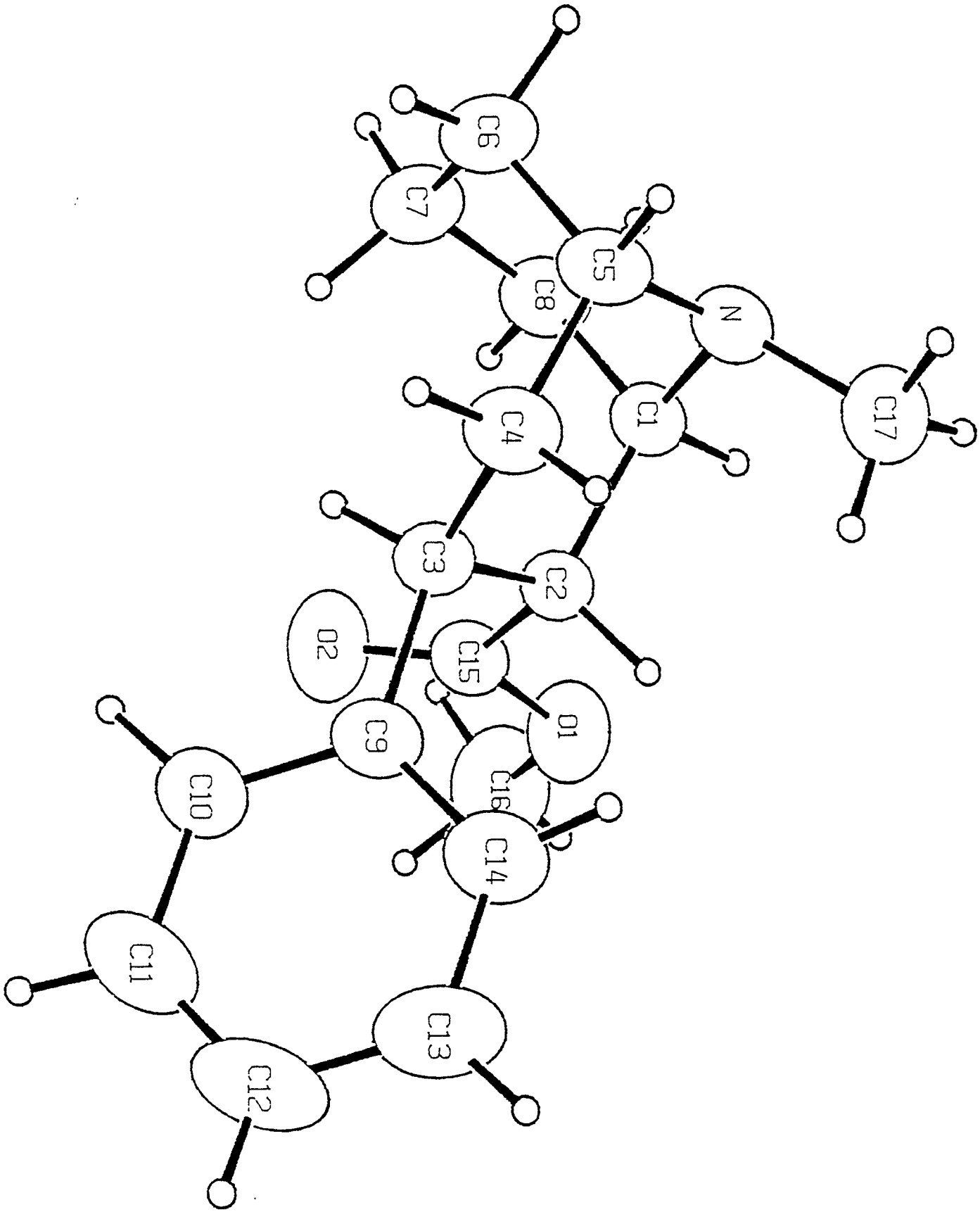
C6
C7
C5
C8
N
C17
C1
C4
C3
C2
O2
C15
O1
C9
C16
C10
C14
C11
C13
C12

Table of Bond Angles in Degrees

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C15	O1	C16	115.2(2)	C4	C5	C6	115.7(2)
C1	N	C5	109.5(1)	C5	C6	C7	114.1(2)
C1	N	C17	114.3(1)	C6	C7	C8	111.7(2)
C5	N	C17	114.1(2)	C1	C8	C7	112.9(2)
N	C1	C2	112.3(1)	C3	C9	C10	119.8(2)
N	C1	C8	108.3(1)	C3	C9	C14	121.9(2)
C2	C1	C8	114.7(1)	C10	C9	C14	118.3(2)
C1	C2	C3	114.3(1)	C9	C10	C11	119.9(2)
C1	C2	C15	109.3(1)	C10	C11	C12	121.3(2)
C3	C2	C15	110.7(1)	C11	C12	C13	118.8(2)
C2	C3	C4	111.3(1)	C12	C13	C14	121.0(2)
C2	C3	C9	111.1(1)	C9	C14	C13	120.7(2)
C4	C3	C9	111.9(1)	O1	C15	O2	122.7(2)
C3	C4	C5	114.3(2)	O1	C15	C2	111.4(1)
N	C5	C4	111.8(1)	O2	C15	C2	125.8(2)
N	C5	C6	107.6(2)				

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
O1	C15	1.337(2)	C3	C9	1.518(2)
O1	C16	1.447(3)	C4	C5	1.532(3)
O2	C15	1.196(2)	C5	C6	1.534(3)
N	C1	1.448(2)	C6	C7	1.512(3)
N	C5	1.476(3)	C7	C8	1.514(3)
N	C17	1.457(3)	C9	C10	1.391(3)
C1	C2	1.568(2)	C9	C14	1.380(3)
C1	C8	1.528(3)	C10	C11	1.393(3)
C2	C3	1.532(2)	C11	C12	1.359(4)
C2	C15	1.506(2)	C12	C13	1.371(3)
C3	C4	1.532(2)	C13	C14	1.382(3)

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Positional Parameters and Their Estimated Standard Deviations

Atom	x	y	z	B(A2)
O1	0.6923(1)	0.95786(9)	0.11439(9)	4.61(2)
O2	0.5484(1)	1.04030(8)	0.21300(9)	4.76(3)
N	0.7810(1)	0.77936(9)	0.39837(9)	3.49(2)
C1	0.7740(2)	0.8638(1)	0.3284(1)	3.11(3)
C2	0.6159(2)	0.8727(1)	0.2570(1)	2.82(2)
C3	0.4785(2)	0.8668(1)	0.3175(1)	2.94(2)
C4	0.5033(2)	0.7885(1)	0.4040(1)	3.64(3)
C5	0.6631(2)	0.7880(1)	0.4670(1)	3.70(3)
C6	0.7029(2)	0.8766(1)	0.5395(1)	4.26(3)
C7	0.7279(2)	0.9710(1)	0.4819(1)	4.17(3)
C8	0.8232(2)	0.9546(1)	0.3941(1)	3.99(3)
C9	0.3319(2)	0.8499(1)	0.2432(1)	3.19(3)
C10	0.2191(2)	0.9211(1)	0.2320(1)	3.72(3)
C11	0.0844(2)	0.9063(2)	0.1649(1)	4.81(4)
C12	0.0603(2)	0.8214(2)	0.1083(1)	5.35(4)
C13	0.1717(2)	0.7506(2)	0.1175(2)	5.72(4)
C14	0.3069(2)	0.7641(1)	0.1848(1)	4.70(4)
C15	0.6113(2)	0.9658(1)	0.1943(1)	3.11(2)
C16	0.7041(3)	1.0464(2)	0.0542(2)	6.47(5)
C17	0.7827(2)	0.6847(1)	0.3451(1)	4.90(4)

Table of Positional Parameters and Their Estimated Standard Deviations (cont.)

Atom	x	y	z	B(A2)
H1	0.842	0.847	0.280	2.5*
H2	0.610	0.814	0.205	3.6*
H3	0.470	0.930	0.349	3.3*
H4A	0.430	0.800	0.448	6.1*
H4B	0.484	0.723	0.377	4.5*
H5	0.670	0.735	0.512	6.7*
H6A	0.624	0.880	0.580	5.4*
H6B	0.806	0.857	0.589	5.7*
H7A	0.624	1.001	0.450	4.7*
H7B	0.772	1.025	0.522	6.6*
H8A	0.926	0.926	0.423	6.8*
H8B	0.822	1.020	0.347	5.6*
H10	0.237	0.989	0.273	4.5*
H11	0.012	0.954	0.162	6.8*
H12	-0.027	0.809	0.071	5.3*
H13	0.167	0.698	0.077	7.8*
H14	0.380	0.715	0.202	8.3*
H16A	0.741	1.033	0.004	8.9*
H16B	0.744	1.107	0.107	9.8*
H16C	0.591	1.073	0.028	8.8*

H17a	0.788	0.634	0.396	8.9*
H17b	0.693	0.679	0.296	9.4*
H17c	0.869	0.682	0.309	8.6*

Starred atoms were refined isotropically..
Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:
(4/3) * [a2*B(1,1) + b2*B(2,2) + c2*B(3,3) + ab(cos gamma)*B(1,2) + ac(cos beta)*B(1,3) + bc(cos alpha)*B(2,3)]

Table of General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
O1	0.0731(8)	0.0564(8)	0.0504(6)	0.0129(7)	0.0265(6)	0.0156(6)
O2	0.0751(8)	0.0418(7)	0.0683(8)	0.0130(7)	0.0241(7)	0.0111(6)
N	0.0456(7)	0.0441(8)	0.0392(7)	0.0075(6)	-0.0033(6)	0.0002(6)
C1	0.0358(7)	0.0450(9)	0.0345(7)	0.0028(7)	0.0010(6)	0.0005(7)
C2	0.0371(7)	0.0358(8)	0.0307(7)	0.0014(6)	0.0021(6)	0.0003(6)
C3	0.0376(7)	0.0391(8)	0.0322(7)	-0.0021(7)	0.0020(6)	-0.0009(6)
C4	0.0483(9)	0.0487(9)	0.0388(8)	-0.0056(8)	0.0051(7)	0.0072(8)
C5	0.056(1)	0.0494(9)	0.0316(7)	0.0013(9)	0.0002(7)	0.0075(7)
C6	0.061(1)	0.065(1)	0.0334(8)	0.003(1)	0.0001(8)	-0.0027(9)
C7	0.057(1)	0.052(1)	0.0435(9)	-0.0034(9)	-0.0051(8)	-0.0131(8)
C8	0.0470(9)	0.052(1)	0.0475(9)	-0.0087(8)	-0.0020(8)	-0.0021(8)
C9	0.0365(7)	0.0442(8)	0.0365(7)	-0.0049(7)	0.0015(6)	0.0038(7)
C10	0.0387(8)	0.059(1)	0.0432(9)	0.0017(8)	0.0079(7)	0.0038(8)
C11	0.0356(8)	0.088(1)	0.058(1)	0.002(1)	0.0035(8)	0.018(1)
C12	0.0441(9)	0.087(1)	0.061(1)	-0.021(1)	-0.0127(9)	0.017(1)
C13	0.077(1)	0.068(1)	0.068(1)	-0.024(1)	-0.017(1)	-0.011(1)
C14	0.055(1)	0.052(1)	0.061(1)	-0.0046(9)	-0.0090(9)	-0.0053(9)
C15	0.0386(7)	0.0424(8)	0.0371(7)	0.0001(7)	0.0023(6)	0.0042(7)
C16	0.108(2)	0.076(1)	0.070(1)	0.011(1)	0.043(1)	0.032(1)
C17	0.087(1)	0.045(1)	0.058(1)	0.017(1)	0.000(1)	-0.0027(9)

The form of the anisotropic displacement parameter is:
exp [-2PI2{h2a2U(1,1) + k2b2U(2,2) + 12c2U(3,3) + 2hkabU(1,2) + 2h1acU(1,3) + 2k1bcU(2,3)}] where a,b, and c are reciprocal lattice constants.

Crystal data for compound **14**

Crystal data:

$C_{22}H_{25}NO$	Mr=319.45
P-1	Mo(k_α) λ=0.71073 Å
a=8.5475(9) Å	α=87.305(1)°
b=13.3728(13) Å	ß=79.047(1)°
c=10.6080(10) Å	Γ=69.217(1)°
V=863.1(1) Å^3	
Z=2	D_c=1.229 g/cm^3

Data collection:

Nonius CAD-4 diffractometer
θ-2θ scans — θmax=30.0°
5333 measured reflections
5020 independent reflections
3956 observed reflections (I>3σ(I))

Structure solution and refinement:

The data were processed and refined using the MolEN software package (Fair, 1995). The structure was solved using the SIR program(Altomare et al. 1994) and refined by full-matrix least-squares technique. All calculation were carried out on a AlphaServer 400 computer.

Refinement on F	$\Delta\rho_{max}$=0.37 e Å^{-3}
R = 0.048	$\Delta\rho_{min}$=-.18 e Å^{-3}
Rw = 0.067	$w=1/\sigma^2(F_o)$
	$(\Delta/\sigma)_{max}$=0.05
3956 reflections	217 parameters

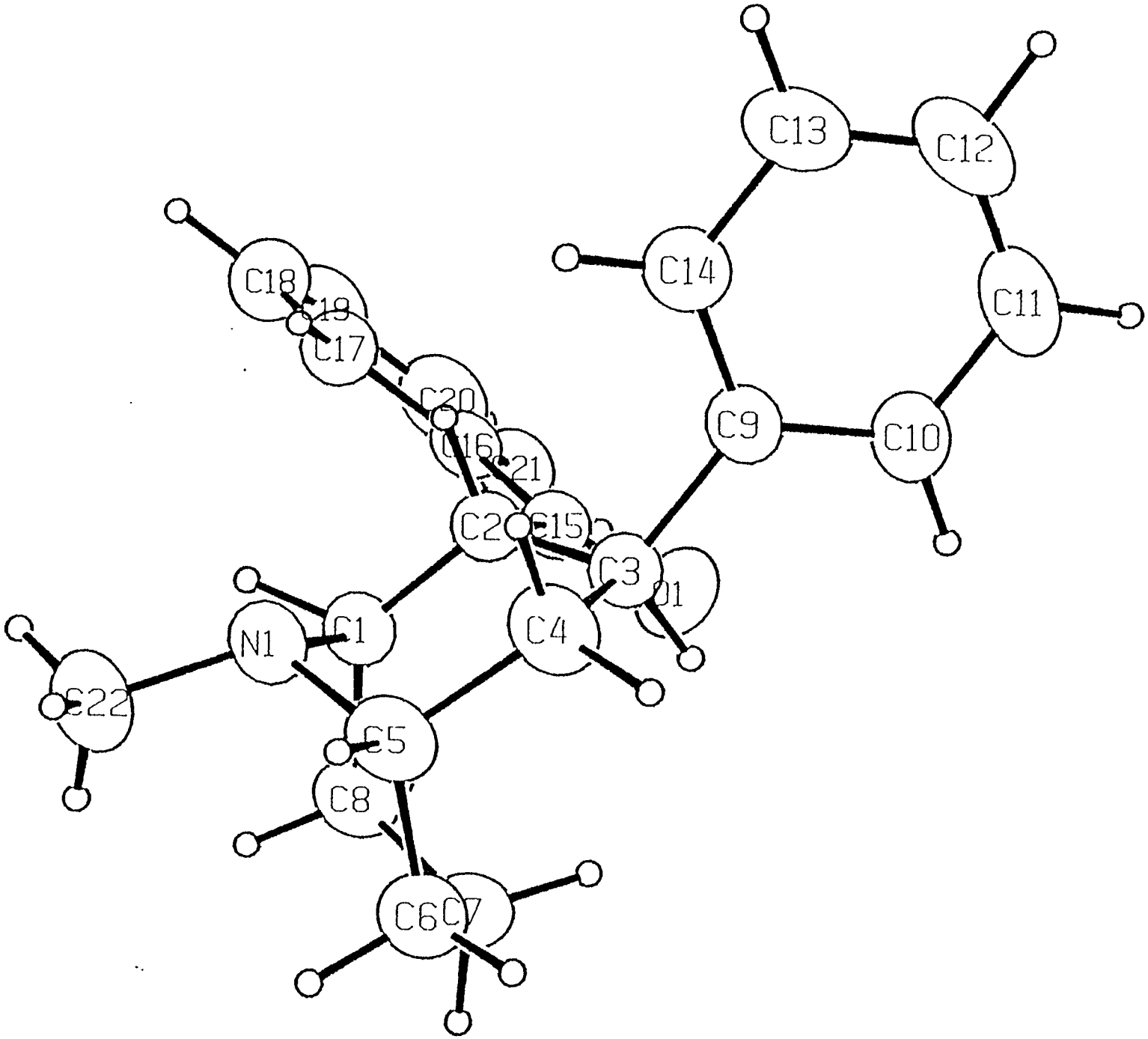
C13
C12
C14
C11
C18
C19
C17
C20
C9
C10
C16
C21
C2
C15
C3
O1
C1
C4
N1
C22
C5
C8
C6
C7

Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
O1	C15	1.215(1)	C9	C10	1.386(1)
N1	C1	1.465(1)	C9	C14	1.397(1)
N1	C5	1.474(1)	C10	C11	1.395(2)
N1	C22	1.455(1)	C11	C12	1.375(2)
C1	C2	1.557(1)	C12	C13	1.378(2)
C1	C8	1.536(1)	C13	C14	1.388(1)
C2	C3	1.547(1)	C15	C16	1.496(1)
C2	C15	1.525(1)	C16	C17	1.389(1)
C3	C4	1.539(2)	C16	C21	1.399(2)
C3	C9	1.520(1)	C17	C18	1.391(2)
C4	C5	1.528(1)	C18	C19	1.377(2)
C5	C6	1.538(2)	C19	C20	1.372(2)
C6	C7	1.520(2)	C20	C21	1.383(2)
C7	C8	1.521(2)			

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Bond Angles in Degrees

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C1	N1	C5	109.52(8)	C3	C9	C10	121.18(9)
C1	N1	C22	113.2(1)	C3	C9	C14	120.84(8)
C5	N1	C22	113.47(8)	C10	C9	C14	117.98(8)
N1	C1	C2	106.85(8)	C9	C10	C11	121.0(1)
N1	C1	C8	112.93(7)	C10	C11	C12	120.1(1)
C2	C1	C8	115.49(8)	C11	C12	C13	119.9(1)
C1	C2	C3	114.75(7)	C12	C13	C14	120.0(1)
C1	C2	C15	110.00(8)	C9	C14	C13	121.0(1)
C3	C2	C15	110.53(7)	O1	C15	C2	121.06(8)
C2	C3	C4	112.38(8)	O1	C15	C16	120.0(1)
C2	C3	C9	110.08(6)	C2	C15	C16	118.87(8)
C4	C3	C9	110.90(9)	C15	C16	C17	123.3(1)
C3	C4	C5	114.6(1)	C15	C16	C21	117.78(8)
N1	C5	C4	107.03(7)	C17	C16	C21	118.88(9)
N1	C5	C6	112.9(1)	C16	C17	C18	120.1(1)
C4	C5	C6	115.64(9)	C17	C18	C19	120.2(1)
C5	C6	C7	113.74(9)	C18	C19	C20	120.2(1)
C6	C7	C8	111.1(1)	C19	C20	C21	120.3(1)
C1	C8	C7	112.8(1)	C16	C21	C20	120.3(1)

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Positional Parameters and Their Estimated Standard Deviations

Atom	x	y	z	B(A2)
O1	-0.25912(9)	-0.29500(8)	0.25970(7)	3.95(2)
N1	-0.2670(1)	0.14163(8)	0.16576(8)	3.34(2)
C1	-0.3024(1)	0.0188(1)	0.13772(9)	2.94(2)
C2	-0.1674(1)	-0.10698(9)	0.18830(8)	2.56(2)
C3	-0.1516(1)	-0.09175(9)	0.32924(8)	2.78(2)
C4	-0.1728(1)	0.0566(1)	0.3642(1)	3.58(2)
C5	-0.3083(1)	0.1688(1)	0.3055(1)	3.57(2)
C6	-0.4941(2)	0.1867(1)	0.3639(1)	4.26(3)
C7	-0.5473(1)	0.0698(1)	0.3292(1)	4.03(2)
C8	-0.4889(1)	0.0327(1)	0.1867(1)	3.63(2)
C9	0.0174(1)	-0.19338(9)	0.35465(8)	2.89(2)
C10	0.0234(1)	-0.2967(1)	0.4433(1)	3.54(2)

Table of Positional Parameters and Their Estimated Standard Deviations (cont.)

Atom	x	y	z	B(A2)
C11	0.1789(2)	-0.3910(1)	0.4649(1)	4.59(3)
C12	0.3291(2)	-0.3828(1)	0.3974(1)	4.98(3)
C13	0.3260(1)	-0.2798(2)	0.3100(1)	4.70(3)
C14	0.1714(1)	-0.1854(1)	0.2890(1)	3.75(2)
C15	-0.2020(1)	-0.23856(9)	0.16919(8)	2.70(2)
C16	-0.1699(1)	-0.29519(9)	0.03588(9)	2.76(2)
C17	-0.0827(1)	-0.2489(1)	-0.0699(1)	3.22(2)
C18	-0.0546(2)	-0.3085(1)	-0.1907(1)	3.97(2)
C19	-0.1125(2)	-0.4138(1)	-0.2061(1)	4.27(2)
C20	-0.1984(1)	-0.4606(1)	-0.1023(1)	4.19(2)
C21	-0.2278(1)	-0.4023(1)	0.0185(1)	3.44(2)
C22	-0.3476(2)	0.2607(1)	0.0923(1)	4.72(3)

Table of Positional Parameters and Their Estimated Standard Deviations (cont.)

Atom	x	y	z	B(A2)
H1	-0.279(1)	0.008(1)	0.044(1)	3.0(2)*
H2	-0.058(1)	-0.112(1)	0.135(1)	2.7(2)*
H3	-0.240(1)	-0.116(1)	0.384(1)	3.0(2)*
H4A	-0.065(1)	0.071(1)	0.328(1)	3.7(2)*
H4B	-0.199(1)	0.066(1)	0.459(1)	3.8(3)*
H5	-0.293(2)	0.255(1)	0.321(1)	4.3(3)*
H6A	-0.569(2)	0.277(2)	0.329(1)	5.8(3)*
H6B	-0.509(1)	0.194(1)	0.456(1)	4.6(3)*
H7A	-0.670(2)	0.101(1)	0.349(1)	5.7(3)*
H7B	-0.494(1)	-0.017(1)	0.383(1)	3.8(3)*
H8A	-0.504(2)	-0.056(1)	0.168(1)	4.1(3)*
H8B	-0.556(2)	0.106(1)	0.138(1)	5.0(3)*

Table of Positional Parameters and Their Estimated Standard Deviations (cont.)

Atom	x	y	z	B(A2)
H10	-0.084(2)	-0.303(1)	0.490(1)	5.0(3)*
H11	0.175(2)	-0.463(1)	0.522(1)	5.5(3)*
H12	0.444(2)	-0.448(2)	0.413(2)	7.0(4)*
H13	0.428(2)	-0.272(1)	0.261(1)	5.3(3)*
H14	0.171(2)	-0.113(1)	0.227(1)	4.8(3)*
H17	-0.039(1)	-0.177(1)	-0.063(1)	4.4(3)*
H18	0.010(2)	-0.275(1)	-0.266(1)	4.6(3)*
H19	-0.090(2)	-0.459(1)	-0.288(1)	5.4(3)*
H20	-0.241(2)	-0.535(1)	-0.103(1)	6.2(4)*
H21	-0.289(1)	-0.433(1)	0.090(1)	4.2(3)*
H22A	-0.321(2)	0.340(2)	0.113(2)	8.4(4)*
H22B	-0.307(2)	0.237(2)	-0.001(2)	6.4(4)*

Table of Positional Parameters and Their Estimated Standard Deviations (cont.)

Atom	x	y	z	B(A2)
H22C	-0.468(2)	0.290(1)	0.111(1)	5.6(4)*

Starred atoms were refined isotropically.
Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:
(4/3) * [a2*B(1,1) + b2*B(2,2) + c2*B(3,3) + ab(cos gamma)*B(1,2) + ac(cos beta)*B(1,3) + bc(cos alpha)*B(2,3)]

Table of General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
O1	0.0614(3)	0.0563(3)	0.0416(3)	-0.0336(2)	-0.0068(3)	0.0024(3)
N1	0.0451(4)	0.0362(3)	0.0449(4)	-0.0119(3)	-0.0121(3)	0.0034(3)
C1	0.0378(4)	0.0400(4)	0.0336(4)	-0.0108(3)	-0.0117(3)	0.0010(3)
C2	0.0327(3)	0.0352(3)	0.0311(3)	-0.0120(2)	-0.0094(3)	-0.0015(3)
C3	0.0355(3)	0.0395(4)	0.0312(4)	-0.0115(3)	-0.0103(3)	-0.0018(3)
C4	0.0507(4)	0.0428(4)	0.0445(4)	-0.0126(3)	-0.0186(3)	-0.0077(4)
C5	0.0499(4)	0.0360(4)	0.0485(5)	-0.0104(3)	-0.0137(4)	-0.0058(4)
C6	0.0508(5)	0.0526(6)	0.0473(5)	-0.0049(5)	-0.0065(4)	-0.0087(5)
C7	0.0367(4)	0.0594(6)	0.0510(5)	-0.0106(4)	-0.0055(4)	0.0007(5)
C8	0.0365(4)	0.0511(5)	0.0507(5)	-0.0118(3)	-0.0166(3)	0.0016(4)
C9	0.0392(3)	0.0403(4)	0.0323(4)	-0.0122(3)	-0.0136(3)	-0.0039(3)
C10	0.0542(5)	0.0441(4)	0.0382(4)	-0.0162(3)	-0.0152(3)	0.0002(4)

Table of General Anisotropic Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C11	0.0755(6)	0.0463(5)	0.0511(5)	-0.0097(5)	-0.0317(4)	0.0024(4)
C12	0.0543(5)	0.0634(7)	0.0636(6)	0.0015(5)	-0.0323(4)	-0.0113(5)
C13	0.0380(4)	0.0763(7)	0.0621(6)	-0.0125(4)	-0.0166(4)	-0.0092(6)
C14	0.0408(4)	0.0585(5)	0.0455(5)	-0.0173(4)	-0.0139(3)	0.0019(4)
C15	0.0315(3)	0.0377(4)	0.0354(4)	-0.0124(3)	-0.0103(3)	-0.0010(3)
C16	0.0331(3)	0.0341(4)	0.0382(4)	-0.0089(3)	-0.0132(3)	-0.0021(3)
C17	0.0441(4)	0.0407(4)	0.0389(4)	-0.0146(3)	-0.0104(3)	-0.0036(4)
C18	0.0568(5)	0.0526(5)	0.0382(4)	-0.0140(4)	-0.0096(4)	-0.0060(4)
C19	0.0629(5)	0.0494(5)	0.0471(5)	-0.0087(4)	-0.0213(4)	-0.0134(4)
C20	0.0611(5)	0.0413(4)	0.0640(5)	-0.0174(3)	-0.0269(4)	-0.0097(4)
C21	0.0443(4)	0.0391(4)	0.0516(5)	-0.0156(3)	-0.0166(3)	-0.0023(4)
C22	0.0670(6)	0.0436(5)	0.0647(7)	-0.0128(5)	-0.0190(5)	0.0135(5)

The form of the anisotropic displacement parameter is:
exp [-2PI2{h2a2U(1,1) + k2b2U(2,2) + l2c2U(3,3) + 2hkabU(1,2) + 2hlacU(1,3) + 2klbcU(2,3)}] where a,b, and c are reciprocal lattice constants.