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Table . Atomic Parameters x,y,z and Beq.
E.S.Ds. refer to the last digit printed.

	x	y	z	Beq
O1	0.8837 (6)	0.6441 (6)	0.3907 (6)	6.9(4)
O2	0.9546 (7)	0.5470 (6)	0.2810 (6)	6.9(5)
O3	0.5965 (7)	0.2886 (6)	0.3693 (6)	6.4(4)
O4	0.5135 (8)	0.5804 (6)	0.1308 (6)	7.7(6)
N	0.5789 (7)	0.4341 (6)	0.2369 (6)	4.9(4)
C1	0.8477 (9)	0.5195 (8)	0.3225 (8)	5.7(6)
C2	0.6893 (10)	0.4488 (8)	0.1987 (8)	5.4(6)
C3	0.6472 (11)	0.3140 (9)	0.1244 (8)	6.6(7)
C4	1.0048 (9)	0.7526 (8)	0.3800 (8)	5.0(6)
C5	1.0809 (9)	0.6809 (8)	0.3565 (8)	5.3(5)
C6	0.5405 (9)	0.3559 (8)	0.3209 (8)	5.3(5)
C7	0.4265 (9)	0.3746 (8)	0.3309 (8)	5.5(5)
C8	0.3528 (10)	0.3208 (9)	0.4016 (9)	6.6(7)
C9	0.2488 (12)	0.3576 (11)	0.3918 (11)	8.2(9)
C10	0.2223 (12)	0.4453 (11)	0.3209 (11)	8.3(9)
C11	0.2978 (11)	0.5013 (10)	0.2519 (10)	7.3(8)
C12	0.4013 (9)	0.4632 (8)	0.2591 (8)	5.6(5)
C13	0.4987 (10)	0.5052 (8)	0.1986 (8)	5.5(6)
C14	1.1015 (8)	0.8659 (8)	0.5027 (7)	4.7(5)
C15	1.1535 (10)	0.9993 (9)	0.4991 (8)	6.1(7)
C16	1.2406 (11)	1.1026 (9)	0.6120 (10)	7.0(7)
C17	1.2783 (11)	1.0794 (10)	0.7335 (9)	7.2(7)
C18	1.2276 (12)	0.9482 (11)	0.7397 (8)	7.5(8)
C19	1.1402 (11)	0.8426 (9)	0.6274 (8)	6.3(7)
C20	1.1570 (9)	0.7386 (8)	0.2771 (8)	5.3(6)
C21	1.0826 (10)	0.6933 (10)	0.1409 (9)	6.9(7)
C22	1.1582 (12)	0.7510 (12)	0.0724 (10)	8.4(9)
C23	1.3079 (13)	0.8509 (13)	0.1402 (11)	9.1(9)
C24	1.3811 (12)	0.8970 (12)	0.2732 (11)	9.0(9)
C25	1.3093 (10)	0.8386 (10)	0.3435 (9)	7.3(7)
C26	0	0	0	26.5(16)
C11	0.0606 (10)	0.0586 (8)	0.1359 (5)	14.2(8)
C12	0.1834 (12)	0.1465 (12)	-0.0023 (11)	18.2(11)
H1	0.861	0.466	0.383	6.3
H2	0.700	0.514	0.149	6.1
H3a	0.548	0.265	0.046	7.1
H3b	0.713	0.331	0.088	7.1
H3c	0.634	0.243	0.165	7.1
H4	0.963	0.780	0.302	5.8
H5	1.149	0.692	0.447	5.9
H8	0.380	0.267	0.459	7.2
H9	0.209	0.341	0.452	8.7
H10	0.156	0.474	0.322	9.3
H11	0.287	0.562	0.199	8.1
H15	1.129	1.008	0.412	6.6
H16	1.274	1.194	0.612	7.6
H17	1.341	1.154	0.811	7.1
H18	1.246	0.937	0.826	8.1
H19	1.099	0.751	0.629	7.1
H21	0.981	0.615	0.094	7.6
H22	1.097	0.707	-0.022	9.1
H23	1.358	0.888	0.093	10.5
H24	1.488	0.963	0.326	9.1
H25	1.363	0.887	0.435	7.5

Beq is the Mean of the Principal Axes of the Thermal Ellipsoid

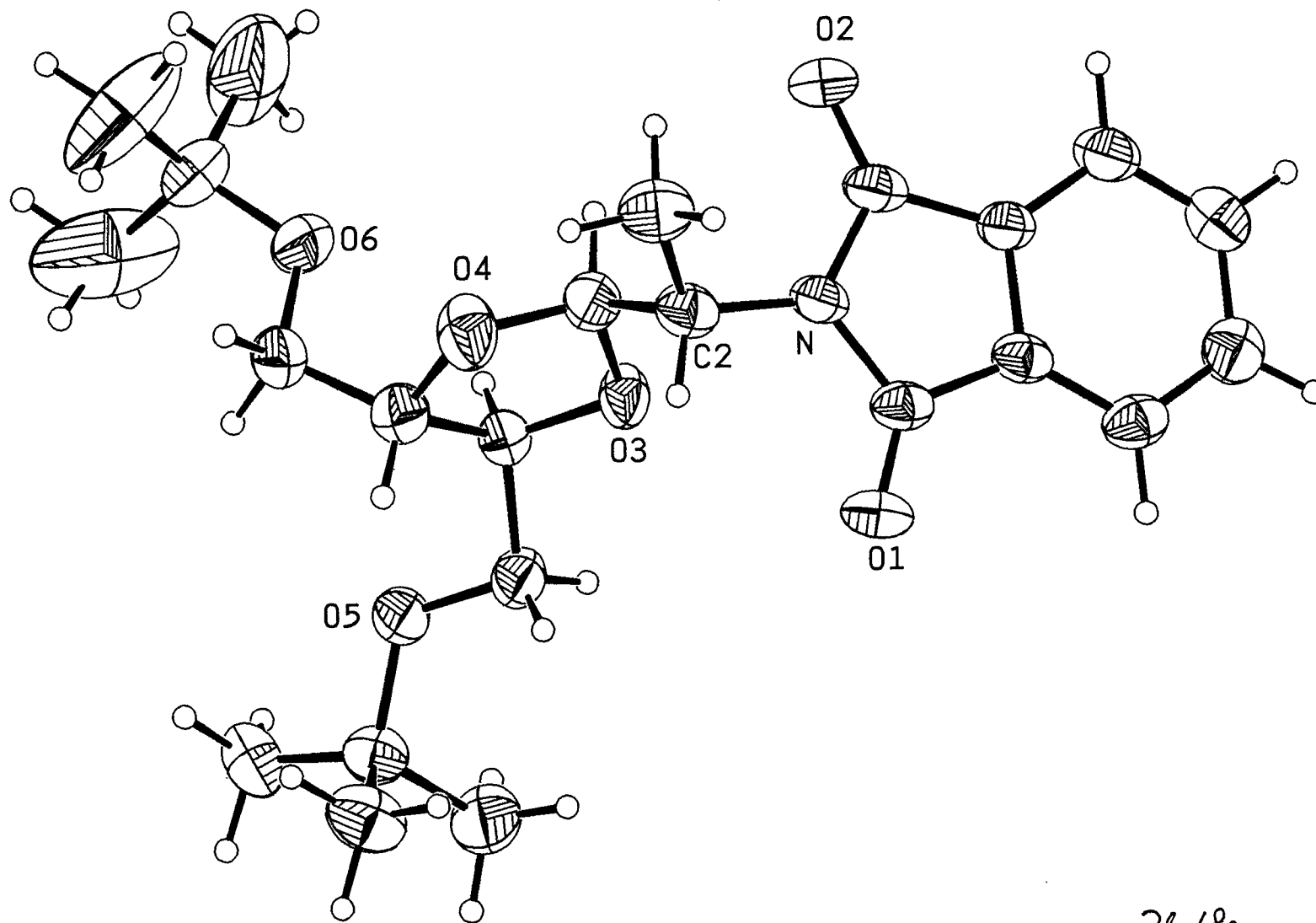
Table of $u(i,j)$ or U values *100.
E.S.Ds. refer to the last digit printed

	u11(U)	u22	u33	u12	u13	u23
O1	6.8(4)	7.2(4)	10.4(5)	1.6(3)	5.3(4)	-0.4(3)
O2	8.0(4)	6.8(4)	10.7(5)	2.5(3)	5.7(4)	0.5(3)
O3	8.2(4)	8.6(4)	9.5(4)	5.6(4)	4.5(4)	5.0(4)
O4	14.0(6)	9.4(5)	7.9(4)	7.8(5)	5.2(4)	4.7(4)
N	6.1(4)	6.4(4)	5.6(4)	3.2(3)	2.5(3)	2.0(3)
C1	6.7(5)	6.6(5)	7.5(6)	2.6(4)	3.9(5)	1.3(4)
C2	7.6(6)	6.6(5)	5.8(5)	3.3(5)	3.3(4)	2.2(4)
C3	9.2(7)	8.0(6)	6.4(5)	4.3(6)	3.1(5)	0.7(5)
C4	5.7(5)	7.0(5)	6.1(5)	3.1(4)	3.0(4)	1.4(4)
C5	6.0(5)	6.3(5)	6.7(5)	2.8(4)	2.8(4)	1.3(4)
C6	5.3(5)	6.5(5)	6.4(5)	2.3(4)	2.4(4)	1.7(4)
C7	5.3(5)	6.5(5)	7.3(5)	2.8(4)	2.1(4)	1.1(4)
C8	7.5(6)	8.5(6)	9.0(7)	3.5(5)	4.8(5)	2.6(5)
C9	8.4(7)	11.1(8)	11.3(8)	4.2(6)	5.7(7)	1.3(7)
C10	8.9(7)	11.8(9)	11.6(8)	6.7(7)	4.3(7)	1.2(7)
C11	9.8(7)	9.6(7)	8.8(7)	6.7(6)	3.3(6)	1.9(6)
C12	6.1(5)	6.8(5)	6.5(5)	3.6(5)	1.6(4)	0.9(4)
C13	8.1(6)	6.1(5)	5.3(5)	4.1(5)	1.8(4)	1.2(4)
C14	5.5(5)	6.7(5)	5.4(4)	3.0(4)	2.6(4)	1.2(4)
C15	8.2(6)	7.3(6)	6.6(5)	3.3(5)	3.7(5)	2.1(4)
C16	10.2(7)	6.4(6)	9.0(7)	3.2(5)	5.2(6)	1.3(5)
C17	8.2(7)	8.0(6)	7.7(6)	2.9(5)	2.7(5)	-0.5(5)
C18	10.6(8)	11.6(8)	5.3(5)	6.0(7)	3.2(5)	1.9(5)
C19	9.7(7)	8.0(6)	6.4(5)	4.7(6)	3.9(5)	2.4(5)
C20	6.0(5)	8.3(6)	6.1(5)	3.9(5)	3.0(4)	1.5(4)
C21	7.6(6)	11.3(8)	6.7(6)	4.4(6)	3.7(5)	1.6(5)
C22	9.8(8)	14.8(10)	6.9(6)	6.1(7)	4.2(6)	2.5(6)
C23	11.7(9)	14.7(10)	9.2(7)	5.3(8)	7.5(7)	3.6(7)
C24	8.4(7)	12.9(9)	10.2(8)	1.9(7)	6.2(7)	0.9(7)
C25	6.9(6)	11.0(8)	7.4(6)	2.6(6)	4.0(5)	0.9(5)
C26	33.5 (20)					
C11	21.9(8)	16.5(7)	5.1(3)	5.1(6)	4.0(4)	-0.5(4)
C12	19.2(10)	24.2(12)	18.9(9)	9.4(9)	6.6(8)	-2.4(8)
H1	8.0					
H2	7.7					
H3a	9.0					
H3b	9.0					
H3c	9.0					
H4	7.3					
H5	7.4					
H8	9.2					
H9	11.0					
H10	11.8					
H11	10.3					
H15	8.4					
H16	9.6					
H17	9.0					
H18	10.2					
H19	9.0					
H21	9.7					
H22	11.6					
H23	13.3					
H24	11.6					
H25	9.5					

Anisotropic Temperature Factors are of the form

Temp= $-2\pi^2(h^2u_{11}^2\sigma_{11}^2 + 2hku_{12}\sigma_{11}\sigma_{12} + k^2u_{22}^2\sigma_{22}^2)$

IC4830



23-18a

Table. Crystal Data and Conditions for Crystallographic
Data Collection and Structure Refinement (25-18a)

TITLE	*** IC4830 ***
Formula	C23 H33 N O6
Formular wt	419.51
Diffractionmeter used	Nonius
Space Group	Monoclinic P 21
a (angstrom)	8.9173(21)
b (angstrom)	11.2624(18)
c (angstrom)	11.8842(23)
beta (deg.)	98.087(17)
V (A**3)	1181.7(4)
Z	2
Dcalc. (g.cm**-3)	1.179
lambda (Angstrom)	1.5418
F(000)	453.
Unit cell detn: #;(2theta range)	25;(40.76 - 75.26 deg.)
Scan type	theta/2theta
Scan width (deg.)	2(0.75+0.15tan(theta))
Scan Speed (deg./min)	2.06-8.24
(2Theta)max.	150.0
h k l ranges	(-11; 11)(0; 14)(0; 14)
mu (cm**-1)	6.569
Crystal size (mm)	0.40 X 0.50 X 0.60
Temperature (K)	298.
# of meas. reflns.	2367
# of obsd relfns. (I>2.0sig(I))	2108
# of unique reflns.	2367
Rf;Rw	0.068;0.062
GoF	4.10
Refinement program	NRCVAX
# of atoms	63
# of refined params.	271 (2108 out of 2367 reflns.)
Minimize function	Sum(w Fo-Fc **2)
Unit weights were used	
g (2nd. ext. coeff.) x 10E4	0.231(7)
(delta/sigma)max.	0.0073
Residual in final D-map (e/A**3)	-0.310; 0.210

NOTE :

$R_f = \text{Sum}(F_o - F_c) / \text{Sum}(F_o)$
 $R_w = \text{Sqrt}[\text{Sum}(w(F_o - F_c)^2) / \text{Sum}(wF_o^2)]$
 $\text{GoF} = \text{Sqrt}[\text{Sum}(w(F_o - F_c)^2) / (\text{No. of reflns} - \text{No. of params.})]$
 3 standard reflections (4,0,0 ; 0,6,0 ; 0,0,6) monitored every
 3600 seconds, intensity variation < 3%.

Table : Bond Distances and Bond Angles of IC4830 2S7Pa

O1-C4	1.218(6)	C5-C6	1.367(9)
O2-C11	1.213(7)	C5-C10	1.390(7)
O3-C3	1.423(7)	C6-C7	1.371(10)
O3-C12	1.444(7)	C7-C8	1.384(9)
O4-C3	1.402(8)	C8-C9	1.372(11)
O4-C18	1.422(7)	C9-C10	1.376(10)
O5-C13	1.389(7)	C10-C11	1.480(10)
O5-C14	1.446(7)	C12-C13	1.500(8)
O6-C19	1.415(8)	C12-C18	1.549(9)
O6-C20	1.406(8)	C14-C15	1.490(10)
N-C2	1.461(9)	C14-C16	1.494(9)
N-C4	1.389(7)	C14-C17	1.539(10)
N-C11	1.390(7)	C18-C19	1.473(10)
C1-C2	1.528(9)	C20-C21	1.459(15)
C2-C3	1.523(8)	C20-C22	1.512(14)
C4-C5	1.489(9)	C20-C23	1.446(16)

C3-O3-C12	105.8(4)	C9-C10-C11	131.8(5)
C3-O4-C18	111.1(5)	O2-C11-N	125.2(7)
C13-O5-C14	118.1(4)	O2-C11-C10	128.0(6)
C19-O6-C20	118.1(6)	N-C11-C10	106.8(5)
C2-N-C4	122.2(5)	O3-C12-C13	107.8(5)
C2-N-C11	126.4(5)	O3-C12-C18	105.0(4)
C4-N-C11	111.3(5)	C13-C12-C18	114.2(5)
N-C2-C1	113.4(5)	O5-C13-C12	107.2(5)
N-C2-C3	110.2(5)	O5-C14-C15	103.8(5)
C1-C2-C3	110.9(5)	O5-C14-C16	110.7(5)
O3-C3-O4	107.0(4)	O5-C14-C17	109.5(5)
O3-C3-C2	108.7(5)	C15-C14-C16	112.9(6)
O4-C3-C2	110.0(5)	C15-C14-C17	110.1(5)
O1-C4-N	124.5(6)	C16-C14-C17	109.8(6)
O1-C4-C5	129.1(5)	O4-C18-C12	103.0(5)
N-C4-C5	106.4(4)	O4-C18-C19	113.8(5)
C4-C5-C6	131.0(5)	C12-C18-C19	114.2(5)
C4-C5-C10	107.7(5)	O6-C19-C18	111.1(6)
C6-C5-C10	121.4(6)	O6-C20-C21	105.7(8)
C5-C6-C7	118.2(5)	O6-C20-C22	109.7(7)
C6-C7-C8	120.5(7)	O6-C20-C23	112.7(7)
C7-C8-C9	121.5(7)	C21-C20-C22	110.6(10)
C8-C9-C10	117.8(5)	C21-C20-C23	110.5(11)
C5-C10-C9	120.4(6)	C22-C20-C23	107.5(12)
C5-C10-C11	107.8(5)		

Table . Atomic Parameters x,y,z and Beq.
E.S.Ds. refer to the last digit printed.

	x	y	z	Beq
O1	0.9410(5)	0.40186	0.0449(3)	5.96(22)
O2	0.9991(5)	0.4132 (5)	0.4327(3)	6.53(24)
O3	1.2313(5)	0.5582 (4)	0.2115(4)	5.37(19)
O4	1.1318(5)	0.7376 (4)	0.2471(4)	6.88(24)
O5	1.5226(4)	0.7039 (4)	0.0842(3)	5.15(18)
O6	1.4147(7)	0.8111 (5)	0.3852(4)	7.8 (3)
N	0.9666(5)	0.4387 (5)	0.2377(4)	4.61(21)
C1	0.8485(8)	0.6280 (8)	0.2911(6)	6.7 (4)
C2	0.9675(7)	0.5682 (6)	0.2294(5)	5.1 (3)
C3	1.1251(7)	0.6161 (6)	0.2716(5)	5.2 (3)
C4	0.9577(6)	0.3661 (6)	0.1426(4)	4.7 (3)
C5	0.9685(5)	0.2416 (6)	0.1854(4)	4.36(24)
C6	0.9685(6)	0.1360 (7)	0.1288(4)	5.2 (3)
C7	0.9758(7)	0.0331 (7)	0.1911(6)	6.0 (3)
C8	0.9882(8)	0.0371 (7)	0.3084(6)	6.4 (3)
C9	0.9867(7)	0.1428 (7)	0.3657(5)	6.0 (3)
C10	0.9814(6)	0.2460 (6)	0.3033(4)	4.46(24)
C11	0.9828(6)	0.3724 (6)	0.3373(4)	5.1 (3)
C12	1.3484(6)	0.6446 (6)	0.2015(4)	4.58(24)
C13	1.4091(7)	0.6210 (6)	0.0922(5)	5.4 (3)
C14	1.5702(6)	0.7229 (6)	-0.0257(5)	5.2 (3)
C15	1.7011(8)	0.8057 (7)	-0.0013(7)	6.6 (4)
C16	1.4436(8)	0.7732 (8)	-0.1076(6)	7.5 (4)
C17	1.6227(9)	0.6044 (7)	-0.0715(7)	7.7 (4)
C18	1.2697(7)	0.7667 (6)	0.2063(5)	5.6 (3)
C19	1.3611(8)	0.8561 (6)	0.2757(6)	6.0 (3)
C20	1.4953(9)	0.8884 (7)	0.4648(6)	7.0 (4)
C21	1.5474(22)	0.8157 (13)	0.5642(10)	21.3 (14)
C22	1.3917(14)	0.9861 (14)	0.4949(12)	17.2 (10)
C23	1.6223(12)	0.9442 (21)	0.4224(10)	20.0 (16)
H1a	0.752	0.601	0.263	7.9
H1b	0.872	0.617	0.370	7.9
H1c	0.852	0.714	0.276	7.9
H2	0.946	0.589	0.151	5.9
H3	1.149	0.602	0.353	6.2
H6	0.962	0.133	0.048	6.1
H7	0.970	-0.042	0.153	6.9
H8	0.996	-0.035	0.351	7.3
H9	0.992	0.145	0.446	6.7
H12	1.426	0.639	0.265	5.3
H13a	1.333	0.623	0.031	6.3
H13b	1.454	0.541	0.097	6.3
H15a	1.740	0.826	-0.071	7.2
H15b	1.669	0.879	0.030	7.2
H15c	1.778	0.772	0.050	7.2
H16a	1.476	0.792	-0.179	8.6
H16b	1.359	0.727	-0.115	8.6
H16c	1.415	0.853	-0.077	8.6
H17a	1.656	0.614	-0.144	8.8
H17b	1.706	0.572	-0.020	8.8
H17c	1.543	0.548	-0.078	8.8
H18	1.247	0.795	0.129	6.4
H19a	1.299	0.926	0.282	7.0
H19b	1.443	0.881	0.237	7.0
H21a	1.611	0.861	0.618	20.5
H21b	1.472	0.777	0.590	20.5

H21c	1.618	0.755	0.536	20.5
H22a	1.446	1.042	0.549	17.5
H22b	1.353	1.032	0.429	17.5
H22c	1.309	0.956	0.528	17.5
H23a	1.670	1.007	0.480	16.3
H23b	1.694	0.902	0.400	16.3
H23c	1.581	1.002	0.358	16.3

Beq is the Mean of the Principal Axes of the Thermal Ellipsoid

Table of u(i,j) or U values *100.
E.S.Ds. refer to the last digit printed

	u11(U)	u22	u33	u12	u13	u23
O1	8.6 (3)	9.9 (3)	4.31(19)	0.4 (3)	1.48(19)	1.07(23)
O2	11.1 (3)	9.5 (3)	4.47(20)	-0.8 (3)	1.95(22)	-0.62(24)
O3	6.76(25)	5.04(22)	9.2 (3)	-0.46(21)	3.29(22)	-1.08(23)
O4	8.7 (3)	5.6 (3)	12.7 (4)	0.7 (3)	4.4 (3)	-0.8 (3)
O5	6.48(22)	6.6 (3)	6.87(23)	-1.05(22)	2.25(19)	-0.55(21)
O6	16.8 (5)	7.1 (3)	5.5 (3)	-1.2 (3)	0.8 (3)	-0.57(25)
N	6.2 (3)	7.0 (3)	4.48(22)	-0.7 (3)	1.31(20)	0.68(24)
C1	7.2 (4)	10.6 (6)	8.1 (4)	1.3 (5)	2.6 (3)	-0.5 (5)
C2	5.6 (3)	7.9 (4)	5.9 (3)	-0.2 (3)	1.4 (3)	0.4 (3)
C3	6.1 (3)	6.9 (4)	7.0 (4)	-0.5 (3)	1.8 (3)	-0.5 (3)
C4	5.0 (3)	8.4 (4)	4.9 (3)	-0.2 (3)	1.50(23)	-0.2 (3)
C5	4.3 (3)	7.5 (4)	4.9 (3)	-0.4 (3)	1.10(21)	0.4 (3)
C6	5.3 (3)	9.0 (5)	5.7 (3)	-0.1 (4)	1.21(25)	-1.1 (4)
C7	6.6 (4)	7.8 (5)	8.5 (4)	-0.3 (4)	1.6 (3)	-0.5 (4)
C8	8.2 (5)	8.3 (5)	8.2 (4)	-0.5 (4)	2.2 (4)	1.2 (4)
C9	8.3 (4)	8.9 (5)	5.8 (3)	-0.9 (4)	1.9 (3)	0.8 (4)
C10	5.6 (3)	7.0 (4)	4.5 (3)	-0.7 (3)	1.10(23)	0.0 (3)
C11	5.9 (3)	9.2 (5)	4.5 (3)	-1.0 (4)	1.34(24)	0.5 (3)
C12	6.3 (3)	5.2 (3)	6.0 (3)	-0.4 (3)	1.28(25)	0.1 (3)
C13	6.9 (4)	6.1 (4)	7.7 (4)	-1.0 (3)	2.4 (3)	-1.6 (3)
C14	5.3 (3)	7.7 (4)	7.0 (4)	0.9 (3)	2.0 (3)	0.1 (3)
C15	7.6 (4)	6.8 (4)	11.3 (6)	0.2 (4)	2.9 (4)	1.7 (4)
C16	7.2 (4)	12.9 (8)	8.5 (5)	-0.2 (5)	1.0 (4)	2.1 (5)
C17	10.5 (6)	8.7 (6)	11.1 (6)	0.3 (5)	5.4 (5)	-2.1 (5)
C18	7.3 (4)	6.8 (4)	7.2 (4)	-0.9 (4)	1.6 (3)	-0.5 (3)
C19	9.8 (5)	5.6 (4)	7.7 (4)	-0.4 (4)	2.6 (4)	-0.1 (3)
C20	9.9 (5)	8.7 (5)	8.0 (5)	0.1 (5)	1.0 (4)	-2.9 (4)
C21	50.3 (27)	14.1 (11)	12.1 (10)	-8.0 (16)	-11.3 (13)	1.7 (9)
C22	15.1 (10)	25.0 (17)	23.9 (14)	5.5 (11)	-2.4 (10)	-16.8 (13)
C23	9.8 (7)	51.9 (34)	13.7 (9)	-7.2 (14)	0.2 (7)	-7.2 (16)
H1a	10.0					
H1b	10.0					
H1c	10.0					
H2	7.4					
H3	7.8					
H6	7.7					
H7	8.7					
H8	9.3					
H9	8.5					
H12	6.7					
H13a	7.9					
H13b	7.9					
H15a	9.1					
H15b	9.1					
H15c	9.1					
H16a	10.9					
H16b	10.9					
H16c	10.9					
H17a	11.1					
H17b	11.1					
H17c	11.1					
H18	8.1					
H19a	8.8					
H19b	8.8					
H21a	25.9					

H21b	25.9
H21c	25.9
H22a	22.2
H22b	22.2
H22c	22.2
H23a	20.6
H23b	20.6
H23c	20.6

Anisotropic Temperature Factors are of the form

Temp= $-2\pi^2(h^2u_{11}^2 + k^2u_{22}^2 + 2hku_{12})$