THE JOURNAL OF PHYSICAL CHEMISTRY B
J. Phys. Chem. B, 1998, 102(36), 6975-6985, DOI:10.1021/jp9818380

P A R S T

IMPLEMENTED ON THE CRAY-2 IN STUTTGART

BY

TH. HILDENBRAND

SOME HINTS FOR HUGE STRUCTURES

BY H. W. POEHLMANN

(TEL. 4334/5)

```
1S422RM
 P bca
0CRYSTAL DATA
 A = 11.3102(0.0034)                          ALPHA=  90.00(0.00)
 B = 10.7439(0.0033)                          BETA =  90.00(0.00)
 C = 39.7299(0.0129)                          GAMMA=  90.00(0.00)
 V =  4827.80( 2.60)  CUBIC-ANGSTROM

0NIGGLI REDUCED CELL:  10.744 11.310 39.730  90.00  90.00  90.00
 NIGGLI MATRIX:       115.4314    127.9206   1578.4650
                        0.0000      0.0000      0.0000
 TRANSFORMATION MATRIX:     0.00    1.00    0.00
                            1.00    0.00    0.00
                            0.00    0.00   -1.00

 N   3. C  28. O   2. H  29.
 M       =   439.556          (ATOMIC WEIGHTS 1977)
 Z       =    8.00
 D(CALC.)=     1.2095         G/CM**3
 F(000)  =  1872.0
 MU      =     0.717          CM**-1 (INT.TAB.VOL.IV,P.55)
 LAMBDA  =     0.7106900      ANGSTROM
0NUMBER OF ATOMS:   62

0ATOMIC COORDINATES
 ATOM            X/A                 Y/B                 Z/C
 N1         0.39056(   31)      0.17508(   31)      0.62823(    8)
 C2         0.39962(   40)      0.24320(   41)      0.65589(   10)
 N3         0.41606(   35)      0.36599(   35)      0.65721(    8)
 C4         0.42340(   35)      0.42065(   38)      0.62739(   10)
 N5         0.41515(   31)      0.36349(   32)      0.59750(    8)
 C6         0.39844(   37)      0.23985(   41)      0.59929(    9)
 C7         0.38206(   37)      0.16778(   38)      0.56797(    9)
 C8         0.42096(   35)      0.20425(   38)      0.53572(   10)
 O8         0.48740(   26)      0.31012(   27)      0.53356(    7)
 C81        0.54158(   55)      0.33861(   52)      0.50203(   12)
 C9         0.39294(   39)      0.13411(   40)      0.50754(   10)
 C10        0.32967(   37)      0.02480(   38)      0.51092(   10)
 O10        0.29591(   27)     -0.04991(   27)      0.48496(    7)
 C11        0.29383(   40)     -0.01565(   44)      0.54243(   11)
 C12        0.32077(   37)      0.05568(   42)      0.56999(   10)
 C13        0.39044(   41)      0.17738(   46)      0.68893(   10)
 C14        0.34515(   51)      0.05804(   52)      0.69115(   13)
 C15        0.33755(   68)     -0.00210(   61)      0.72172(   15)
 C16        0.37813(   71)      0.05569(   69)      0.75026(   15)
 C17        0.42294(   70)      0.17374(   68)      0.74891(   14)
 C18        0.42872(   56)      0.23484(   60)      0.71825(   12)
 C19        0.43691(   36)      0.55788(   41)      0.62681(   10)
 C20        0.43534(   48)      0.62721(   47)      0.65635(   12)
 C21        0.43910(   50)      0.75431(   51)      0.65571(   14)
 C22        0.44888(   46)      0.81694(   50)      0.62510(   14)
 C23        0.45232(   48)      0.75027(   50)      0.59586(   13)
 C24        0.44751(   44)      0.62206(   45)      0.59636(   11)
```

C25	0.32232(47)	-0.01246(48)	0.45082(10)
C26	0.28297(52)	-0.11882(49)	0.42876(11)
C27	0.29589(54)	-0.09186(51)	0.39154(12)
C28	0.27680(51)	-0.20904(51)	0.37042(12)
C29	0.27959(65)	-0.18701(66)	0.33288(13)
C30	0.27061(89)	-0.31044(94)	0.31389(19)
H81	0.58678(359)	0.41538(403)	0.50369(95)
H82	0.59033(398)	0.25638(465)	0.49663(112)
H83	0.47595(421)	0.35758(420)	0.48580(118)
H9	0.41453(306)	0.16114(325)	0.48558(90)
H11	0.25180(372)	-0.09563(395)	0.54313(96)
H12	0.29844(297)	0.02853(311)	0.59164(87)
H14	0.31532(387)	0.02256(416)	0.67116(120)
H15	0.30923(436)	-0.09202(490)	0.72302(124)
H16	0.37615(513)	0.01969(545)	0.77126(160)
H17	0.46762(438)	0.21568(464)	0.76607(129)
H18	0.45675(505)	0.32079(526)	0.71368(136)
H20	0.42642(364)	0.58304(390)	0.67619(105)
H21	0.43236(398)	0.80299(426)	0.67491(119)
H22	0.45355(343)	0.90823(392)	0.62404(98)
H23	0.45620(467)	0.78829(483)	0.57157(146)
H24	0.45089(299)	0.57189(331)	0.57914(87)
H251	0.28053(347)	0.06711(381)	0.44734(88)
H252	0.41038(373)	0.00616(360)	0.44878(90)
H261	0.33160(430)	-0.19753(451)	0.43658(113)
H262	0.19916(432)	-0.14166(414)	0.43416(105)
H271	0.23629(452)	-0.02946(450)	0.38532(115)
H272	0.38068(400)	-0.05272(403)	0.38664(103)
H281	0.33954(510)	-0.27536(493)	0.37688(131)
H282	0.19748(471)	-0.24970(448)	0.37645(119)
H291	0.20864(549)	-0.12908(552)	0.32913(142)
H292	0.35159(612)	-0.13628(614)	0.32715(167)
H301	0.34330(668)	-0.37001(649)	0.32043(173)
H302	0.19167(686)	-0.35985(687)	0.32061(177)
H303	0.26984(574)	-0.29050(602)	0.29306(155)

0ORTHOGONAL COORDINATES (ANGSTROM)

ORTHOGONALISATION MATRIX:

A B COSGAMMA	C COSBETA	11.31020	0.00000	0.00000
0 B SINGAMMA	-C SINBETA COSALPHA*	0.00000	10.74390	0.00000
0 0	C SINBETA SINALPHA*	0.00000	0.00000	39.72990

ATOM	X	Y	Z
N1	4.4173(0.0035)	1.8810(0.0034)	24.9595(0.0035)
C2	4.5198(0.0045)	2.6129(0.0045)	26.0584(0.0042)
N3	4.7057(0.0040)	3.9322(0.0039)	26.1109(0.0035)
C4	4.7887(0.0040)	4.5194(0.0042)	24.9261(0.0042)
N5	4.6954(0.0035)	3.9053(0.0035)	23.7386(0.0035)
C6	4.5064(0.0042)	2.5769(0.0045)	23.8097(0.0039)
C7	4.3212(0.0042)	1.8026(0.0042)	22.5654(0.0039)
C8	4.7611(0.0040)	2.1944(0.0042)	21.2841(0.0042)
O8	5.5126(0.0030)	3.3319(0.0030)	21.1983(0.0031)
C81	6.1254(0.0062)	3.6380(0.0057)	19.9456(0.0050)
C9	4.4442(0.0044)	1.4409(0.0044)	20.1645(0.0042)
C10	3.7286(0.0042)	0.2664(0.0042)	20.2988(0.0042)
O10	3.3468(0.0031)	-0.5362(0.0030)	19.2674(0.0031)
C11	3.3233(0.0045)	-0.1681(0.0048)	21.5507(0.0046)
C12	3.6280(0.0042)	0.5982(0.0046)	22.6456(0.0042)
C13	4.4160(0.0046)	1.9058(0.0050)	27.3711(0.0042)
C14	3.9037(0.0058)	0.6236(0.0057)	27.4593(0.0054)
C15	3.8178(0.0077)	-0.0226(0.0066)	28.6739(0.0061)
C16	4.2767(0.0080)	0.5983(0.0075)	29.8078(0.0061)
C17	4.7835(0.0079)	1.8666(0.0074)	29.7541(0.0058)
C18	4.8489(0.0063)	2.5231(0.0065)	28.5360(0.0050)
C19	4.9415(0.0041)	5.9938(0.0045)	24.9031(0.0042)
C20	4.9238(0.0054)	6.7387(0.0051)	26.0767(0.0050)
C21	4.9663(0.0057)	8.1042(0.0055)	26.0513(0.0058)
C22	5.0769(0.0052)	8.7771(0.0054)	24.8352(0.0058)
C23	5.1158(0.0054)	8.0608(0.0054)	23.6735(0.0054)
C24	5.0614(0.0050)	6.6834(0.0049)	23.6933(0.0046)
C25	3.6455(0.0053)	-0.1339(0.0052)	17.9110(0.0042)
C26	3.2004(0.0059)	-1.2766(0.0053)	17.0346(0.0046)
C27	3.3466(0.0061)	-0.9869(0.0055)	15.5558(0.0050)
C28	3.1307(0.0058)	-2.2459(0.0055)	14.7167(0.0050)
C29	3.1622(0.0074)	-2.0092(0.0071)	13.2253(0.0054)
C30	3.0607(0.0101)	-3.3353(0.0101)	12.4708(0.0077)
H81	6.6366(0.0406)	4.4628(0.0433)	20.0116(0.0378)

H82	6.6768(0.0450)	2.7545(0.0500)	19.7311(0.0445)
H83	5.3831(0.0476)	3.8418(0.0451)	19.3008(0.0469)
H9	4.6884(0.0346)	1.7313(0.0349)	19.2920(0.0358)
H11	2.8479(0.0421)	-1.0274(0.0424)	21.5785(0.0382)
H12	3.3754(0.0336)	0.3065(0.0334)	23.5058(0.0346)
H14	3.5663(0.0438)	0.2424(0.0447)	26.6651(0.0477)
H15	3.4975(0.0493)	-0.9887(0.0527)	28.7255(0.0493)
H16	4.2543(0.0580)	0.2115(0.0586)	30.6421(0.0636)
H17	5.2889(0.0495)	2.3172(0.0499)	30.4359(0.0513)
H18	5.1659(0.0571)	3.4465(0.0565)	28.3544(0.0541)
H20	4.8229(0.0412)	6.2641(0.0419)	26.8650(0.0417)
H21	4.8901(0.0450)	8.6272(0.0458)	26.8141(0.0473)
H22	5.1297(0.0388)	9.7579(0.0421)	24.7930(0.0390)
H23	5.1597(0.0528)	8.4693(0.0519)	22.7084(0.0580)
H24	5.0997(0.0338)	6.1443(0.0356)	23.0092(0.0346)
H251	3.1729(0.0392)	0.7210(0.0409)	17.7728(0.0350)
H252	4.6415(0.0422)	0.0662(0.0387)	17.8300(0.0358)
H261	3.7505(0.0486)	-2.1222(0.0485)	17.3453(0.0449)
H262	2.2525(0.0489)	-1.5220(0.0445)	17.2491(0.0417)
H271	2.6725(0.0511)	-0.3165(0.0484)	15.3087(0.0457)
H272	4.3056(0.0452)	-0.5664(0.0433)	15.3612(0.0409)
H281	3.8403(0.0577)	-2.9584(0.0530)	14.9734(0.0521)
H282	2.2335(0.0533)	-2.6828(0.0481)	14.9563(0.0473)
H291	2.3598(0.0621)	-1.3868(0.0593)	13.0763(0.0564)
H292	3.9766(0.0692)	-1.4642(0.0660)	12.9976(0.0664)
H301	3.8828(0.0756)	-3.9754(0.0697)	12.7307(0.0687)
H302	2.1678(0.0776)	-3.8662(0.0738)	12.7378(0.0703)
H303	3.0519(0.0649)	-3.1211(0.0647)	11.6432(0.0616)

OTHERMAL PARAMETERS, U(I,J)X10**4

EXP(-2*PI**2(U11*H**2*(A*)**2+...+2*U12*H*K*(A*)*(B*)+...)

ATOM	U11	U22	U33	U23	U13	U12
N1	480(20)	370(20)	290(20)	30(20)	20(20)	0(20)
C2	420(30)	360(20)	330(20)	80(20)	10(20)	50(20)
N3	570(30)	480(20)	280(20)	50(20)	-19(20)	-19(20)
C4	320(20)	430(30)	350(20)	20(20)	-9(20)	-19(20)
N5	450(20)	370(20)	280(20)	20(20)	-29(20)	-19(20)
C6	330(20)	440(30)	280(20)	50(20)	20(20)	30(20)
C7	400(30)	350(20)	250(20)	10(20)	0(20)	0(20)
C8	360(20)	350(20)	310(20)	30(20)	-19(20)	0(20)
O8	590(20)	410(20)	320(10)	-119(20)	70(10)	0(10)
C81	700(40)	450(30)	420(30)	-149(30)	130(30)	10(20)
C9	440(30)	380(20)	240(20)	0(20)	30(20)	10(20)
C10	350(20)	390(20)	340(20)	10(20)	0(20)	-19(20)
O10	630(20)	480(20)	300(10)	-119(20)	10(10)	-39(10)
C11	440(30)	410(30)	390(20)	-69(20)	50(20)	0(20)
C12	440(30)	470(30)	210(20)	-19(20)	30(20)	60(20)
C13	570(30)	530(30)	300(20)	20(30)	70(20)	30(20)
C14	810(40)	550(30)	380(30)	30(30)	90(30)	50(30)
C15	1390(60)	550(40)	540(30)	40(40)	260(40)	140(30)
C16	1600(70)	850(50)	330(30)	90(50)	170(40)	140(40)
C17	1390(60)	910(50)	340(30)	-179(50)	-69(30)	50(30)
C18	930(50)	750(40)	300(20)	-79(40)	-9(30)	40(30)
C19	370(20)	440(20)	320(20)	-19(20)	-39(20)	0(20)
C20	690(40)	430(30)	410(30)	20(30)	-39(20)	-29(20)
C21	720(40)	430(30)	580(30)	10(30)	-49(30)	-189(30)
C22	620(40)	370(30)	720(40)	-69(30)	20(30)	100(30)
C23	620(40)	470(30)	460(30)	-59(30)	10(20)	30(30)
C24	560(30)	410(30)	390(30)	-29(20)	10(20)	-89(20)
C25	500(30)	490(30)	360(20)	-19(30)	0(20)	-59(20)
C26	580(40)	540(30)	340(20)	-99(30)	-89(20)	-89(20)
C27	590(30)	580(30)	360(20)	-9(30)	-29(20)	-79(20)
C28	510(30)	650(30)	420(20)	-19(30)	-9(20)	-139(30)
C29	760(50)	910(50)	410(30)	150(40)	0(30)	-189(30)
C30	1070(70)	1220(70)	610(40)	200(60)	-139(40)	-489(50)
H81	400(100)					
H82	600(100)					
H83	600(200)					
H9	300(100)					
H11	500(100)					
H12	300(100)					
H14	600(200)					
H15	800(200)					
H16	1100(200)					
H17	700(200)					
H18	900(200)					
H20	500(100)					

H21	600(100)
H22	400(100)
H23	900(200)
H24	200(100)
H251	400(100)
H252	400(100)
H261	700(200)
H262	600(100)
H271	700(200)
H272	500(100)
H281	900(200)
H282	700(200)
H291	1100(200)
H292	1300(300)
H301	1400(300)
H302	1400(300)
H303	1000(200)

0PRINCIPAL AXES OF THE THERMAL ELLIPSOIDS AND U-EQUIV.(X10**4 A**2)
AND B-EQUIV.(A**2)

ATOM	R1	R2	R3	U-EQUIV.	B-EQUIV.	RMAX/RMIN
N1	482(20)	380(21)	278(21)	380(12)	3.00(0.09)	1.73
C2	470(27)	381(26)	260(24)	370(14)	2.92(0.11)	1.81
N3	577(30)	485(22)	267(21)	443(13)	3.50(0.11)	2.16
C4	439(30)	346(22)	315(22)	367(14)	2.90(0.11)	1.39
N5	461(21)	367(23)	272(20)	367(12)	2.90(0.09)	1.69
C6	463(30)	323(23)	264(22)	350(14)	2.76(0.11)	1.76
C7	400(30)	351(20)	249(20)	333(14)	2.63(0.11)	1.61
C8	374(26)	356(25)	289(23)	340(12)	2.68(0.09)	1.29
O8	612(18)	480(22)	228(20)	440(11)	3.47(0.08)	2.69
C81	759(40)	552(38)	259(35)	523(21)	4.13(0.17)	2.93
C9	446(31)	379(20)	236(20)	353(13)	2.79(0.11)	1.89
C10	400(24)	344(24)	336(24)	360(12)	2.84(0.10)	1.19
O10	646(18)	525(22)	240(18)	470(10)	3.71(0.08)	2.69
C11	494(30)	429(29)	317(26)	413(16)	3.26(0.12)	1.56
C12	517(31)	400(28)	203(21)	373(16)	2.95(0.12)	2.54
C13	603(28)	515(31)	282(21)	467(15)	3.68(0.12)	2.14
C14	839(39)	542(33)	360(31)	580(20)	4.58(0.15)	2.33
C15	1486(58)	527(40)	467(34)	827(26)	6.53(0.21)	3.18
C16	1651(70)	831(51)	298(33)	927(31)	7.32(0.24)	5.54
C17	1403(59)	952(53)	285(37)	880(29)	6.95(0.23)	4.92
C18	940(49)	754(39)	286(23)	660(20)	5.21(0.16)	3.28
C19	444(22)	390(24)	296(24)	377(12)	2.97(0.09)	1.50
C20	700(40)	434(36)	396(35)	510(20)	4.03(0.15)	1.77
C21	824(40)	571(31)	335(36)	577(20)	4.55(0.16)	2.46
C22	733(39)	655(41)	322(32)	570(21)	4.50(0.16)	2.28
C23	626(40)	523(39)	401(36)	517(21)	4.08(0.16)	1.56
C24	604(28)	403(29)	353(30)	453(18)	3.58(0.14)	1.71
C25	556(28)	438(31)	356(22)	450(16)	3.55(0.13)	1.56
C26	652(34)	552(32)	255(30)	487(18)	3.84(0.14)	2.56
C27	666(28)	510(30)	354(21)	510(16)	4.03(0.12)	1.88
C28	737(35)	441(30)	402(30)	527(16)	4.16(0.13)	1.83
C29	1063(51)	656(44)	361(36)	693(26)	5.47(0.21)	2.95
C30	1695(74)	655(68)	550(48)	967(39)	7.63(0.31)	3.08

0BOND DISTANCES (ANGSTROM)
(CORRECTIONS FOLLOWING BUSING & LEVY, ACTA CRYST.(1964).17.142)

		UNCORRECTED DISTANCE	LOWER BOUND	UPPER BOUND	RIDING MOTION	NON-CORRELATED MOTION
N1	- C2	1.3243(52)	1.3244	1.4364	1.3282	1.3804
N1	- C6	1.3469(50)	1.3470	1.4677	1.3501	1.4073
C2	- N3	1.3333(58)	1.3335	1.4516	1.3379	1.3925
C2	- C13	1.4946(59)	1.4951	1.6218	1.5024	1.5585
N3	- C4	1.3249(52)	1.3258	1.4597	1.3361	1.3928
C4	- N5	1.3402(52)	1.3402	1.4527	1.3428	1.3965
C4	- C19	1.4825(60)	1.4825	1.5746	1.4829	1.5285
N5	- C6	1.3436(56)	1.3439	1.4436	1.3483	1.3937
C6	- C7	1.4772(54)	1.4773	1.5709	1.4785	1.5241
C7	- C8	1.4102(54)	1.4103	1.5122	1.4112	1.4613
C7	- C12	1.3920(61)	1.3920	1.4814	1.3931	1.4367
C8	- O8	1.3660(50)	1.3664	1.4766	1.3725	1.4215
C8	- C9	1.3863(57)	1.3864	1.4894	1.3891	1.4379
O8	- C81	1.4277(58)	1.4280	1.5739	1.4341	1.5009
C81	- H81	0.9726(429)				
C81	- H82	1.0633(488)				
C81	- H83	1.0042(475)				
C9	- C10	1.3818(60)	1.3818	1.4816	1.3840	1.4317
C9	- H9	0.9514(358)				

C10	- O10	1.3616(49)	1.3633	1.4962	1.3769	1.4298
C10	- C11	1.3858(60)	1.3859	1.4993	1.3889	1.4426
O10	- C25	1.4460(50)	1.4460	1.5842	1.4480	1.5151
C11	- C12	1.3708(61)	1.3709	1.4944	1.3736	1.4326
C11	- H11	0.9824(426)				
C12	- H12	0.9427(346)				
C13	- C14	1.3835(75)	1.3842	1.5259	1.3936	1.4551
C13	- C18	1.3876(68)	1.3903	1.5688	1.4098	1.4796
C14	- C15	1.3784(81)	1.3806	1.6185	1.4014	1.4996
C14	- H14	0.9433(470)				
C15	- C16	1.3718(91)	1.3725	1.6353	1.3853	1.5039
C15	- H15	1.0191(527)				
C16	- C17	1.3669(105)	1.3670	1.6125	1.3715	1.4897
C16	- H16	0.9199(630)				
C17	- C18	1.3853(79)	1.3866	1.6381	1.4035	1.5123
C17	- H17	0.9608(509)				
C18	- H18	0.9931(569)				
C19	- C20	1.3902(64)	1.3910	1.5251	1.4010	1.4581
C19	- C24	1.3976(61)	1.3980	1.5192	1.4044	1.4586
C20	- C21	1.3664(75)	1.3668	1.5428	1.3741	1.4548
C20	- H20	0.9256(420)				
C21	- C22	1.3943(78)	1.3946	1.5524	1.4012	1.4735
C21	- H21	0.9280(471)				
C22	- C23	1.3653(76)	1.3653	1.5334	1.3657	1.4494
C22	- H22	0.9831(424)				
C23	- C24	1.3787(72)	1.3788	1.5259	1.3830	1.4524
C23	- H23	1.0488(573)				
C24	- H24	0.8718(352)				
C25	- C26	1.5073(70)	1.5076	1.6457	1.5138	1.5767
C25	- H251	0.9866(408)				
C25	- H252	1.0191(424)				
C26	- C27	1.5139(66)	1.5140	1.6600	1.5170	1.5870
C26	- H261	1.0555(485)				
C26	- H262	1.0024(486)				
C27	- C28	1.5283(75)	1.5283	1.6659	1.5285	1.5971
C27	- H271	0.9823(498)				
C27	- H272	1.0651(452)				
C28	- C29	1.5105(71)	1.5123	1.6976	1.5289	1.6049
C28	- H281	1.0378(554)				
C28	- H282	1.0262(524)				
C29	- C30	1.5291(117)	1.5307	1.7177	1.5467	1.6242
C29	- H291	1.0264(614)				
C29	- H292	1.0060(685)				
C30	- H301	1.0738(738)				
C30	- H302	1.0725(769)				
C30	- H303	0.8549(623)				

NUMBER OF INTERATOMIC CONTACTS: 65

OBOND ANGLES (DEGREES)
(E.S.D.FOLLOWING CRUICKSHANK, INTERNAT.TABLES,II,1959,P.331)

			ANGLE	E.S.D.
C2	- N1	- C6	114.69	0.37
N1	- C2	- C13	117.51	0.39
N1	- C2	- N3	126.17	0.39
N3	- C2	- C13	116.31	0.38
C2	- N3	- C4	114.34	0.38
N3	- C4	- C19	117.46	0.38
N3	- C4	- N5	125.79	0.39
N5	- C4	- C19	116.69	0.37
C4	- N5	- C6	114.58	0.35
N1	- C6	- N5	124.42	0.36
N5	- C6	- C7	119.42	0.37
N1	- C6	- C7	116.10	0.37
C6	- C7	- C12	117.87	0.36
C6	- C7	- C8	125.49	0.37
C8	- C7	- C12	116.63	0.36
C7	- C8	- C9	120.76	0.38
C7	- C8	- O8	117.39	0.37
O8	- C8	- C9	121.85	0.37
C8	- O8	- C81	118.02	0.35
O8	- C81	- H83	106.84	2.75
O8	- C81	- H82	102.80	2.60
O8	- C81	- H81	110.36	2.33
H82	- C81	- H83	114.99	3.61
H81	- C81	- H83	105.07	3.54
H81	- C81	- H82	116.47	3.48

C8	- C9	- H9	121.07	2.14
C8	- C9	- C10	120.13	0.39
C10	- C9	- H9	118.78	2.17
C9	- C10	- C11	120.39	0.40
C9	- C10	- O10	124.94	0.38
O10	- C10	- C11	114.67	0.38
C10	- O10	- C25	119.25	0.35
C10	- C11	- H11	116.19	2.32
C10	- C11	- C12	118.77	0.42
C12	- C11	- H11	125.03	2.30
C7	- C12	- C11	123.26	0.41
C11	- C12	- H12	119.75	2.08
C7	- C12	- H12	116.98	2.11
C2	- C13	- C18	120.34	0.46
C2	- C13	- C14	121.34	0.41
C14	- C13	- C18	118.31	0.46
C13	- C14	- H14	116.95	2.88
C13	- C14	- C15	120.91	0.51
C15	- C14	- H14	122.01	2.77
C14	- C15	- H15	120.57	2.86
C14	- C15	- C16	119.69	0.61
C16	- C15	- H15	119.49	2.87
C15	- C16	- H16	123.45	3.71
C15	- C16	- C17	120.77	0.58
C17	- C16	- H16	115.77	3.87
C16	- C17	- H17	127.04	3.10
C16	- C17	- C18	119.45	0.61
C18	- C17	- H17	112.14	3.04
C13	- C18	- C17	120.84	0.57
C17	- C18	- H18	128.06	3.21
C13	- C18	- H18	111.09	3.17
C4	- C19	- C24	120.86	0.40
C4	- C19	- C20	121.23	0.40
C20	- C19	- C24	117.87	0.43
C19	- C20	- H20	116.46	2.64
C19	- C20	- C21	121.29	0.47
C21	- C20	- H20	122.11	2.64
C20	- C21	- H21	123.05	2.94
C20	- C21	- C22	120.07	0.51
C22	- C21	- H21	116.84	2.88
C21	- C22	- H22	121.54	2.37
C21	- C22	- C23	119.42	0.51
C23	- C22	- H22	119.04	2.36
C22	- C23	- H23	125.43	2.88
C22	- C23	- C24	120.72	0.49
C24	- C23	- H23	113.83	3.06
C19	- C24	- C23	120.58	0.44
C23	- C24	- H24	127.21	2.35
C19	- C24	- H24	112.21	2.38
O10	- C25	- H252	109.34	2.14
O10	- C25	- H251	105.88	2.17
O10	- C25	- C26	105.87	0.37
H251	- C25	- H252	106.68	3.22
C26	- C25	- H252	113.03	2.19
C26	- C25	- H251	115.72	2.19
C25	- C26	- H262	109.90	2.54
C25	- C26	- H261	106.40	2.56
C25	- C26	- C27	113.23	0.43
H261	- C26	- H262	103.51	3.68
C27	- C26	- H262	110.31	2.57
C27	- C26	- H261	112.98	2.57
C26	- C27	- H272	109.94	2.33
C26	- C27	- H271	108.06	2.82
C26	- C27	- C28	111.41	0.43
H271	- C27	- H272	107.60	3.74
C28	- C27	- H272	110.62	2.35
C28	- C27	- H271	109.10	2.84
C27	- C28	- H282	110.24	2.78
C27	- C28	- H281	109.46	3.04
C27	- C28	- C29	114.21	0.47
H281	- C28	- H282	104.34	4.09
C29	- C28	- H282	108.39	2.81
C29	- C28	- H281	109.72	3.01
C28	- C29	- H292	108.98	3.86
C28	- C29	- H291	102.83	3.29
C28	- C29	- C30	110.48	0.54

H291	- C29	- H292		105.75	5.08
C30	- C29	- H292		114.33	3.88
C30	- C29	- H291		113.72	3.38
C29	- C30	- H303		105.13	4.41
C29	- C30	- H302		111.21	3.99
C29	- C30	- H301		110.28	3.89
H302	- C30	- H303		110.89	5.80
H301	- C30	- H303		113.04	5.74
H301	- C30	- H302		106.39	5.54

NUMBER OF ANGLES: 110

OTORSION ANGLES (DEGREES)
(RIGHT-HAND RULE,KLYNE & PRELOG.(1960).EXPERIENTIA,16,521)
(E.S.D.'S. FOLLOWING STANFORD & WASER,ACTA CRYST.(1972).A28,213)

				ANGLE	E.S.D.
C2	-N1	-C6	-C7	-176.72	0.37
C2	-N1	-C6	-N5	0.55	0.61
C6	-N1	-C2	-C13	179.41	0.38
C6	-N1	-C2	-N3	-0.45	0.64
N1	-C2	-C13	-C14	-15.98	0.67
N1	-C2	-C13	-C18	163.33	0.46
N1	-C2	-N3	-C4	0.02	0.65
N3	-C2	-C13	-C14	163.89	0.46
N3	-C2	-C13	-C18	-16.80	0.66
C13	-C2	-N3	-C4	-179.84	0.38
C2	-N3	-C4	-N5	0.36	0.63
C2	-N3	-C4	-C19	177.63	0.38
N3	-C4	-C19	-C20	-3.48	0.63
N3	-C4	-C19	-C24	178.77	0.41
N3	-C4	-N5	-C6	-0.27	0.62
N5	-C4	-C19	-C20	174.03	0.42
N5	-C4	-C19	-C24	-3.71	0.61
C19	-C4	-N5	-C6	-177.55	0.36
C4	-N5	-C6	-N1	-0.23	0.60
C4	-N5	-C6	-C7	176.96	0.37
N5	-C6	-C7	-C8	23.20	0.63
N1	-C6	-C7	-C8	-159.38	0.40
N5	-C6	-C7	-C12	-155.18	0.40
N1	-C6	-C7	-C12	22.24	0.56
C6	-C7	-C12	-H12	-4.94	2.39
C6	-C7	-C12	-C11	175.97	0.41
C6	-C7	-C8	-O8	5.47	0.62
C6	-C7	-C8	-C9	-174.96	0.40
C8	-C7	-C12	-H12	176.53	2.34
C8	-C7	-C12	-C11	-2.56	0.64
C12	-C7	-C8	-C9	3.44	0.61
C12	-C7	-C8	-O8	-176.13	0.37
C7	-C8	-C9	-C10	-2.24	0.64
C7	-C8	-C9	-H9	175.85	2.50
C7	-C8	-O8	-C81	171.16	0.39
O8	-C8	-C9	-C10	177.32	0.38
O8	-C8	-C9	-H9	-4.60	2.56
C9	-C8	-O8	-C81	-8.41	0.59
C8	-O8	-C81	-H81	-179.53	2.58
C8	-O8	-C81	-H82	-54.66	2.63
C8	-O8	-C81	-H83	66.76	2.83
C8	-C9	-C10	-O10	178.89	0.39
C8	-C9	-C10	-C11	-0.05	0.65
H9	-C9	-C10	-C11	-178.19	2.45
H9	-C9	-C10	-O10	0.76	2.51
C9	-C10	-C11	-C12	0.98	0.66
C9	-C10	-C11	-H11	-177.78	2.69
C9	-C10	-O10	-C25	-2.78	0.62
O10	-C10	-C11	-C12	-178.07	0.39
O10	-C10	-C11	-H11	3.17	2.73
C11	-C10	-O10	-C25	176.22	0.39
C10	-O10	-C25	-C26	175.41	0.37
C10	-O10	-C25	-H251	-61.22	2.38
C10	-O10	-C25	-H252	53.36	2.38
C10	-C11	-C12	-C7	0.39	0.69
C10	-C11	-C12	-H12	-178.67	2.41
H11	-C11	-C12	-C7	179.03	2.95
H11	-C11	-C12	-H12	-0.04	3.84
C2	-C13	-C18	-H18	2.57	3.54
C2	-C13	-C18	-C17	-178.63	0.53
C2	-C13	-C14	-C15	179.70	0.52

C2	-C13	-C14	-H14	-4.33	3.19
C14	-C13	-C18	-H18	-178.09	3.49
C14	-C13	-C18	-C17	0.70	0.84
C18	-C13	-C14	-H14	176.35	3.14
C18	-C13	-C14	-C15	0.37	0.82
C13	-C14	-C15	-C16	-1.67	0.95
C13	-C14	-C15	-H15	-175.94	3.34
H14	-C14	-C15	-H15	8.30	4.75
H14	-C14	-C15	-C16	-177.43	3.31
C14	-C15	-C16	-C17	1.90	1.06
C14	-C15	-C16	-H16	-179.22	4.54
H15	-C15	-C16	-H16	-4.89	5.68
H15	-C15	-C16	-C17	176.24	3.32
C15	-C16	-C17	-C18	-0.84	1.07
C15	-C16	-C17	-H17	-166.37	3.82
H16	-C16	-C17	-H17	14.67	5.74
H16	-C16	-C17	-C18	-179.80	4.21
C16	-C17	-C18	-C13	-0.47	0.98
C16	-C17	-C18	-H18	178.09	4.15
H17	-C17	-C18	-C13	167.09	3.28
H17	-C17	-C18	-H18	-14.34	5.33
C4	-C19	-C24	-H24	-4.67	2.55
C4	-C19	-C24	-C23	175.76	0.44
C4	-C19	-C20	-C21	-175.16	0.46
C4	-C19	-C20	-H20	0.74	2.97
C20	-C19	-C24	-H24	177.51	2.50
C20	-C19	-C24	-C23	-2.06	0.70
C24	-C19	-C20	-H20	178.55	2.91
C24	-C19	-C20	-C21	2.65	0.73
C19	-C20	-C21	-C22	-2.28	0.82
C19	-C20	-C21	-H21	175.15	3.43
H20	-C20	-C21	-H21	-0.52	4.66
H20	-C20	-C21	-C22	-177.96	3.09
C20	-C21	-C22	-C23	1.26	0.83
C20	-C21	-C22	-H22	-178.60	2.79
H21	-C21	-C22	-H22	3.81	4.29
H21	-C21	-C22	-C23	-176.32	3.23
C21	-C22	-C23	-C24	-0.70	0.82
C21	-C22	-C23	-H23	177.48	3.68
H22	-C22	-C23	-H23	-2.65	4.61
H22	-C22	-C23	-C24	179.17	2.71
C22	-C23	-C24	-C19	1.13	0.78
C22	-C23	-C24	-H24	-178.37	2.91
H23	-C23	-C24	-C19	-177.24	3.27
H23	-C23	-C24	-H24	3.26	4.41
O10	-C25	-C26	-C27	175.82	0.40
O10	-C25	-C26	-H261	-59.48	2.73
O10	-C25	-C26	-H262	51.96	2.80
H251	-C25	-C26	-H262	-64.95	3.75
H251	-C25	-C26	-H261	-176.40	3.68
H251	-C25	-C26	-C27	58.90	2.56
H252	-C25	-C26	-H262	171.62	3.66
H252	-C25	-C26	-H261	60.18	3.63
H252	-C25	-C26	-C27	-64.52	2.45
C25	-C26	-C27	-C28	169.61	0.44
C25	-C26	-C27	-H271	-70.56	3.03
C25	-C26	-C27	-H272	46.62	2.55
H261	-C26	-C27	-H272	-74.44	3.78
H261	-C26	-C27	-H271	168.39	4.11
H261	-C26	-C27	-C28	48.56	2.86
H262	-C26	-C27	-H272	170.25	3.73
H262	-C26	-C27	-H271	53.07	4.10
H262	-C26	-C27	-C28	-66.76	2.81
C26	-C27	-C28	-C29	175.76	0.48
C26	-C27	-C28	-H281	-60.78	3.24
C26	-C27	-C28	-H282	53.45	3.02
H271	-C27	-C28	-H282	-65.77	4.25
H271	-C27	-C28	-H281	-180.00	4.39
H271	-C27	-C28	-C29	56.54	3.06
H272	-C27	-C28	-H282	176.05	3.89
H272	-C27	-C28	-H281	61.83	4.08
H272	-C27	-C28	-C29	-61.63	2.56
C27	-C28	-C29	-C30	175.06	0.56
C27	-C28	-C29	-H291	-63.24	3.46
C27	-C28	-C29	-H292	48.65	4.11
H281	-C28	-C29	-H292	-74.67	5.19

H281	-C28	-C29	-H291	173.44	4.68
H281	-C28	-C29	-C30	51.74	3.26
H282	-C28	-C29	-H292	171.97	5.02
H282	-C28	-C29	-H291	60.08	4.53
H282	-C28	-C29	-C30	-61.62	3.00
C28	-C29	-C30	-H301	-60.13	4.16
C28	-C29	-C30	-H302	57.65	4.33
C28	-C29	-C30	-H303	177.72	4.48
H291	-C29	-C30	-H303	62.69	5.80
H291	-C29	-C30	-H302	-57.38	5.65
H291	-C29	-C30	-H301	-175.15	5.48
H292	-C29	-C30	-H303	-58.92	6.19
H292	-C29	-C30	-H302	-178.99	6.01
H292	-C29	-C30	-H301	63.23	5.92

NUMBER OF TORSION ANGLES: 151

INTERATOMIC CONTACTS GREATER THAN 2.00 AND LESS THAN 3.50 ANGSTROM.
INVOLVING ATOMS OF THE ORIGINAL SET.
(CORRECTIONS FOLLOWING BUSING & LEVY, ACTA CRYST.(1964).17,142)

		UNCORRECTED DISTANCE	LOWER BOUND	UPPER BOUND	RIDING MOTION	NON-CORRELATED MOTION
N1	...N3	2.3698(49)	2.3699	2.4381	2.3719	2.4040
N1	...C4	2.6646(53)	2.6647	2.7188	2.6663	2.6918
N1	...N5	2.3802(47)	2.3803	2.4470	2.3812	2.4136
N1	...C7	2.3973(48)	2.3974	2.4638	2.3994	2.4306
N1	...C12	2.7609(53)	2.7609	2.8190	2.7616	2.7900
N1	...C13	2.4117(51)	2.4121	2.4922	2.4169	2.4521
N1	...C14	2.8450(62)	2.8460	2.9218	2.8538	2.8839
N1	...H12	2.3828(340)				
N1	...H14	2.5137(461)				
C2	...C4	2.2337(59)	2.2337	2.3020	2.2360	2.2679
C2	...N5	2.6613(53)	2.6613	2.7234	2.6618	2.6924
C2	...C6	2.2490(54)	2.2490	2.3178	2.2492	2.2834
C2	...C14	2.5099(70)	2.5109	2.5913	2.5188	2.5511
C2	...C18	2.5009(63)	2.5042	2.5955	2.5186	2.5499
C2	...H14	2.6261(450)				
C2	...H18	2.5267(547)				
N3	...N5	2.3724(46)	2.3727	2.4509	2.3773	2.4118
N3	...C6	2.6780(51)	2.6784	2.7387	2.6832	2.7086
N3	...C13	2.4038(59)	2.4038	2.4830	2.4039	2.4434
N3	...C18	2.8084(63)	2.8091	2.8982	2.8165	2.8537
N3	...C19	2.4010(57)	2.4014	2.4691	2.4061	2.4352
N3	...C20	2.8152(64)	2.8155	2.8844	2.8196	2.8499
N3	...H18	2.3412(544)				
N3	...H20	2.4537(421)				
C4	...C6	2.2582(59)	2.2582	2.3148	2.2600	2.2865
C4	...C20	2.5034(65)	2.5044	2.5729	2.5118	2.5387
C4	...C24	2.5054(63)	2.5057	2.5711	2.5100	2.5384
C4	...H20	2.6085(420)				
C4	...H24	2.5321(352)				
N5	...C7	2.4368(53)	2.4368	2.4944	2.4384	2.4656
N5	...C8	2.9927(52)	2.9927	3.0407	2.9944	3.0167
N5	...O8	2.7294(43)	2.7298	2.7961	2.7346	2.7630
N5	...C19	2.4038(55)	2.4038	2.4654	2.4038	2.4346
N5	...C24	2.8024(60)	2.8027	2.8629	2.8066	2.8328
N5	...H24	2.3893(356)				
C6	...C8	2.5671(54)	2.5671	2.6236	2.5683	2.5954
C6	...O8	2.8986(47)	2.8988	2.9582	2.9015	2.9285
C6	...C12	2.4581(61)	2.4581	2.5101	2.4598	2.4841
C6	...H12	2.5547(338)				
C7	...O8	2.3722(49)	2.3724	2.4362	2.3757	2.4043
C7	...C9	2.4311(54)	2.4311	2.4954	2.4326	2.4633
C7	...C10	2.8015(55)	2.8015	2.8523	2.8018	2.8269
C7	...C11	2.4309(62)	2.4312	2.4928	2.4352	2.4620
C7	...H9	3.2947(359)				
C7	...H11	3.3397(422)				
C7	...H12	2.0043(339)				
C8	...C81	2.3951(69)	2.3958	2.4658	2.4021	2.4308
C8	...C10	2.3988(58)	2.3988	2.4561	2.3998	2.4274
C8	...C11	2.7785(62)	2.7787	2.8319	2.7812	2.8053
C8	...C12	2.3845(59)	2.3845	2.4431	2.3847	2.4138
C8	...H81	3.2066(417)				
C8	...H82	2.5289(453)				
C8	...H83	2.6522(464)				

C8	...H9	2.0465(359)				
C8	...H12	3.2281(342)				
O8	...C9	2.4054(52)	2.4059	2.4723	2.4110	2.4391
O8	...H9	2.6220(355)				
O8	...H24	3.3704(354)				
C81	...C9	2.7752(73)	2.7759	2.8344	2.7817	2.8052
C81	...H9	2.4754(353)				
C9	...O10	2.4327(52)	2.4335	2.5015	2.4399	2.4675
C9	...C11	2.4014(62)	2.4015	2.4650	2.4031	2.4332
C9	...C12	2.7445(58)	2.7445	2.8051	2.7455	2.7748
C9	...C25	2.8629(61)	2.8631	2.9227	2.8669	2.8929
C9	...H82	2.6264(465)				
C9	...H83	2.7188(458)				
C9	...H11	3.2619(418)				
C9	...H251	2.8027(365)				
C9	...H252	2.7164(368)				
C10	...C12	2.3723(57)	2.3725	2.4416	2.3761	2.4071
C10	...C25	2.4225(57)	2.4229	2.4935	2.4278	2.4582
C10	...H9	2.0200(353)				
C10	...H11	2.0217(409)				
C10	...H12	3.2266(348)				
C10	...H251	2.6261(356)				
C10	...H252	2.6398(368)				
O10	...C11	2.3129(52)	2.3133	2.3996	2.3187	2.3565
O10	...C26	2.3569(53)	2.3569	2.4560	2.3571	2.4065
O10	...H9	2.6348(350)				
O10	...H11	2.4148(386)				
O10	...H252	2.0262(389)				
O10	...H261	2.5245(465)				
O10	...H262	2.4985(437)				
C11	...H9	3.2516(356)				
C11	...H12	2.0126(348)				
C12	...H11	2.0952(415)				
C13	...C15	2.4028(80)	2.4063	2.5195	2.4230	2.4629
C13	...C16	2.7687(76)	2.7736	2.8897	2.7930	2.8317
C13	...C17	2.4115(69)	2.4162	2.5463	2.4367	2.4813
C13	...H15	3.3250(521)				
C13	...H17	3.2131(513)				
C14	...C16	2.3780(80)	2.3812	2.5300	2.4000	2.4556
C14	...C17	2.7542(82)	2.7571	2.8758	2.7730	2.8165
C14	...C18	2.3792(83)	2.3795	2.4811	2.3841	2.4303
C14	...H15	2.0899(516)				
C14	...H16	3.2284(636)				
C14	...H18	3.2192(567)				
C15	...C17	2.3809(97)	2.3812	2.5264	2.3875	2.4538
C15	...C18	2.7500(93)	2.7510	2.8544	2.7602	2.8027
C15	...H14	2.0417(480)				
C15	...H16	2.0296(636)				
C15	...H17	3.2777(506)				
C16	...C18	2.3769(93)	2.3791	2.5161	2.3946	2.4476
C16	...H14	3.2415(479)				
C16	...H15	2.0729(518)				
C16	...H17	2.0913(505)				
C16	...H18	3.3189(566)				
C17	...H15	3.2962(523)				
C17	...H18	2.1451(559)				
C18	...H14	3.2167(460)				
C18	...H16	3.1831(611)				
C19	...C21	2.4027(70)	2.4041	2.4843	2.4136	2.4442
C19	...C22	2.7874(70)	2.7893	2.8579	2.7989	2.8236
C19	...C23	2.4114(69)	2.4121	2.4824	2.4182	2.4472
C19	...H21	3.2542(465)				
C19	...H23	3.3155(548)				
C20	...C22	2.3917(74)	2.3917	2.4877	2.3927	2.4397
C20	...C23	2.7497(71)	2.7497	2.8283	2.7513	2.7890
C20	...C24	2.3880(65)	2.3881	2.4752	2.3910	2.4317
C20	...H21	2.0277(462)				
C20	...H22	3.2873(419)				
C20	...H24	3.1295(349)				
C21	...C23	2.3829(76)	2.3829	2.4767	2.3840	2.4298
C21	...C24	2.7546(72)	2.7548	2.8329	2.7579	2.7938
C21	...H20	2.0171(422)				
C21	...H22	2.0844(413)				
C21	...H23	3.3683(582)				
C22	...C24	2.3849(72)	2.3855	2.4808	2.3920	2.4331
C22	...H20	3.2403(422)				

C22	...H23	2.1505(581)				
C22	...H24	3.2041(357)				
C23	...H21	3.1993(475)				
C23	...H22	2.0332(415)				
C23	...H24	2.0284(359)				
C24	...H20	3.2081(420)				
C24	...H22	3.2661(420)				
C24	...H23	2.0419(536)				
C25	...C27	2.5227(64)	2.5228	2.6079	2.5261	2.5653
C25	...H9	2.5443(355)				
C25	...H261	2.0700(485)				
C25	...H262	2.0749(465)				
C25	...H271	2.7843(466)				
C25	...H272	2.6692(415)				
C26	...C28	2.5133(67)	2.5133	2.6053	2.5138	2.5593
C26	...H251	2.1298(406)				
C26	...H252	2.1242(403)				
C26	...H271	2.0443(469)				
C26	...H272	2.1274(427)				
C26	...H281	2.7361(529)				
C26	...H282	2.6891(486)				
C27	...C29	2.5516(74)	2.5520	2.6546	2.5582	2.6033
C27	...H251	2.8039(377)				
C27	...H252	2.8209(380)				
C27	...H261	2.1573(463)				
C27	...H262	2.0858(443)				
C27	...H281	2.1142(534)				
C27	...H282	2.1152(499)				
C27	...H291	2.6985(575)				
C27	...H292	2.6775(667)				
C28	...C30	2.4972(95)	2.4998	2.6216	2.5152	2.5607
C28	...H261	2.7034(454)				
C28	...H262	2.7764(430)				
C28	...H271	2.0695(486)				
C28	...H272	2.1486(440)				
C28	...H291	2.0058(580)				
C28	...H292	2.0693(670)				
C28	...H301	2.7388(699)				
C28	...H302	2.7329(727)				
C28	...H303	3.1967(620)				
C29	...H271	2.7287(473)				
C29	...H272	2.8197(427)				
C29	...H281	2.1016(532)				
C29	...H282	2.0767(490)				
C29	...H301	2.1516(707)				
C29	...H302	2.1621(748)				
C30	...H281	2.6482(532)				
C30	...H282	2.6996(486)				
C30	...H291	2.1574(602)				
C30	...H292	2.1489(673)				
H81	...H9	3.4314(547)				
H82	...H9	2.2789(577)				
H83	...H9	2.2219(572)				
H9	...H251	2.3719(517)				
H9	...H252	2.2164(514)				
H11	...H12	2.4025(524)				
H12	...H14	3.1657(589)				
H14	...H15	2.4011(687)				
H15	...H16	2.3847(796)				
H16	...H17	2.3552(768)				
H17	...H18	2.3713(747)				
H18	...H20	3.2055(699)				
H20	...H21	2.3646(621)				
H21	...H22	2.3282(615)				
H22	...H23	2.4509(690)				
H23	...H24	2.3451(630)				
H251	...H261	2.9327(633)				
H251	...H262	2.4804(605)				
H251	...H271	2.7200(587)				
H251	...H272	2.9591(559)				
H252	...H261	2.4121(622)				
H252	...H262	2.9269(626)				
H252	...H271	3.2218(613)				
H252	...H272	2.5706(547)				
H261	...H271	2.9275(667)				
H261	...H272	2.5817(626)				

```
H261  ...H281   2.5166( 691)
H261  ...H282   2.8848( 673)
H262  ...H271   2.3226( 632)
H262  ...H272   2.9483( 629)
H262  ...H281   3.1246( 696)
H262  ...H282   2.5700( 636)
H271  ...H281   2.9079( 726)
H271  ...H282   2.4323( 684)
H271  ...H291   2.4954( 735)
H271  ...H292   2.8912( 819)
H272  ...H281   2.4675( 685)
H272  ...H282   2.9893( 672)
H272  ...H291   3.1112( 728)
H272  ...H292   2.5496( 782)
H281  ...H291   2.8742( 798)
H281  ...H292   2.4809( 844)
H281  ...H301   2.4629( 865)
H281  ...H302   2.9358( 909)
H281  ...H303   3.4261( 810)
H282  ...H291   2.2869( 745)
H282  ...H292   2.8913( 837)
H282  ...H301   3.0569( 864)
H282  ...H302   2.5153( 855)
H282  ...H303   3.4407( 781)
H291  ...H301   3.0232( 931)
H291  ...H302   2.5097( 946)
H291  ...H303   2.3538( 864)
H292  ...H301   2.5271( 960)
H292  ...H302   3.0181(1008)
H292  ...H303   2.3312( 922)
NUMBER OF CONTACTS:   235


I HOPE THAT YOU SUCCEEDED IN USING THIS PROGRAM
AND THAT THE RESULTS OF THE CALCULATIONS ARE USEFUL TO HAVE
A BETTER UNDERSTANDING OF YOUR STRUCTURE. BEST WISHES^
```

```
data_c:\sonja\s499rm\s499rm

_audit_creation_method            SHELXL
_chemical_name_systematic
;
 2-(4-methoxy-phenyl)-4,6-diphenyl-1,3,5-triazine
;
_chemical_name_common             ?
_chemical_formula_moiety          ?
_chemical_formula_structural      ?
_chemical_formula_analytical      ?
_chemical_formula_sum             'C22 H17 N3 O'
_chemical_formula_weight          339.39
_chemical_melting_point           ?
_chemical_compound_source         ?

loop_
 _atom_type_symbol
 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
 'C'  'C'   0.0033   0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting            monoclinic
_symmetry_space_group_name_H-M    P2(1)/c

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y-1/2, z-1/2'

_cell_length_a                    10.841(3)
_cell_length_b                    3.9140(10)
_cell_length_c                    40.479(9)
_cell_angle_alpha                 90.00
_cell_angle_beta                  95.49(2)
_cell_angle_gamma                 90.00
_cell_volume                      1709.7(7)
_cell_formula_units_Z             4
_cell_measurement_temperature     293(2)
_cell_measurement_reflns_used     21
_cell_measurement_theta_min       10
_cell_measurement_theta_max       12.5

_exptl_crystal_description        plates
_exptl_crystal_colour             colourless
_exptl_crystal_size_max           1.2
_exptl_crystal_size_mid           0.1
_exptl_crystal_size_min           0.04
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.318
_exptl_crystal_density_method     ?
_exptl_crystal_F_000              712
_exptl_absorpt_coefficient_mu     0.083
_exptl_absorpt_correction_type    none
```

```
_exptl_absorpt_correction_T_min   ?
_exptl_absorpt_correction_T_max   ?

_exptl_special_details
;
 ?
;

_diffrn_ambient_temperature       293(2)
_diffrn_radiation_wavelength      0.71073
_diffrn_radiation_type            MoK\a
_diffrn_radiation_source          'fine-focus sealed tube'
_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device        Nicolet P3
_diffrn_measurement_method        Wyckoff - scan
_diffrn_standards_number          3
_diffrn_standards_interval_count  50
_diffrn_standards_interval_time   ?
_diffrn_standards_decay_%         ?
_diffrn_reflns_number             2389
_diffrn_reflns_av_R_equivalents   0.0461
_diffrn_reflns_av_sigmaI/netI     0.1595
_diffrn_reflns_limit_h_min        0
_diffrn_reflns_limit_h_max        12
_diffrn_reflns_limit_k_min        0
_diffrn_reflns_limit_k_max        4
_diffrn_reflns_limit_l_min        -46
_diffrn_reflns_limit_l_max        46
_diffrn_reflns_theta_min          1.01
_diffrn_reflns_theta_max          22.49
_reflns_number_total              2245
_reflns_number_observed           891
_reflns_observed_criterion        >2sigma(I)

_computing_data_collection        Siemens P3/V Data Collection System
_computing_cell_refinement        Siemens P3/V Data Collection System
_computing_data_reduction         SHELXTL PLUS - XDISK
_computing_structure_solution     'SHELXS-86 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-93 (Sheldrick, 1993)'
_computing_molecular_graphics     SHELXTL -XP
_computing_publication_material   ?

_refine_special_details
;
 Refinement on F^2^ for ALL reflections except for 475 with very negative F^2^
 or flagged by the user for potential systematic errors.  Weighted R-factors
 wR and all goodnesses of fit S are based on F^2^, conventional R-factors R
 are based on F, with F set to zero for negative F^2^. The observed criterion
 of F^2^ > 2sigma(F^2^) is used only for calculating _R_factor_obs etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme
 'calc w=1/[\s^2^(Fo^2^)+(0.0564P)^2^+4.0160P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     ?
_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.0140(24)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
```

```
_refine_ls_number_reflns          1770
_refine_ls_number_parameters      236
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.2716
_refine_ls_R_factor_obs           0.1148
_refine_ls_wR_factor_all          0.2745
_refine_ls_wR_factor_obs          0.1883
_refine_ls_goodness_of_fit_all    1.118
_refine_ls_goodness_of_fit_obs    1.424
_refine_ls_restrained_S_all       1.209
_refine_ls_restrained_S_obs       1.424
_refine_ls_shift/esd_max          0.045
_refine_ls_shift/esd_mean         0.013

loop_
 _atom_site_label
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_U_iso_or_equiv
 _atom_site_thermal_displace_type
 _atom_site_occupancy
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_group
N1 N 0.3528(6) 0.9205(24) 0.1139(2) 0.056(3) Uani 1 d . .
C2 C 0.4241(9) 1.0409(28) 0.1400(2) 0.046(3) Uani 1 d . .
N3 N 0.5454(7) 1.1166(24) 0.1411(2) 0.055(3) Uani 1 d . .
C4 C 0.5952(9) 1.0638(29) 0.1127(2) 0.052(3) Uani 1 d . .
N5 N 0.5335(7) 0.9426(23) 0.0845(2) 0.051(2) Uani 1 d . .
C6 C 0.4143(9) 0.8717(29) 0.0868(2) 0.053(3) Uani 1 d . .
C7 C 0.3638(9) 1.0857(30) 0.1704(2) 0.057(3) Uani 1 d . .
C8 C 0.2434(9) 0.9813(32) 0.1735(2) 0.063(3) Uani 1 d . .
H8 H 0.1998(9) 0.8751(32) 0.1554(2) 0.075 Uiso 1 calc R .
C9 C 0.1857(9) 1.0255(33) 0.2014(3) 0.069(4) Uani 1 d . .
H9 H 0.1044(9) 0.9519(33) 0.2021(3) 0.083 Uiso 1 calc R .
C10 C 0.2467(10) 1.1780(30) 0.2284(2) 0.055(3) Uani 1 d . .
C11 C 0.3667(9) 1.2923(29) 0.2276(2) 0.060(3) Uani 1 d . .
H11 H 0.4095(9) 1.3969(29) 0.2459(2) 0.072 Uiso 1 calc R .
C12 C 0.4206(10) 1.2438(31) 0.1982(3) 0.067(3) Uani 1 d . .
H12 H 0.5009(10) 1.3240(31) 0.1972(3) 0.081 Uiso 1 calc R .
C13 C 0.7289(9) 1.1282(28) 0.1124(2) 0.052(3) Uani 1 d . .
C14 C 0.7957(9) 1.2846(30) 0.1389(2) 0.061(3) Uani 1 d . .
H14 H 0.7550(9) 1.3586(30) 0.1568(2) 0.074 Uiso 1 calc R .
C15 C 0.9212(10) 1.3331(36) 0.1393(3) 0.080(4) Uani 1 d . .
H15 H 0.9645(10) 1.4364(36) 0.1576(3) 0.096 Uiso 1 calc R .
C16 C 0.9843(10) 1.2299(31) 0.1128(3) 0.069(4) Uani 1 d . .
H16 H 1.0692(10) 1.2646(31) 0.1131(3) 0.083 Uiso 1 calc R .
C17 C 0.9186(9) 1.0747(32) 0.0860(3) 0.069(4) Uani 1 d . .
H17 H 0.9595(9) 0.9992(32) 0.0682(3) 0.083 Uiso 1 calc R .
C18 C 0.7911(10) 1.0311(29) 0.0857(2) 0.060(3) Uani 1 d . .
H18 H 0.7470(10) 0.9351(29) 0.0671(2) 0.072 Uiso 1 calc R .
C19 C 0.3450(8) 0.7543(26) 0.0565(2) 0.038(2) Uani 1 d . .
C20 C 0.3920(9) 0.7511(29) 0.0263(2) 0.056(3) Uani 1 d . .
H20 H 0.4727(9) 0.8273(29) 0.0251(2) 0.068 Uiso 1 calc R .
C21 C 0.3244(9) 0.6387(27) -0.0029(2) 0.060(3) Uani 1 d . .
H21 H 0.3597(9) 0.6416(27) -0.0229(2) 0.072 Uiso 1 calc R .
C22 C 0.2054(10) 0.5241(32) -0.0015(3) 0.068(4) Uani 1 d . .
H22 H 0.1594(10) 0.4510(32) -0.0207(3) 0.082 Uiso 1 calc R .
C23 C 0.1534(9) 0.5162(32) 0.0282(3) 0.070(4) Uani 1 d . .
H23 H 0.0730(9) 0.4361(32) 0.0291(3) 0.084 Uiso 1 calc R .
C24 C 0.2227(8) 0.6302(25) 0.0571(2) 0.050(3) Uani 1 d . .
H24 H 0.1874(8) 0.6241(25) 0.0772(2) 0.060 Uiso 1 calc R .
O25 O 0.1777(9) 1.2015(26) 0.2556(2) 0.105(4) Uani 1 d . .
C26 C 0.2297(14) 1.3580(43) 0.2818(4) 0.144(6) Uani 1 d . .
```

```
H26A H 0.1738(14) 1.3589(43) 0.2988(4) 0.216 Uiso 1 calc R .
H26B H 0.2487(14) 1.5889(43) 0.2761(4) 0.216 Uiso 1 calc R .
H26C H 0.3046(14) 1.2412(43) 0.2897(4) 0.216 Uiso 1 calc R .

loop_
 _atom_site_aniso_label
 _atom_site_aniso_U_11
 _atom_site_aniso_U_22
 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
N1 0.041(5) 0.081(8) 0.043(5) 0.012(5) -0.010(4) -0.003(5)
C2 0.043(6) 0.053(8) 0.044(6) 0.014(6) 0.009(5) 0.012(6)
N3 0.047(5) 0.081(8) 0.038(5) -0.011(5) 0.004(4) 0.004(6)
C4 0.053(6) 0.062(8) 0.037(6) 0.003(6) -0.013(5) -0.013(7)
N5 0.041(5) 0.059(7) 0.055(5) 0.003(5) 0.004(4) -0.003(5)
C6 0.040(6) 0.063(9) 0.055(7) 0.001(7) -0.002(5) 0.002(7)
C7 0.058(7) 0.063(9) 0.048(7) -0.005(7) -0.003(6) -0.002(7)
C8 0.057(7) 0.088(10) 0.042(6) 0.007(7) 0.001(5) 0.000(7)
C9 0.046(7) 0.097(11) 0.067(8) -0.001(8) 0.015(6) -0.023(7)
C10 0.059(7) 0.070(9) 0.039(6) -0.008(7) 0.019(5) 0.014(7)
C11 0.058(7) 0.072(9) 0.051(7) -0.006(7) 0.002(5) 0.003(7)
C12 0.060(7) 0.073(9) 0.069(7) -0.010(8) 0.004(6) 0.018(7)
C13 0.047(6) 0.055(8) 0.053(7) 0.010(7) -0.007(6) -0.010(7)
C14 0.047(7) 0.078(9) 0.060(7) -0.004(7) 0.007(6) 0.004(7)
C15 0.052(7) 0.107(12) 0.075(8) 0.014(9) -0.024(6) -0.006(9)
C16 0.047(7) 0.067(9) 0.095(9) 0.021(8) 0.008(7) -0.015(7)
C17 0.044(7) 0.086(10) 0.078(8) 0.000(8) 0.010(6) -0.002(7)
C18 0.065(8) 0.068(9) 0.046(6) 0.003(7) 0.002(5) 0.011(7)
C19 0.047(6) 0.026(7) 0.041(6) 0.007(5) 0.007(5) -0.005(5)
C20 0.054(7) 0.069(9) 0.044(6) -0.007(6) -0.007(5) -0.018(7)
C21 0.057(7) 0.070(9) 0.054(7) -0.013(7) 0.007(5) 0.002(7)
C22 0.068(8) 0.081(10) 0.057(7) 0.001(7) 0.007(6) 0.004(8)
C23 0.053(7) 0.088(10) 0.067(7) -0.012(8) -0.008(6) -0.009(7)
C24 0.056(7) 0.040(7) 0.058(7) 0.003(6) 0.019(6) -0.012(6)
O25 0.156(9) 0.108(8) 0.049(5) -0.023(5) -0.003(5) 0.007(7)
C26 0.157(15) 0.118(16) 0.161(15) 0.036(14) 0.037(13) 0.029(13)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
;

loop_
 _geom_bond_atom_site_label_1
 _geom_bond_atom_site_label_2
 _geom_bond_distance
 _geom_bond_site_symmetry_2
 _geom_bond_publ_flag
N1 C2 1.335(11) . ?
N1 C6 1.348(11) . ?
C2 N3 1.345(10) . ?
C2 C7 1.456(11) . ?
N3 C4 1.334(10) . ?
C4 N5 1.351(10) . ?
C4 C13 1.471(12) . ?
N5 C6 1.334(10) . ?
C6 C19 1.451(12) . ?
C7 C12 1.377(13) . ?
C7 C8 1.385(12) . ?
```

```
C8 C9 1.353(12) . ?
C8 H8 0.93 . ?
C9 C10 1.362(12) . ?
C9 H9 0.93 . ?
C10 C11 1.378(12) . ?
C10 O25 1.390(11) . ?
C11 C12 1.389(12) . ?
C11 H11 0.93 . ?
C12 H12 0.93 . ?
C13 C14 1.379(12) . ?
C13 C18 1.384(12) . ?
C14 C15 1.372(12) . ?
C14 H14 0.93 . ?
C15 C16 1.388(13) . ?
C15 H15 0.93 . ?
C16 C17 1.380(13) . ?
C16 H16 0.93 . ?
C17 C18 1.391(12) . ?
C17 H17 0.93 . ?
C18 H18 0.93 . ?
C19 C20 1.369(11) . ?
C19 C24 1.415(11) . ?
C20 C21 1.400(11) . ?
C20 H20 0.93 . ?
C21 C22 1.373(12) . ?
C21 H21 0.93 . ?
C22 C23 1.375(12) . ?
C22 H22 0.93 . ?
C23 C24 1.402(12) . ?
C23 H23 0.93 . ?
C24 H24 0.93 . ?
O25 C26 1.31(2) . ?
C26 H26A 0.96 . ?
C26 H26B 0.96 . ?
C26 H26C 0.96 . ?

loop_
 _geom_angle_atom_site_label_1
 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
 _geom_angle
 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
C2 N1 C6 113.6(8) . . ?
N1 C2 N3 126.4(8) . . ?
N1 C2 C7 116.0(9) . . ?
N3 C2 C7 117.5(10) . . ?
C4 N3 C2 114.4(8) . . ?
N3 C4 N5 125.0(9) . . ?
N3 C4 C13 117.3(9) . . ?
N5 C4 C13 117.6(9) . . ?
C6 N5 C4 114.7(8) . . ?
N5 C6 N1 125.8(9) . . ?
N5 C6 C19 115.6(9) . . ?
N1 C6 C19 118.4(9) . . ?
C12 C7 C8 114.2(10) . . ?
C12 C7 C2 122.8(10) . . ?
C8 C7 C2 123.0(10) . . ?
C9 C8 C7 123.6(10) . . ?
C9 C8 H8 118.2(7) . . ?
C7 C8 H8 118.2(6) . . ?
C8 C9 C10 120.0(10) . . ?
C8 C9 H9 120.0(7) . . ?
C10 C9 H9 120.0(6) . . ?
C9 C10 C11 120.6(9) . . ?
```

```
C9 C10 O25 114:1(10) . . ?
C11 C10 O25 125.3(10) . . ?
C10 C11 C12 116.9(10) . . ?
C10 C11 H11 121.6(6) . . ?
C12 C11 H11 121.6(7) . . ?
C7 C12 C11 124.8(11) . . ?
C7 C12 H12 117.6(6) . . ?
C11 C12 H12 117.6(7) . . ?
C14 C13 C18 118.2(10) . . ?
C14 C13 C4 121.0(10) . . ?
C18 C13 C4 120.8(10) . . ?
C15 C14 C13 121.1(10) . . ?
C15 C14 H14 119.4(7) . . ?
C13 C14 H14 119.4(6) . . ?
C14 C15 C16 120.8(11) . . ?
C14 C15 H15 119.6(7) . . ?
C16 C15 H15 119.6(7) . . ?
C17 C16 C15 118.7(10) . . ?
C17 C16 H16 120.6(7) . . ?
C15 C16 H16 120.6(7) . . ?
C16 C17 C18 119.9(10) . . ?
C16 C17 H17 120.0(7) . . ?
C18 C17 H17 120.0(7) . . ?
C13 C18 C17 121.1(10) . . ?
C13 C18 H18 119.4(6) . . ?
C17 C18 H18 119.4(7) . . ?
C20 C19 C24 116.3(9) . . ?
C20 C19 C6 123.5(9) . . ?
C24 C19 C6 120.2(9) . . ?
C19 C20 C21 123.2(9) . . ?
C19 C20 H20 118.4(6) . . ?
C21 C20 H20 118.4(6) . . ?
C22 C21 C20 119.0(10) . . ?
C22 C21 H21 120.5(6) . . ?
C20 C21 H21 120.5(6) . . ?
C23 C22 C21 120.6(11) . . ?
C23 C22 H22 119.7(7) . . ?
C21 C22 H22 119.7(6) . . ?
C22 C23 C24 119.4(10) . . ?
C22 C23 H23 120.3(7) . . ?
C24 C23 H23 120.3(6) . . ?
C23 C24 C19 121.5(9) . . ?
C23 C24 H24 119.3(6) . . ?
C19 C24 H24 119.3(6) . . ?
C26 O25 C10 116.8(12) . . ?
O25 C26 H26A 109.5(8) . . ?
O25 C26 H26B 109.5(9) . . ?
H26A C26 H26B 109.5 . . ?
O25 C26 H26C 109.5(9) . . ?
H26A C26 H26C 109.5 . . ?
H26B C26 H26C 109.47(6) . . ?

loop_
 _geom_torsion_atom_site_label_1
 _geom_torsion_atom_site_label_2
 _geom_torsion_atom_site_label_3
 _geom_torsion_atom_site_label_4
 _geom_torsion
 _geom_torsion_site_symmetry_1
 _geom_torsion_site_symmetry_2
 _geom_torsion_site_symmetry_3
 _geom_torsion_site_symmetry_4
 _geom_torsion_publ_flag
 C6 N1 C2 N3 0.9(16) . . . . ?
 C6 N1 C2 C7 -177.6(10) . . . . ?
 N1 C2 N3 C4 0.4(16) . . . . ?
```

```
 C7 C2 N3 C4 178.8(10) . . . . ?
 C2 N3 C4 N5 -0.5(16) . . . . ?
 C2 N3 C4 C13 -177.6(10) . . . . ?
 N3 C4 N5 C6 -0.7(16) . . . . ?
 C13 C4 N5 C6 176.4(10) . . . . ?
 C4 N5 C6 N1 2.1(16) . . . . ?
 C4 N5 C6 C19 177.6(10) . . . . ?
 C2 N1 C6 N5 -2.2(16) . . . . ?
 C2 N1 C6 C19 -177.6(10) . . . . ?
 N1 C2 C7 C12 -172.2(11) . . . . ?
 N3 C2 C7 C12 9.1(16) . . . . ?
 N1 C2 C7 C8 6.0(16) . . . . ?
 N3 C2 C7 C8 -172.6(11) . . . . ?
 C12 C7 C8 C9 -0.7(18) . . . . ?
 C2 C7 C8 C9 -179.1(12) . . . . ?
 C7 C8 C9 C10 -0.4(19) . . . . ?
 C8 C9 C10 C11 0.8(18) . . . . ?
 C8 C9 C10 O25 -178.8(11) . . . . ?
 C9 C10 C11 C12 0.0(17) . . . . ?
 O25 C10 C11 C12 179.6(11) . . . . ?
 C8 C7 C12 C11 1.6(17) . . . . ?
 C2 C7 C12 C11 180.0(11) . . . . ?
 C10 C11 C12 C7 -1.3(17) . . . . ?
 N3 C4 C13 C14 -9.5(15) . . . . ?
 N5 C4 C13 C14 173.2(10) . . . . ?
 N3 C4 C13 C18 170.1(11) . . . . ?
 N5 C4 C13 C18 -7.2(15) . . . . ?
 C18 C13 C14 C15 -2.1(17) . . . . ?
 C4 C13 C14 C15 177.5(11) . . . . ?
 C13 C14 C15 C16 0.9(19) . . . . ?
 C14 C15 C16 C17 -0.5(19) . . . . ?
 C15 C16 C17 C18 1.4(18) . . . . ?
 C14 C13 C18 C17 3.0(17) . . . . ?
 C4 C13 C18 C17 -176.6(10) . . . . ?
 C16 C17 C18 C13 -2.7(18) . . . . ?
 N5 C6 C19 C20 -7.3(16) . . . . ?
 N1 C6 C19 C20 168.5(11) . . . . ?
 N5 C6 C19 C24 171.8(10) . . . . ?
 N1 C6 C19 C24 -12.4(15) . . . . ?
 C24 C19 C20 C21 1.1(16) . . . . ?
 C6 C19 C20 C21 -179.7(11) . . . . ?
 C19 C20 C21 C22 -0.3(17) . . . . ?
 C20 C21 C22 C23 -0.7(18) . . . . ?
 C21 C22 C23 C24 0.7(19) . . . . ?
 C22 C23 C24 C19 0.2(17) . . . . ?
 C20 C19 C24 C23 -1.0(15) . . . . ?
 C6 C19 C24 C23 179.8(11) . . . . ?
 C9 C10 O25 C26 -177.3(13) . . . . ?
 C11 C10 O25 C26 3.1(18) . . . . ?

_refine_diff_density_max    0.282
_refine_diff_density_min   -0.193
_refine_diff_density_rms    0.048
```

Table 1. Crystal data and structure refinement for 1.

Identification code	c:\sonja\s499rm\s499rm
Empirical formula	C22 H17 N3 O
Formula weight	339.39
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system	monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 10.841(3) A alpha = 90 deg. b = 3.914(1) A beta = 95.49(2) deg. c = 40.479(9) A gamma = 90 deg.
Volume, Z	1709.7(7) A^3, 4
Density (calculated)	1.318 Mg/m^3
Absorption coefficient	0.083 mm^-1
F(000)	712
Crystal size	1.2 x 0.1 x 0.04 mm
Theta range for data collection	1.01 to 22.49 deg.
Limiting indices	0<=h<=12, 0<=k<=4, -46<=l<=46
Reflections collected	2389
Independent reflections	2245 [R(int) = 0.0461]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1770 / 0 / 236
Goodness-of-fit on F^2	1.118
Final R indices [I>2sigma(I)]	R1 = 0.1148, wR2 = 0.1883
R indices (all data)	R1 = 0.2716, wR2 = 0.2745
Extinction coefficient	0.014(2)
Largest diff. peak and hole	0.282 and -0.193 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	3528(6)	9205(24)	1139(2)	56(3)
C(2)	4241(9)	10409(28)	1400(2)	46(3)
N(3)	5454(7)	11166(24)	1411(2)	55(3)
C(4)	5952(9)	10638(29)	1127(2)	52(3)
N(5)	5335(7)	9426(23)	845(2)	51(2)
C(6)	4143(9)	8717(29)	868(2)	53(3)
C(7)	3638(9)	10857(30)	1704(2)	57(3)
C(8)	2434(9)	9813(32)	1735(2)	63(3)
C(9)	1857(9)	10255(33)	2014(3)	69(4)
C(10)	2467(10)	11780(30)	2284(2)	55(3)
C(11)	3667(9)	12923(29)	2276(2)	60(3)
C(12)	4206(10)	12438(31)	1982(3)	67(3)
C(13)	7289(9)	11282(28)	1124(2)	52(3)
C(14)	7957(9)	12846(30)	1389(2)	61(3)
C(15)	9212(10)	13331(36)	1393(3)	80(4)
C(16)	9843(10)	12299(31)	1128(3)	69(4)
C(17)	9186(9)	10747(32)	860(3)	69(4)
C(18)	7911(10)	10311(29)	857(2)	60(3)
C(19)	3450(8)	7543(26)	565(2)	38(2)
C(20)	3920(9)	7511(29)	263(2)	56(3)
C(21)	3244(9)	6387(27)	-29(2)	60(3)
C(22)	2054(10)	5241(32)	-15(3)	68(4)
C(23)	1534(9)	5162(32)	282(3)	70(4)
C(24)	2227(8)	6302(25)	571(2)	50(3)
O(25)	1777(9)	12015(26)	2556(2)	105(4)
C(26)	2297(14)	13580(43)	2818(4)	144(6)

Table 3. Bond lengths [A] and angles [deg] for 1.

N(1)-C(2)	1.335(11)
N(1)-C(6)	1.348(11)
C(2)-N(3)	1.345(10)
C(2)-C(7)	1.456(11)
N(3)-C(4)	1.334(10)
C(4)-N(5)	1.351(10)
C(4)-C(13)	1.471(12)
N(5)-C(6)	1.334(10)
C(6)-C(19)	1.451(12)
C(7)-C(12)	1.377(13)
C(7)-C(8)	1.385(12)
C(8)-C(9)	1.353(12)
C(8)-H(8)	0.93
C(9)-C(10)	1.362(12)
C(9)-H(9)	0.93
C(10)-C(11)	1.378(12)
C(10)-O(25)	1.390(11)
C(11)-C(12)	1.389(12)
C(11)-H(11)	0.93
C(12)-H(12)	0.93
C(13)-C(14)	1.379(12)
C(13)-C(18)	1.384(12)
C(14)-C(15)	1.372(12)
C(14)-H(14)	0.93
C(15)-C(16)	1.388(13)
C(15)-H(15)	0.93
C(16)-C(17)	1.380(13)
C(16)-H(16)	0.93
C(17)-C(18)	1.391(12)
C(17)-H(17)	0.93
C(18)-H(18)	0.93
C(19)-C(20)	1.369(11)
C(19)-C(24)	1.415(11)
C(20)-C(21)	1.400(11)
C(20)-H(20)	0.93
C(21)-C(22)	1.373(12)
C(21)-H(21)	0.93
C(22)-C(23)	1.375(12)
C(22)-H(22)	0.93
C(23)-C(24)	1.402(12)
C(23)-H(23)	0.93
C(24)-H(24)	0.93
O(25)-C(26)	1.31(2)
C(26)-H(26A)	0.96
C(26)-H(26B)	0.96
C(26)-H(26C)	0.96

C(2)-N(1)-C(6)	113.6(8)
N(1)-C(2)-N(3)	126.4(8)
N(1)-C(2)-C(7)	116.0(9)
N(3)-C(2)-C(7)	117.5(10)
C(4)-N(3)-C(2)	114.4(8)
N(3)-C(4)-N(5)	125.0(9)
N(3)-C(4)-C(13)	117.3(9)
N(5)-C(4)-C(13)	117.6(9)
C(6)-N(5)-C(4)	114.7(8)
N(5)-C(6)-N(1)	125.8(9)
N(5)-C(6)-C(19)	115.6(9)
N(1)-C(6)-C(19)	118.4(9)
C(12)-C(7)-C(8)	114.2(10)
C(12)-C(7)-C(2)	122.8(10)
C(8)-C(7)-C(2)	123.0(10)

C(9)-C(8)-C(7)	123.6(10)
C(9)-C(8)-H(8)	118.2(7)
C(7)-C(8)-H(8)	118.2(6)
C(8)-C(9)-C(10)	120.0(10)
C(8)-C(9)-H(9)	120.0(7)
C(10)-C(9)-H(9)	120.0(6)
C(9)-C(10)-C(11)	120.6(9)
C(9)-C(10)-O(25)	114.1(10)
C(11)-C(10)-O(25)	125.3(10)
C(10)-C(11)-C(12)	116.9(10)
C(10)-C(11)-H(11)	121.6(6)
C(12)-C(11)-H(11)	121.6(7)
C(7)-C(12)-C(11)	124.8(11)
C(7)-C(12)-H(12)	117.6(6)
C(11)-C(12)-H(12)	117.6(7)
C(14)-C(13)-C(18)	118.2(10)
C(14)-C(13)-C(4)	121.0(10)
C(18)-C(13)-C(4)	120.8(10)
C(15)-C(14)-C(13)	121.1(10)
C(15)-C(14)-H(14)	119.4(7)
C(13)-C(14)-H(14)	119.4(6)
C(14)-C(15)-C(16)	120.8(11)
C(14)-C(15)-H(15)	119.6(7)
C(16)-C(15)-H(15)	119.6(7)
C(17)-C(16)-C(15)	118.7(10)
C(17)-C(16)-H(16)	120.6(7)
C(15)-C(16)-H(16)	120.6(7)
C(16)-C(17)-C(18)	119.9(10)
C(16)-C(17)-H(17)	120.0(7)
C(18)-C(17)-H(17)	120.0(7)
C(13)-C(18)-C(17)	121.1(10)
C(13)-C(18)-H(18)	119.4(6)
C(17)-C(18)-H(18)	119.4(7)
C(20)-C(19)-C(24)	116.3(9)
C(20)-C(19)-C(6)	123.5(9)
C(24)-C(19)-C(6)	120.2(9)
C(19)-C(20)-C(21)	123.2(9)
C(19)-C(20)-H(20)	118.4(6)
C(21)-C(20)-H(20)	118.4(6)
C(22)-C(21)-C(20)	119.0(10)
C(22)-C(21)-H(21)	120.5(6)
C(20)-C(21)-H(21)	120.5(6)
C(23)-C(22)-C(21)	120.6(11)
C(23)-C(22)-H(22)	119.7(7)
C(21)-C(22)-H(22)	119.7(6)
C(22)-C(23)-C(24)	119.4(10)
C(22)-C(23)-H(23)	120.3(7)
C(24)-C(23)-H(23)	120.3(6)
C(23)-C(24)-C(19)	121.5(9)
C(23)-C(24)-H(24)	119.3(6)
C(19)-C(24)-H(24)	119.3(6)
C(26)-O(25)-C(10)	116.8(12)
O(25)-C(26)-H(26A)	109.5(8)
O(25)-C(26)-H(26B)	109.5(9)
H(26A)-C(26)-H(26B)	109.5
O(25)-C(26)-H(26C)	109.5(9)
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.47(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 1.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	41(5)	81(8)	43(5)	12(5)	-10(4)	-3(5)
C(2)	43(6)	53(8)	44(6)	14(6)	9(5)	12(6)
N(3)	47(5)	81(8)	38(5)	-11(5)	4(4)	4(6)
C(4)	53(6)	62(8)	37(6)	3(6)	-13(5)	-13(7)
N(5)	41(5)	59(7)	55(5)	3(5)	4(4)	-3(5)
C(6)	40(6)	63(9)	55(7)	1(7)	-2(5)	2(7)
C(7)	58(7)	63(9)	48(7)	-5(7)	-3(6)	-2(7)
C(8)	57(7)	88(10)	42(6)	7(7)	1(5)	0(7)
C(9)	46(7)	97(11)	67(8)	-1(8)	15(6)	-23(7)
C(10)	59(7)	70(9)	39(6)	-8(7)	19(5)	14(7)
C(11)	58(7)	72(9)	51(7)	-6(7)	2(5)	3(7)
C(12)	60(7)	73(9)	69(7)	-10(8)	4(6)	18(7)
C(13)	47(6)	55(8)	53(7)	10(7)	-7(6)	-10(7)
C(14)	47(7)	78(9)	60(7)	-4(7)	7(6)	4(7)
C(15)	52(7)	107(12)	75(8)	14(9)	-24(6)	-6(9)
C(16)	47(7)	67(9)	95(9)	21(8)	8(7)	-15(7)
C(17)	44(7)	86(10)	78(8)	0(8)	10(6)	-2(7)
C(18)	65(8)	68(9)	46(6)	3(7)	2(5)	11(7)
C(19)	47(6)	26(7)	41(6)	7(5)	7(5)	-5(5)
C(20)	54(7)	69(9)	44(6)	-7(6)	-7(5)	-18(7)
C(21)	57(7)	70(9)	54(7)	-13(7)	7(5)	2(7)
C(22)	68(8)	81(10)	57(7)	1(7)	7(6)	4(8)
C(23)	53(7)	88(10)	67(7)	-12(8)	-8(6)	-9(7)
C(24)	56(7)	40(7)	58(7)	3(6)	19(6)	-12(6)
O(25)	156(9)	108(8)	49(5)	-23(5)	-3(5)	7(7)
C(26)	157(15)	118(16)	161(15)	36(14)	37(13)	29(13)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1.

	x	y	z	U(eq)
H(8)	1998(9)	8751(32)	1554(2)	75
H(9)	1044(9)	9519(33)	2021(3)	83
H(11)	4095(9)	13969(29)	2459(2)	72
H(12)	5009(10)	13240(31)	1972(3)	81
H(14)	7550(9)	13586(30)	1568(2)	74
H(15)	9645(10)	14364(36)	1576(3)	96
H(16)	10692(10)	12646(31)	1131(3)	83
H(17)	9595(9)	9992(32)	682(3)	83
H(18)	7470(10)	9351(29)	671(2)	72
H(20)	4727(9)	8273(29)	251(2)	68
H(21)	3597(9)	6416(27)	-229(2)	72
H(22)	1594(10)	4510(32)	-207(3)	82
H(23)	730(9)	4361(32)	291(3)	84
H(24)	1874(8)	6241(25)	772(2)	60
H(26A)	1738(14)	13589(43)	2988(4)	216
H(26B)	2487(14)	15889(43)	2761(4)	216
H(26C)	3046(14)	12412(43)	2897(4)	216