EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{32}H_{29}O_5N$
Formula Weight	507.58
Crystal Color, Habit	colorless, platelet
Crystal Dimensions	0.10 X 0.10 X 0.10 mm
Crystal System	triclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	3920 (4.7 - 54.6°)
Indexing Images	2 oscillations at 1.7 minutes
Camera Radius	127.40 mm
Lattice Parameters	a = 10.3133(3) Å b = 17.3740(6) Å c = 7.9204(4) Å α = 101.164(3)° β = 106.457(3)° γ = 89.030(4)° V = 1334.23(10) Å^3
Space Group	$P\bar{1}$ (#2)
Z value	2
D_{calc}	1.263 g/cm^3
F_{000}	536.00
μ(MoKα)	0.85 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID Imaging Plate

Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Temperature	23.0 °C
Voltage, Current	50 kV, 40 mA
Collimator Size	0.8 mm
Detector Aperture	270.0 mm x 256.0 mm
Data Images	44 exposures at 1.0 minutes per degree
Oscillation Range (ϕ=0.0°,χ=45.0°)	ω 130.0 - 190.0° with 5.0° step
Oscillation Range (ϕ=180.0°,χ=45.0°)	ω 0.0 - 160.0° with 5.0° step
Camera Radius	127.40 mm
Pixel Size	0.100 mm
$2\theta_{max}$	54.9°
No. of Reflections Measured	Total: 7179 Unique: 5672 (R_{int} = 0.027)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.8829 - 0.9915)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR88)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = \frac{1}{\sigma^2(Fo^2)}$
p-factor	0.0500
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>-10.00σ(I))	5668
No. Variables	459
Reflection/Parameter Ratio	12.35
Residuals: R; Rw	0.081 ; 0.148

Residuals: R1	0.059
No. of Reflections to calc R1	3020
Goodness of Fit Indicator	1.41
Max Shift/Error in Final Cycle	0.433
Maximum peak in Final Diff. Map	0.35 $e^-/\AA^3$
Minimum peak in Final Diff. Map	-0.33 $e^-/\AA^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
O(1)	0.6630(2)	-0.0172(1)	0.3503(3)	7.19(6)
O(2)	0.8946(2)	0.29370(9)	0.4650(2)	4.78(4)
O(3)	0.6796(2)	0.3165(1)	0.3120(2)	6.13(5)
O(4)	0.8510(2)	0.1465(1)	0.8627(2)	6.24(5)
O(5)	0.6732(2)	0.1841(1)	0.6525(2)	6.28(5)
N(1)	0.8610(2)	0.1470(1)	0.5781(2)	4.51(5)
C(1)	0.7951(2)	0.1613(1)	0.3959(3)	3.99(5)
C(2)	0.8864(3)	0.2167(1)	0.3478(3)	4.63(6)
C(3)	1.0315(3)	0.1911(2)	0.3795(4)	6.00(8)
C(4)	1.0921(3)	0.1763(2)	0.5675(5)	6.27(8)
C(5)	1.0019(3)	0.1207(2)	0.6128(4)	5.87(8)
C(6)	0.7587(3)	0.0838(1)	0.2544(3)	4.74(6)
C(7)	0.6407(3)	0.0390(1)	0.2769(3)	4.92(6)
C(8)	0.5000(3)	0.0661(1)	0.2131(3)	4.50(6)
C(9)	0.4691(3)	0.1271(2)	0.1185(3)	5.69(7)
C(10)	0.3359(4)	0.1494(2)	0.0581(4)	6.97(9)
C(11)	0.2325(4)	0.1109(2)	0.0927(4)	7.04(9)
C(12)	0.2612(4)	0.0523(2)	0.1878(5)	7.04(9)
C(13)	0.3932(3)	0.0292(2)	0.2485(4)	5.82(7)
C(14)	0.7837(3)	0.3372(1)	0.4324(3)	4.61(6)
C(15)	0.8038(2)	0.4129(1)	0.5644(3)	4.34(6)
C(16)	0.9300(3)	0.4493(1)	0.6469(3)	4.49(6)
C(17)	0.9479(2)	0.5225(1)	0.7683(3)	4.44(6)
C(18)	1.0775(3)	0.5621(2)	0.8529(4)	5.61(7)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(19)	1.0891(4)	0.6325(2)	0.9667(4)	6.56(9)
C(20)	0.9748(4)	0.6673(2)	1.0047(4)	6.99(9)
C(21)	0.8500(4)	0.6309(2)	0.9298(4)	6.53(8)
C(22)	0.8307(3)	0.5573(1)	0.8070(3)	4.96(6)
C(23)	0.7014(3)	0.5179(2)	0.7226(4)	5.64(7)
C(24)	0.6881(3)	0.4483(2)	0.6022(4)	5.32(7)
C(25)	0.8002(3)	0.1577(1)	0.7101(3)	4.61(6)
C(26)	0.5953(4)	0.1987(2)	0.7823(5)	7.05(9)
C(27)	0.5044(2)	0.2645(1)	0.7390(3)	4.68(6)
C(28)	0.5010(4)	0.3279(2)	0.8748(4)	7.14(9)
C(29)	0.4118(5)	0.3905(2)	0.8270(7)	8.7(1)
C(30)	0.3368(4)	0.3856(2)	0.6531(6)	8.1(1)
C(31)	0.3438(4)	0.3241(2)	0.5243(6)	7.9(1)
C(32)	0.4261(3)	0.2643(2)	0.5664(4)	6.33(8)
H(1)	1.164(3)	0.536(1)	0.829(3)	6.3(6)
H(2)	0.707(2)	0.186(1)	0.394(2)	3.5(4)
H(3)	0.844(2)	0.222(1)	0.220(3)	5.3(5)
H(4)	1.027(2)	0.142(2)	0.295(3)	5.8(6)
H(5)	1.088(3)	0.231(2)	0.349(4)	8.2(7)
H(6)	1.184(3)	0.157(2)	0.590(4)	7.8(7)
H(7)	1.106(2)	0.225(2)	0.652(3)	6.3(6)
H(8)	1.028(3)	0.115(1)	0.728(4)	6.5(7)
H(9)	0.994(3)	0.061(2)	0.534(3)	7.0(6)
H(10)	0.839(2)	0.050(1)	0.272(3)	5.3(5)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(11)	0.740(2)	0.096(1)	0.138(3)	5.7(6)
H(12)	1.007(2)	0.424(1)	0.625(3)	4.7(5)
H(13)	1.174(3)	0.657(2)	1.021(4)	7.2(7)
H(14)	0.990(3)	0.715(2)	1.091(4)	8.8(8)
H(15)	0.765(3)	0.655(2)	0.953(4)	9.0(8)
H(16)	0.613(3)	0.543(2)	0.747(3)	7.3(6)
H(17)	0.602(3)	0.421(1)	0.544(3)	5.8(6)
H(18)	0.425(3)	-0.011(2)	0.325(3)	6.4(6)
H(19)	0.540(3)	0.153(2)	0.094(3)	6.2(6)
H(20)	0.325(4)	0.191(2)	-0.012(5)	11.0(9)
H(21)	0.136(3)	0.121(2)	0.052(4)	8.4(8)
H(22)	0.186(4)	0.024(2)	0.204(4)	10.5(9)
H(23)	0.416(4)	0.431(2)	0.912(5)	10.8(10)
H(24)	0.273(4)	0.431(2)	0.631(5)	11.8(10)
H(25)	0.286(5)	0.320(3)	0.393(6)	14(1)
H(26)	0.443(4)	0.211(2)	0.461(5)	13.1(10)
H(27)	0.548(3)	0.324(2)	0.984(4)	8.8(9)
H(28)	0.659(4)	0.206(2)	0.915(6)	12(1)
H(29)	0.534(3)	0.146(2)	0.756(4)	9.4(8)

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters

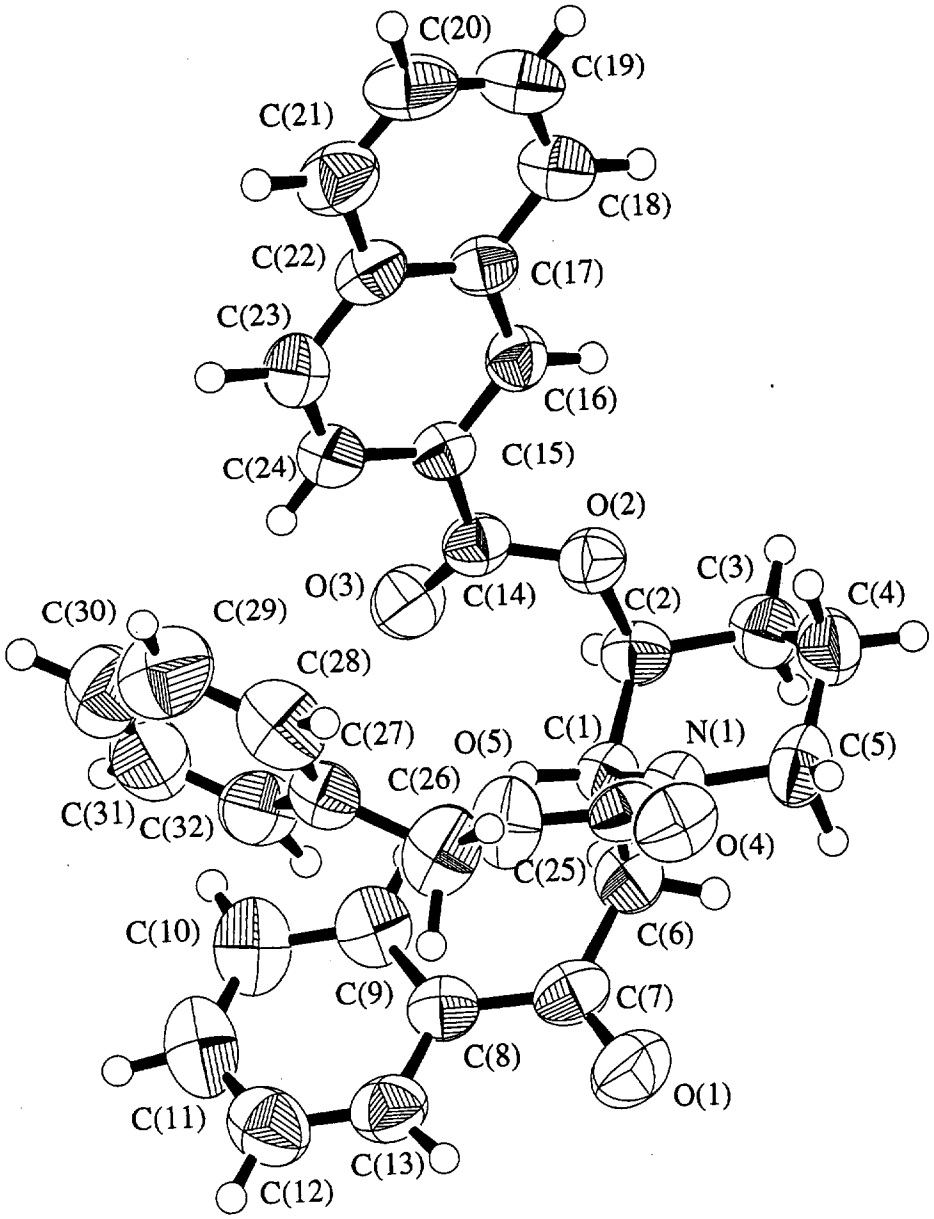
atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	0.105(2)	0.070(1)	0.105(1)	0.013(1)	0.031(1)	0.033(1)
O(2)	0.063(1)	0.0535(10)	0.0601(10)	0.0015(8)	0.0146(8)	0.0043(8)
O(3)	0.080(1)	0.071(1)	0.066(1)	0.0016(10)	-0.003(1)	0.0097(9)
O(4)	0.107(1)	0.080(1)	0.0514(10)	0.004(1)	0.0166(10)	0.0227(9)
O(5)	0.085(1)	0.108(1)	0.062(1)	0.026(1)	0.0413(10)	0.030(1)
N(1)	0.065(1)	0.058(1)	0.046(1)	0.0075(10)	0.0147(10)	0.0071(9)
C(1)	0.057(1)	0.050(1)	0.042(1)	0.004(1)	0.015(1)	0.0024(10)
C(2)	0.069(2)	0.055(1)	0.051(1)	-0.001(1)	0.022(1)	0.001(1)
C(3)	0.072(2)	0.075(2)	0.085(2)	0.003(2)	0.039(2)	-0.001(2)
C(4)	0.059(2)	0.077(2)	0.094(2)	0.010(2)	0.021(2)	0.002(2)
C(5)	0.073(2)	0.074(2)	0.068(2)	0.022(2)	0.009(2)	0.013(2)
C(6)	0.067(2)	0.057(2)	0.050(1)	0.001(1)	0.020(1)	-0.006(1)
C(7)	0.087(2)	0.048(1)	0.048(1)	-0.001(1)	0.019(1)	-0.001(1)
C(8)	0.071(2)	0.053(1)	0.043(1)	-0.003(1)	0.018(1)	-0.003(1)
C(9)	0.079(2)	0.089(2)	0.053(1)	0.005(2)	0.023(1)	0.018(1)
C(10)	0.092(2)	0.118(3)	0.058(2)	0.022(2)	0.024(2)	0.024(2)
C(11)	0.076(2)	0.125(3)	0.056(2)	0.020(2)	0.016(2)	-0.003(2)
C(12)	0.080(2)	0.091(2)	0.094(2)	-0.007(2)	0.034(2)	-0.004(2)
C(13)	0.085(2)	0.056(2)	0.080(2)	-0.001(2)	0.030(2)	0.002(1)
C(14)	0.067(2)	0.056(1)	0.052(1)	0.000(1)	0.014(1)	0.016(1)
C(15)	0.061(2)	0.050(1)	0.055(1)	0.002(1)	0.016(1)	0.012(1)
C(16)	0.056(2)	0.055(1)	0.062(1)	0.005(1)	0.021(1)	0.014(1)
C(17)	0.068(2)	0.051(1)	0.054(1)	-0.003(1)	0.022(1)	0.013(1)
C(18)	0.076(2)	0.065(2)	0.072(2)	-0.011(1)	0.024(2)	0.007(1)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(19)	0.093(2)	0.076(2)	0.078(2)	-0.023(2)	0.025(2)	0.004(2)
C(20)	0.121(3)	0.061(2)	0.079(2)	-0.017(2)	0.035(2)	-0.008(2)
C(21)	0.101(2)	0.061(2)	0.089(2)	0.007(2)	0.039(2)	0.004(2)
C(22)	0.079(2)	0.050(1)	0.067(1)	0.006(1)	0.030(1)	0.015(1)
C(23)	0.064(2)	0.068(2)	0.084(2)	0.009(1)	0.026(2)	0.012(1)
C(24)	0.061(2)	0.062(2)	0.076(2)	0.000(1)	0.014(1)	0.016(1)
C(25)	0.076(2)	0.044(1)	0.052(1)	-0.001(1)	0.015(1)	0.006(1)
C(26)	0.110(3)	0.102(2)	0.087(2)	0.029(2)	0.064(2)	0.041(2)
C(27)	0.063(2)	0.069(2)	0.052(1)	-0.003(1)	0.028(1)	0.011(1)
C(28)	0.095(2)	0.118(3)	0.063(2)	-0.004(2)	0.038(2)	0.004(2)
C(29)	0.138(3)	0.097(3)	0.118(3)	0.019(3)	0.083(3)	0.002(2)
C(30)	0.098(3)	0.112(3)	0.124(3)	0.026(2)	0.062(3)	0.043(3)
C(31)	0.081(2)	0.115(3)	0.107(3)	0.003(2)	0.024(2)	0.034(2)
C(32)	0.082(2)	0.083(2)	0.073(2)	-0.004(2)	0.013(2)	0.022(2)

The general temperature factor expression:

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


C(20)
C(19)
C(21)
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