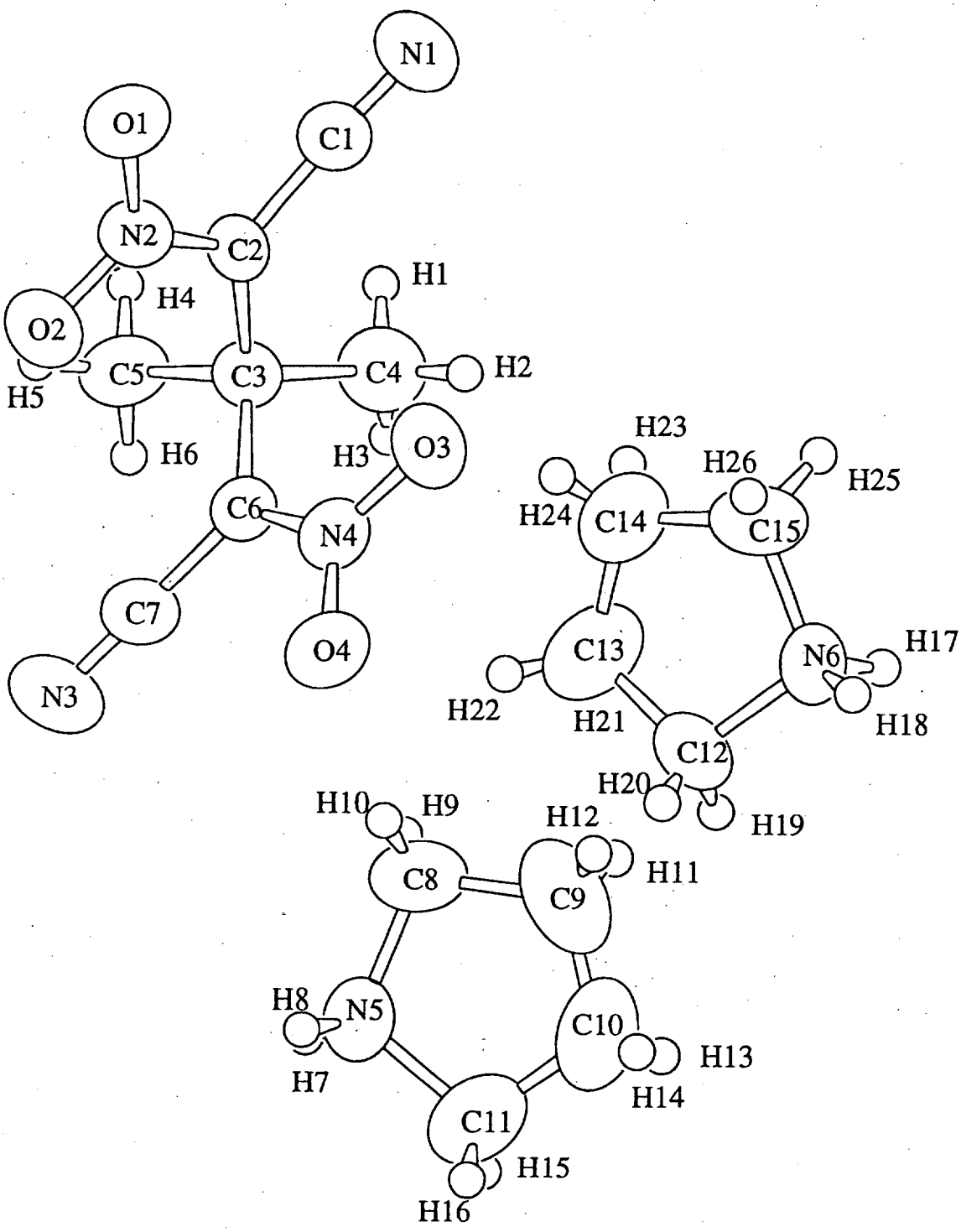

Figure 1. Atomic numbering with thermal ellipsoids drawn at 50% probability

Table 1. Experimental Details

A. Crystal Data

Empirical Formula	$C_7H_6N_4O_4 \cdot (C_4H_{10}N)_2$
Formula Weight	354.41
Crystal Color ,Habit	Colorless, prism
Crystal Dimensions	0.40 X 0.40 X 0.15mm
Crystal System	triclinic
No. of Reflections Used for Unit Cell Determination (2θ range)	17 (20.2°- 24.1°)
Omega Scan Peak Width at Half-height	0.23°
Lattice Parameters	a = 10.223(4) Å b = 10.397(3) Å c = 10.201(3) Å α = 114.38(2)° β = 103.62(3)° γ = 80.41(3)° V = 956.7(6) Å^3
Space Group	$P\bar{1}$(#2)
Z value	2
D_{calc}	1.230 g/cm^3
F_{000}	380.00
μ (Mo$K\alpha$)	0.91 cm^{-1}

B: Intensity Measurements

Diffractometer	Rigaku AFC7R
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Temperature	20.0°C
Scan Type	ω-2θ
Scan Rate	16.0°/min(in ω) - up to 5 scans
Scan Width	(0.94 + 0.30 tan θ)°
$2\theta_{max}$	55.0°
No. of Reflection Measured	Total: 4661 Unique: 4414 (R_{int} = 0.038)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.8825 - 1.0779)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (MITHRIL90)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma\omega(\|F_o\|-\|F_c\|)^2$
Least Squares Weights	$1/\sigma^2(F_o) = 4F_o^2/\sigma^2(F_o^2)$
p-factor	0.01

C. Structure Solution and Refinement(continued)

No. Observations($I > 3.00\sigma(I)$)	1619
No. Variables	226
Residuals: R; Rw	0.056; 0.050
Goodness of Fit Indicator	2.38
Max Shift/Error in Final Cycle	0.10
Maximum peak in Final Diff. Map	0.32 $e^-/Å^3$
Minimum Peak in Final Diff. Map	-0.30 $e^-/Å^3$

Table 2. Intramolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance	atom	atom	distance
O(1)	N(2)	1.313(4)	C(1)	C(2)	1.414(6)
O(2)	N(2)	1.272(4)	C(2)	C(3)	1.515(6)
O(3)	N(4)	1.279(4)	C(3)	C(4)	1.534(6)
O(4)	N(4)	1.297(4)	C(3)	C(5)	1.540(6)
N(1)	C(1)	1.137(6)	C(3)	C(6)	1.523(6)
N(2)	C(2)	1.331(5)	C(6)	C(7)	1.414(6)
N(3)	C(7)	1.139(5)	N(4)	C(6)	1.331(5)
C(8)	C(9)	1.443(8)	C(9)	C(10)	1.37(1)
N(5)	C(8)	1.500(6)	C(10)	C(11)	1.425(9)
N(5)	C(11)	1.499(6)	C(12)	C(13)	1.453(9)
N(6)	C(12)	1.465(6)	C(13)	C(14)	1.366(9)
N(6)	C(15)	1.473(6)	C(14)	C(15)	1.436(8)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parenthes.

Table 3. Intramolecular Bond Angles Involving the Nonhydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	C(1)	C(2)	177.0(6)	N(2)	C(2)	C(1)	115.5(4)
N(2)	C(2)	C(3)	121.7(4)	N(3)	C(7)	C(6)	178.6(6)
N(4)	C(6)	C(7)	115.5(4)	N(4)	C(6)	C(3)	122.3(4)
O(1)	N(2)	O(2)	117.3(4)	O(1)	N(2)	C(2)	120.5(4)
O(2)	N(2)	C(2)	122.2(4)	O(3)	N(4)	O(4)	118.4(4)
O(3)	N(4)	C(6)	121.0(4)	O(4)	N(4)	C(6)	120.6(4)
C(1)	C(2)	C(3)	122.8(4)	C(2)	C(3)	C(4)	110.4(4)
C(2)	C(3)	C(5)	108.5(4)	C(2)	C(3)	C(6)	110.1(4)
C(4)	C(3)	C(5)	108.7(4)	C(4)	C(3)	C(6)	109.1(4)
C(5)	C(3)	C(6)	109.9(4)	C(3)	C(6)	C(7)	122.2(4)
N(5)	C(8)	C(9)	104.5(5)	N(5)	C(11)	C(10)	105.1(5)
C(8)	N(5)	C(11)	107.3(4)	C(8)	C(9)	C(10)	111.2(7)
C(9)	C(10)	C(11)	111.4(7)	N(6)	C(12)	C(13)	103.1(5)
N(6)	C(15)	C(14)	107.3(5)	C(12)	N(6)	C(15)	106.1(4)
C(12)	C(13)	C(14)	112.1(7)	C(13)	C(14)	C(15)	107.3(6)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table 4. Torsion Angles(°) except for pyrrolidium ions

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
O(1)	N(2)	C(2)	C(1)	1.4(6)	N(4)	C(6)	C(3)	C(5)	-176.1(4)
O(1)	N(2)	C(2)	C(3)	-177.8(4)	O(2)	N(2)	C(2)	C(1)	-177.3(4)
O(2)	N(2)	C(2)	C(3)	3.4(7)	O(3)	N(4)	C(6)	C(3)	0.6(7)

Table 4. Torsion Angles(°) except for pyrrolidium ions (continued)

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
O(3)	N(4)	C(6)	C(7)	-176.9(4)	C(1)	C(2)	C(3)	C(4)	6.2(6)
O(4)	N(4)	C(6)	C(3)	179.6(4)	C(1)	C(2)	C(3)	C(5)	-112.9(5)
O(4)	N(4)	C(6)	C(7)	2.2(6)	C(1)	C(2)	C(3)	C(6)	126.8(5)
N(1)	C(1)	C(2)	N(2)	161(12)	C(2)	C(3)	C(6)	C(7)	120.6(5)
N(1)	C(1)	C(2)	C(3)	-19(12)	C(4)	C(3)	C(6)	C(7)	-118.0(5)
N(2)	C(2)	C(3)	C(4)	-174.6(4)	C(5)	C(3)	C(6)	C(7)	1.2(6)
N(2)	C(2)	C(3)	C(5)	66.3(5)	N(2)	C(2)	C(3)	C(6)	-54.0(6)
N(4)	C(6)	C(3)	C(2)	-56.7(6)	N(4)	C(6)	C(3)	C(4)	64.7(5)

The sign is positive if when looking from atom 2 to atom 3 a clock-wise motion of atom 1 would superimpose it on atom 4.

Table 5. Positional parameters and B_{eq}

atom	x	y	z	B_{eq}
O(1)	1.1077(3)	0.2930(3)	1.0464(4)	4.9(1)
O(2)	0.9337(3)	0.3100(4)	1.1478(4)	4.8(1)
O(3)	0.7751(3)	0.0585(3)	0.7577(4)	5.1(1)
O(4)	0.6639(3)	0.0057(3)	0.8883(4)	4.9(1)
N(1)	1.0012(5)	0.3114(5)	0.7178(5)	7.0(2)
N(2)	0.9766(4)	0.3108(4)	1.0408(5)	3.8(1)
N(3)	0.5654(5)	0.2973(5)	1.1545(5)	6.6(2)
N(4)	0.7094(4)	0.1003(4)	0.8624(4)	3.9(1)
C(1)	0.9561(5)	0.3187(5)	0.8126(6)	4.3(1)
C(2)	0.8934(5)	0.3263(5)	0.9256(5)	3.4(1)
C(3)	0.7421(4)	0.3522(5)	0.9183(5)	3.5(1)
C(4)	0.6706(5)	0.3517(6)	0.7679(6)	5.4(2)
C(5)	0.7118(4)	0.4985(5)	1.0368(6)	4.7(1)
C(6)	0.6897(4)	0.2375(5)	0.9443(5)	3.4(1)

Table 5. Positional parameters and B_{eq} (continued)

atom	x	y	z	B_{eq}
C(7)	0.6216(5)	0.2693(5)	1.0611(6)	4.1(1)
H(1)	0.7042	0.4255	0.7548	5.9
H(2)	0.6886	0.2544	0.6881	8.3
H(3)	0.5859	0.3705	0.7626	8.0
H(4)	0.7432	0.5745	1.0204	5.7
H(5)	0.7650	0.5058	1.1317	6.4
H(6)	0.6111	0.5144	1.0336	6.5
N(5)	0.2331(4)	0.0537(4)	0.8663(4)	4.6(1)
N(6)	0.2032(4)	0.2470(4)	0.3165(4)	4.2(1)
C(8)	0.3292(6)	0.0772(6)	0.7891(7)	7.0(2)
C(9)	0.294(1)	-0.020(1)	0.6389(9)	11.2(3)
C(10)	0.188(1)	-0.096(1)	0.620(1)	16.0(4)
C(11)	0.1374(6)	-0.0497(6)	0.7524(8)	6.8(2)
C(12)	0.1397(6)	0.3057(7)	0.4460(6)	6.9(2)
C(13)	0.205(1)	0.436(1)	0.536(1)	19.7(4)
C(14)	0.3229(8)	0.4369(8)	0.4946(8)	10.5(3)
C(15)	0.3306(6)	0.3152(7)	0.3607(7)	7.9(2)
H(7)	0.1846	0.1401	0.9155	5.5
H(8)	0.2824	0.0156	0.9354	5.5
H(9)	0.3134	0.1717	0.7904	8.4
H(10)	0.4190	0.0598	0.8268	23.3
H(11)	0.2712	0.0277	0.5747	14.0
H(12)	0.3700	-0.0873	0.6135	14.0
H(13)	0.1180	-0.0790	0.5471	20.1
H(14)	0.2166	-0.1923	0.5893	20.1
H(15)	0.0486	-0.0054	0.7428	8.3
H(16)	0.1368	-0.1282	0.7774	8.3
H(17)	0.1465	0.2666	0.2376	5.0
H(18)	0.2210	0.1470	0.2872	5.0
H(19)	0.0459	0.3317	0.4202	8.3
H(20)	0.1496	0.2412	0.4914	8.3

Table 5. Positional parameters and B_{eq} (continued)

atom	x	y	z	B_{eq}
H(21)	0.1509	0.5125	0.5463	23.3
H(22)	0.2380	0.4287	0.6360	14.0
H(23)	0.3133	0.5226	0.4756	12.6
H(24)	0.4005	0.4397	0.5662	12.6
H(25)	0.3426	0.3430	0.2869	9.7
H(26)	0.4048	0.2524	0.3783	9.7

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

Table 6. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	0.034(2)	0.073(3)	0.073(3)	-0.000(2)	0.007(2)	0.026(2)
O(2)	0.057(2)	0.081(3)	0.053(2)	-0.003(2)	0.011(2)	0.035(2)
O(3)	0.073(3)	0.056(2)	0.057(2)	0.001(2)	0.028(2)	0.009(2)
O(4)	0.069(2)	0.046(2)	0.072(3)	-0.013(2)	0.009(2)	0.024(2)
N(1)	0.081(4)	0.127(5)	0.065(3)	-0.028(3)	0.026(3)	0.030(3)
N(2)	0.039(3)	0.048(3)	0.056(3)	0.001(2)	0.014(2)	0.019(2)
N(3)	0.085(4)	0.091(4)	0.086(4)	-0.010(3)	0.042(3)	0.032(3)
N(4)	0.044(3)	0.047(3)	0.052(3)	-0.004(2)	0.007(2)	0.014(2)
C(1)	0.045(3)	0.063(4)	0.055(3)	-0.008(3)	0.013(3)	0.018(3)
C(2)	0.042(3)	0.050(3)	0.037(3)	-0.003(2)	0.008(2)	0.019(3)
C(3)	0.040(3)	0.044(3)	0.049(3)	0.001(2)	0.012(2)	0.019(3)
C(4)	0.055(4)	0.087(4)	0.072(4)	-0.000(3)	0.001(3)	0.050(4)
C(5)	0.043(3)	0.049(3)	0.082(4)	0.000(2)	0.018(3)	0.021(3)
C(6)	0.040(3)	0.041(3)	0.045(3)	-0.005(2)	0.009(2)	0.011(3)
C(7)	0.047(3)	0.050(3)	0.062(4)	-0.005(2)	0.017(3)	0.020(3)

Table 6. Anisotropic Displacement Parameters(continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(5)	0.055(3)	0.057(3)	0.052(3)	0.001(2)	0.007(2)	0.015(2)
N(6)	0.064(3)	0.044(2)	0.044(3)	-0.003(2)	0.010(2)	0.011(2)
C(8)	0.074(4)	0.079(5)	0.104(5)	-0.023(3)	0.043(4)	0.008(4)
C(9)	0.165(9)	0.17(1)	0.081(6)	-0.031(7)	0.057(6)	0.019(6)
C(10)	0.24(1)	0.25(1)	0.081(6)	-0.16(1)	0.036(7)	-0.032(7)
C(11)	0.077(5)	0.074(5)	0.101(5)	-0.019(4)	0.001(4)	0.030(4)
C(12)	0.081(4)	0.125(6)	0.058(4)	-0.030(4)	0.028(3)	0.020(4)
C(13)	0.20(1)	0.29(1)	0.143(8)	-0.18(1)	0.116(8)	-0.130(8)
C(14)	0.146(7)	0.137(7)	0.091(6)	-0.086(6)	0.035(5)	-0.015(5)
C(15)	0.089(5)	0.099(5)	0.103(5)	-0.039(4)	0.052(4)	0.002(4)

The general temperature factor expression:

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

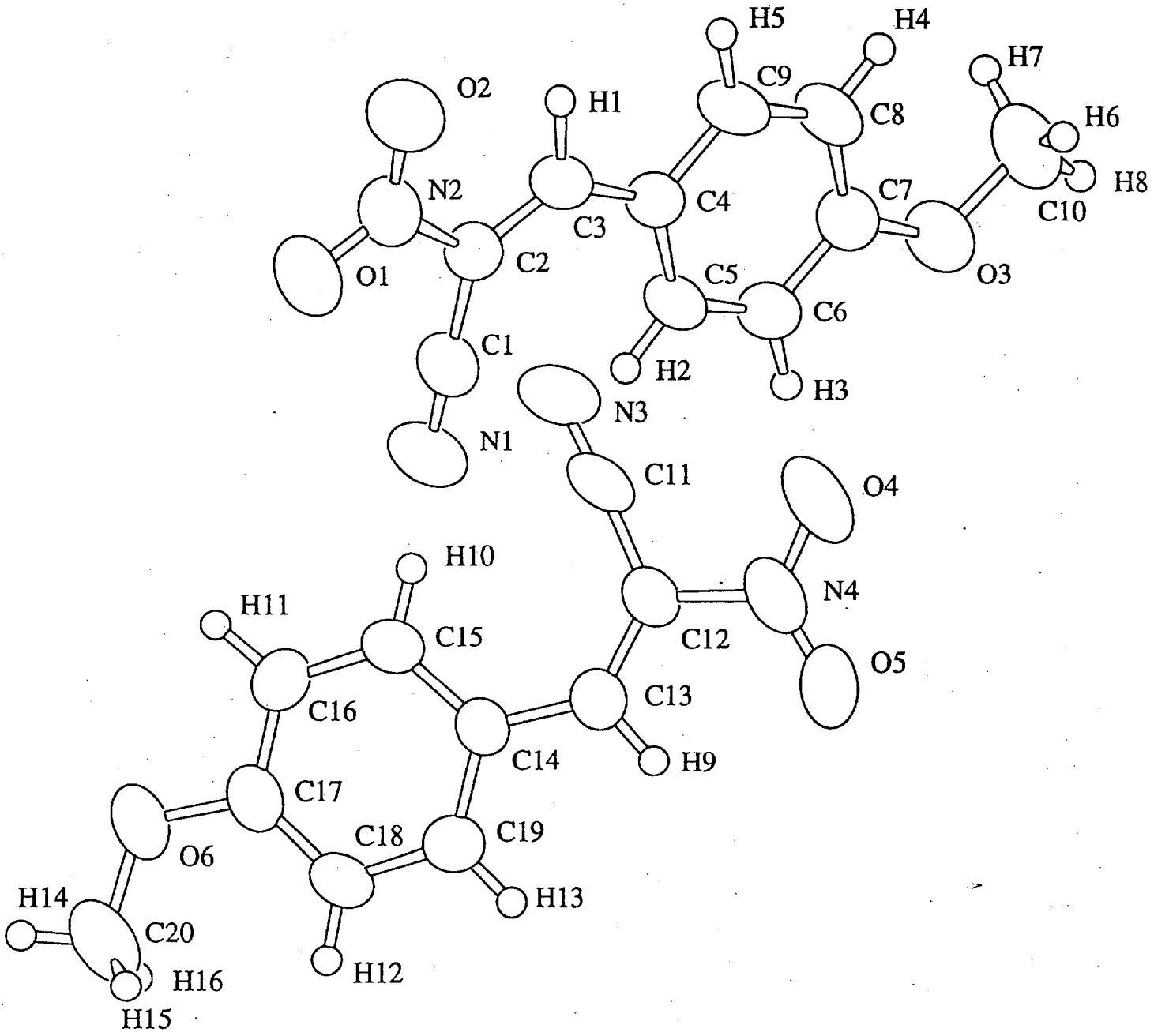

Figure 1. Atomic numbering with thermal ellipsoids drawn at 50% probability

Table 1. Experimental Details

A. Crystal Data

Empirical Formula	$C_{10}H_8N_2O_3$
Formula Weight	204.19
Crystal Color ,Habit	dark yellow, prism
Crystal Dimensions	0.30 X 0.30 X 0.15mm
Crystal System	triclinic
No. of Reflections Used for Unit Cell Determination (2θ range)	17 (22.4°- 24.5°)
Omega Scan Peak Width at Half-height	0.24°
Lattice Parameters	a = 6.843(1) Å b = 9.130(2) Å c = 16.093(3) Å α = 89.91(2)° β = 95.82(3)° γ = 90.40(3)° V = 1000.2(3) Å^3
Space Group	$P\bar{1}$(#2)
Z value	4
D_{calc}	1.356 g/cm^3
F_{000}	424.00
μ (Mo$K\alpha$)	1.02 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC7R
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Temperature	20.0°C
Scan Type	ω-2θ
Scan Rate	16.0°/min(in ω) - up to 5 scans
Scan Width	(1.26 + 0.30 tan θ)°
$2\theta_{max}$	55.0°
No. of Reflection Measured	Total: 4963 Unique: 4581 (R_{int} = 0.037)
Corrections	Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR88)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma\omega(\|F_o\|-\|F_c\|)^2$
Least Squares Weights	$1/\sigma^2(F_o) = 4F_o^2/\sigma^2(F_o^2)$
p-factor	0.00
No. Observations($I > 3.00\sigma(I)$)	1429

C. Structure Solution and Refinement(continued)

No. Variables	271
Residuals: R; Rw	0.042; 0.036
Goodness of Fit Indicator	1.63
Max Shift/Error in Final Cycle	0.40
Maximum peak in Final Diff. Map	0.12 $e^-/Å^3$
Minimum Peak in Final Diff. Map	-0.25 $e^-/Å^3$

Table 2. Intramolecular Distances Involving the Nonhydrogen Atom

atom	atom	distance	atom	atom	distance
O(1)	N(2)	1.219(4)	O(4)	N(4)	1.225(5)
O(2)	N(2)	1.224(4)	O(5)	N(4)	1.221(5)
O(3)	C(7)	1.348(5)	O(6)	C(17)	1.360(5)
O(3)	C(10)	1.436(5)	O(6)	C(20)	1.432(6)
N(1)	C(1)	1.132(5)	N(3)	C(11)	1.125(6)
N(2)	C(2)	1.473(5)	N(4)	C(12)	1.473(5)
C(1)	C(2)	1.428(6)	C(11)	C(12)	1.428(6)
C(2)	C(3)	1.341(6)	C(12)	C(13)	1.347(6)
C(3)	C(4)	1.436(6)	C(13)	C(14)	1.428(6)
C(4)	C(5)	1.406(6)	C(14)	C(15)	1.406(6)
C(4)	C(9)	1.397(6)	C(14)	C(19)	1.401(5)
C(5)	C(6)	1.363(6)	C(15)	C(16)	1.364(6)
C(6)	C(7)	1.394(6)	C(16)	C(17)	1.404(6)
C(7)	C(8)	1.389(6)	C(17)	C(18)	1.374(6)
C(8)	C(9)	1.376(6)	C(18)	C(19)	1.378(6)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parenthes.

Table 3. Intramolecular Bond Angles Involving the Nonhydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
C(7)	O(3)	C(10)	118.5(4)	C(17)	O(6)	C(20)	118.0(4)
O(3)	C(7)	C(6)	115.9(4)	O(6)	C(17)	C(16)	114.2(4)
O(3)	C(7)	C(8)	124.0(4)	O(6)	C(17)	C(18)	125.4(4)
C(6)	C(7)	C(8)	120.1(5)	C(16)	C(17)	C(18)	120.4(4)
C(7)	C(8)	C(9)	118.7(4)	C(17)	C(18)	C(19)	119.2(4)
C(4)	C(9)	C(8)	122.6(4)	C(14)	C(19)	C(18)	122.2(4)
C(3)	C(4)	C(9)	117.7(4)	C(13)	C(14)	C(19)	117.6(4)
C(3)	C(4)	C(5)	125.2(4)	C(13)	C(14)	C(15)	125.4(4)
C(2)	C(3)	C(4)	131.0(4)	C(12)	C(13)	C(14)	131.0(4)
O(1)	N(2)	O(2)	124.6(4)	O(4)	N(4)	O(5)	125.3(5)
O(1)	N(2)	C(2)	116.7(4)	O(4)	N(4)	C(12)	115.9(4)
O(2)	N(2)	C(2)	118.7(4)	O(5)	N(4)	C(12)	118.7(4)
N(1)	C(1)	C(2)	179.8(5)	N(3)	C(11)	C(12)	178.1(5)
N(2)	C(2)	C(1)	113.0(4)	N(4)	C(12)	C(11)	113.3(4)
N(2)	C(2)	C(3)	119.0(4)	N(4)	C(12)	C(13)	118.8(4)
C(1)	C(2)	C(3)	127.9(4)	C(11)	C(12)	C(13)	127.9(4)
C(4)	C(5)	C(6)	121.3(4)	C(14)	C(15)	C(16)	121.6(4)
C(5)	C(4)	C(9)	117.0(4)	C(15)	C(14)	C(19)	117.0(4)
C(5)	C(6)	C(7)	120.3(4)	C(15)	C(16)	C(17)	119.6(4)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table 4. Torsion Angles(°)

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
O(1)	N(2)	C(2)	C(1)	-2.5(6)	O(4)	N(4)	C(12)	C(11)	-3.5(6)
O(1)	N(2)	C(2)	C(3)	178.1(5)	O(4)	N(4)	C(12)	C(13)	174.3(4)
O(2)	N(2)	C(2)	C(1)	177.3(4)	O(5)	N(4)	C(12)	C(11)	176.6(5)
O(2)	N(2)	C(2)	C(3)	-2.1(7)	O(5)	N(4)	C(12)	C(13)	-5.5(7)
N(2)	C(2)	C(3)	C(4)	178.4(5)	N(4)	C(12)	C(13)	C(14)	-177.8(5)
C(1)	C(2)	C(3)	C(4)	-0.8(9)	C(11)	C(12)	C(13)	C(14)	-0.3(9)
C(2)	C(3)	C(4)	C(5)	-2.3(9)	C(12)	C(13)	C(14)	C(15)	1.3(8)
C(2)	C(3)	C(4)	C(9)	177.7(5)	C(12)	C(13)	C(14)	C(19)	179.8(5)
C(3)	C(4)	C(5)	C(6)	-179.8(5)	C(13)	C(14)	C(15)	C(16)	177.7(5)
C(3)	C(4)	C(9)	C(8)	-179.6(5)	C(13)	C(14)	C(19)	C(18)	-178.0(5)
C(4)	C(5)	C(6)	C(7)	0.1(8)	C(14)	C(15)	C(16)	C(17)	-0.2(8)
C(4)	C(9)	C(8)	C(7)	-1.4(8)	C(14)	C(19)	C(18)	C(17)	0.6(7)
C(5)	C(4)	C(9)	C(8)	0.5(8)	C(15)	C(14)	C(19)	C(18)	0.6(7)
C(5)	C(6)	C(7)	C(8)	-1.1(8)	C(15)	C(16)	C(17)	C(18)	1.5(8)
C(6)	C(5)	C(4)	C(9)	0.2(7)	C(16)	C(15)	C(14)	C(19)	-0.8(7)
C(6)	C(7)	C(8)	C(9)	1.7(8)	C(16)	C(17)	C(18)	C(19)	-1.6(7)
O(3)	C(7)	C(6)	C(5)	179.1(4)	O(6)	C(17)	C(16)	C(15)	-179.0(5)
O(3)	C(7)	C(8)	C(9)	-178.5(5)	O(6)	C(17)	C(18)	C(19)	178.9(5)
C(6)	C(7)	O(3)	C(10)	-177.2(5)	C(16)	C(17)	O(6)	C(20)	177.2(5)
C(8)	C(7)	O(3)	C(10)	3.0(7)	C(18)	C(17)	O(6)	C(20)	-3.2(7)

The sign is positive if when looking from atom 2 to atom 3 a clock-wise motion of atom 1 would superimpose it on atom 4.

Table 5. Positional parameters and B_{eq}

atom	x	y	z	B_{eq}
O(1)	0.5718(5)	0.3078(4)	0.7859(2)	6.5(1)
O(2)	0.5783(5)	0.4447(4)	0.8957(2)	6.2(1)
O(3)	-0.4246(5)	0.1372(4)	1.0834(2)	5.6(1)
N(1)	0.1898(6)	0.0873(5)	0.7612(3)	6.5(1)
N(2)	0.5052(6)	0.3485(5)	0.8493(3)	4.9(1)
C(1)	0.2493(7)	0.1706(5)	0.8094(3)	4.5(1)
C(2)	0.3239(7)	0.2757(5)	0.8704(3)	3.8(1)
C(3)	0.2480(7)	0.3137(5)	0.9408(3)	4.2(1)
C(4)	0.0738(7)	0.2645(5)	0.9754(3)	3.8(1)
C(5)	-0.0631(7)	0.1631(5)	0.9378(3)	4.3(1)
C(6)	-0.2253(7)	0.1228(5)	0.9752(3)	4.5(1)
C(7)	-0.2590(7)	0.1822(5)	1.0521(3)	4.2(1)
C(8)	-0.1256(7)	0.2811(5)	1.0918(3)	4.8(1)
C(9)	0.0362(7)	0.3215(5)	1.0527(3)	5.0(1)
C(10)	-0.4721(8)	0.1995(6)	1.1607(3)	6.5(2)
H(1)	0.3296	0.3847	0.9780	4.3
H(2)	-0.0472	0.1227	0.8837	5.1
H(3)	-0.3261	0.0572	0.9467	6.5
H(4)	-0.1428	0.3200	1.1444	5.4
H(5)	0.1283	0.3901	1.0814	6.3
H(6)	-0.4914	0.3077	1.1500	8.7
H(7)	-0.3587	0.1755	1.2065	6.5
H(8)	-0.5889	0.1557	1.1704	6.3
O(4)	-0.3032(6)	0.6409(4)	0.7132(2)	7.1(1)
O(5)	-0.4889(6)	0.5485(5)	0.6086(3)	7.4(1)
O(6)	0.3400(5)	0.0419(4)	0.4084(2)	5.9(1)
N(3)	0.1400(7)	0.4993(5)	0.7363(3)	6.9(1)
N(4)	-0.3335(7)	0.5601(5)	0.6526(3)	5.4(1)
C(11)	0.0038(8)	0.4883(5)	0.6913(3)	4.7(1)
C(12)	-0.1657(7)	0.4712(5)	0.6325(3)	3.9(1)
C(13)	-0.1844(6)	0.3896(5)	0.5625(3)	3.9(1)
C(14)	-0.0473(6)	0.2980(5)	0.5264(3)	3.7(1)

Table 5. Positional parameters and B_{eq} (continued)

C(15)	0.1489(7)	0.2759(5)	0.5588(3)	4.4(1)
C(16)	0.2721(6)	0.1902(5)	0.5187(3)	4.9(1)
C(17)	0.2028(7)	0.1224(5)	0.4431(3)	4.2(1)
C(18)	0.0109(7)	0.1392(5)	0.4103(3)	4.3(1)
C(19)	-0.1114(6)	0.2265(5)	0.4516(3)	4.2(1)
C(20)	0.2847(8)	-0.0259(6)	0.3293(3)	6.6(2)
H(9)	-0.3171	0.3960	0.5358	3.4
H(10)	0.1909	0.3161	0.6105	5.2
H(11)	0.4127	0.1768	0.5396	5.6
H(12)	-0.0386	0.0994	0.3586	5.3
H(13)	-0.2433	0.2414	0.4264	6.3
H(14)	0.4097	-0.0578	0.3134	15.2
H(15)	0.2360	0.0447	0.2843	8.5
H(16)	0.1867	-0.0980	0.3340	5.3

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

Table 6. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	0.082(3)	0.091(3)	0.080(3)	-0.009(2)	0.037(2)	-0.015(2)
O(2)	0.078(3)	0.074(3)	0.084(3)	-0.029(2)	0.016(2)	-0.019(2)
O(3)	0.070(3)	0.077(3)	0.071(3)	-0.018(2)	0.026(2)	-0.017(2)
N(1)	0.098(4)	0.079(3)	0.071(3)	-0.012(3)	0.009(3)	-0.032(3)
N(2)	0.061(3)	0.060(3)	0.064(3)	0.001(2)	0.013(2)	-0.002(2)
C(1)	0.061(3)	0.058(3)	0.054(3)	-0.003(3)	0.014(3)	-0.006(3)
C(2)	0.048(3)	0.043(3)	0.052(3)	-0.003(2)	0.004(2)	-0.003(2)
C(3)	0.057(3)	0.053(3)	0.049(3)	-0.002(3)	-0.002(3)	-0.011(2)
C(4)	0.048(3)	0.046(3)	0.051(3)	-0.005(2)	0.003(2)	-0.009(2)
C(5)	0.062(3)	0.056(3)	0.048(3)	-0.004(3)	0.007(3)	-0.018(2)
C(6)	0.054(3)	0.060(3)	0.056(3)	-0.008(3)	0.004(3)	-0.016(3)
C(7)	0.055(3)	0.052(3)	0.056(3)	-0.003(3)	0.009(3)	-0.004(3)

Table 6. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(8)	0.071(4)	0.065(4)	0.049(3)	-0.012(3)	0.018(3)	-0.018(3)
C(9)	0.071(4)	0.065(4)	0.054(3)	-0.016(3)	0.005(3)	-0.025(3)
C(10)	0.089(4)	0.082(4)	0.082(4)	-0.010(3)	0.041(3)	-0.013(3)
O(4)	0.114(3)	0.078(3)	0.083(3)	0.014(2)	0.040(2)	-0.023(2)
O(5)	0.066(3)	0.127(4)	0.093(3)	0.025(3)	0.023(2)	-0.020(3)
O(6)	0.074(2)	0.083(3)	0.071(2)	0.021(2)	0.019(2)	-0.019(2)
N(3)	0.110(4)	0.092(4)	0.057(3)	0.018(3)	-0.015(3)	-0.022(3)
N(4)	0.081(4)	0.071(3)	0.058(3)	0.009(3)	0.032(3)	-0.003(3)
C(11)	0.088(4)	0.054(3)	0.038(3)	0.012(3)	0.007(3)	-0.012(2)
C(12)	0.058(3)	0.047(3)	0.044(3)	0.003(2)	0.011(2)	-0.002(2)
C(13)	0.049(3)	0.053(3)	0.048(3)	-0.000(2)	0.011(2)	0.000(2)
C(14)	0.047(3)	0.048(3)	0.044(3)	0.001(2)	0.009(2)	-0.003(2)
C(15)	0.056(3)	0.068(4)	0.044(3)	0.001(3)	0.001(3)	-0.012(3)
C(16)	0.046(3)	0.072(4)	0.066(3)	0.011(3)	-0.003(3)	-0.011(3)
C(17)	0.059(3)	0.048(3)	0.056(3)	0.007(3)	0.016(3)	-0.002(2)
C(18)	0.064(4)	0.055(3)	0.045(3)	-0.002(3)	0.005(3)	-0.014(2)
C(19)	0.050(3)	0.059(3)	0.051(3)	-0.006(3)	0.002(2)	-0.007(3)
C(20)	0.104(5)	0.080(4)	0.073(4)	0.009(3)	0.035(3)	-0.014(3)

The general temperature factor expression:

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