Figure 1. ORTEP view of **6**

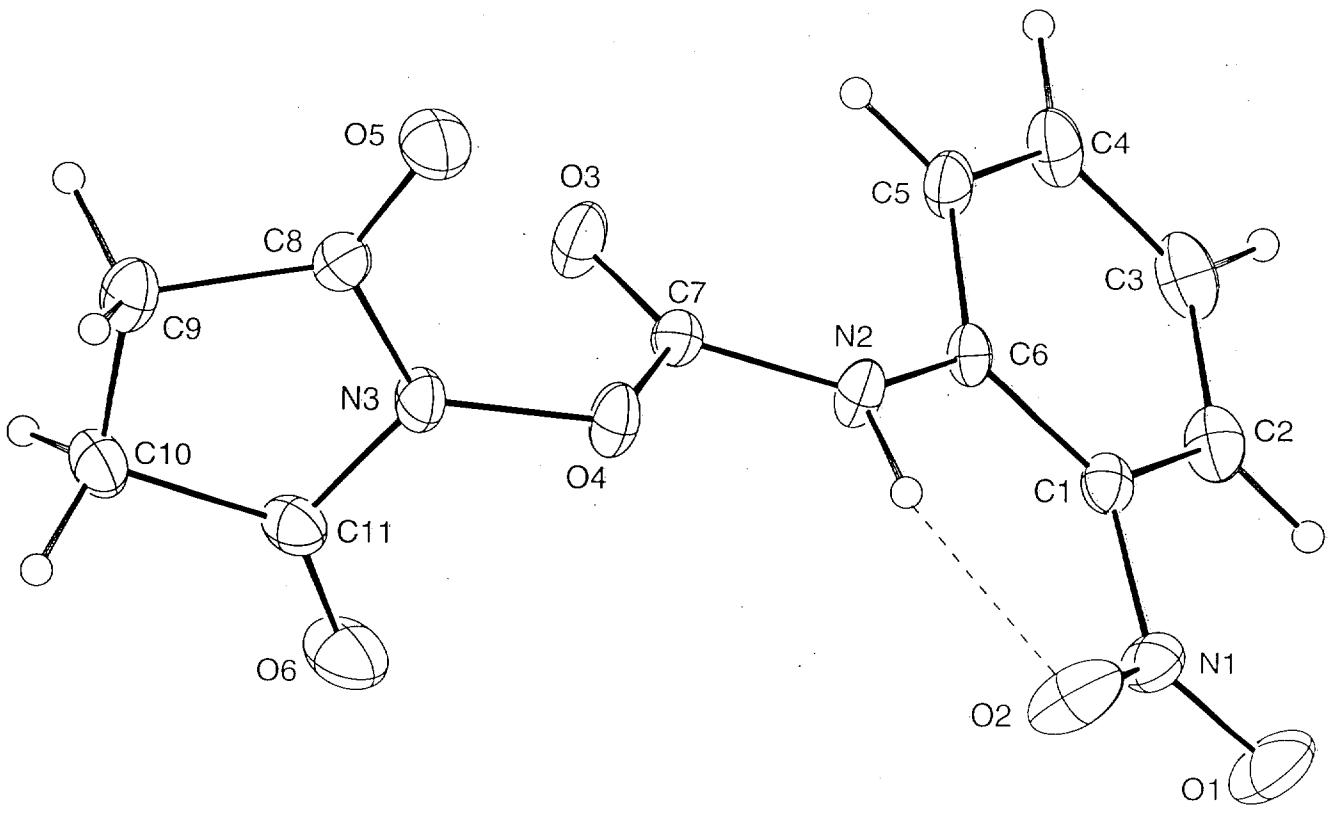

Table 1. Crystal data and Structure Refinement for **6**.

Color / Shape	yellow / fragment
Empirical formula	C11 H9 N3 O6
Formula weight	279.21
Temperature	293(2) K
Crystal system	monoclinic
Space group	P $2_1/a$
Unit cell dimensions	a = 12.530(1) Å $\alpha = 90°$
	b = 10.077(2) Å $\beta = 94.50(1)°$
	c = 9.572(2) Å $\gamma = 90°$
Volume	1204.9(4) A^3
Z / Calculated density	4 / 1.539 Mg/m^3
Absorption coefficient	0.077 mm^{-1}
Diffractometer	Nonius Kappa CCD
Radiation / Wavelength	AgKα (graphite monochrom.) / 0.56090 Å
F(000)	576
Crystal size	.40 x .30 x .30 mm
θ range for data collection	4.18 to 19.27°
Index ranges	$0 \le h \le 14, 0 \le k \le 11, -11 \le l \le 11$
Reflections collected / unique	8346 / 2162 [R_{int} = 0.043]
Completeness to θ = 19.27°	99.8%
Absorption correction	none
Refinement method	Full-matrix least-squares on F^2
Computing	Collect / DENZO / maXus / SHELXL97
Data / restraints / parameters	2035 / 1 / 209
Goodness-of-fit on F^2 1.050	
SHELXL97 weight parameters	0.0375, 0.5285
Final R indices [I>2σ(I)]	R1 = 0.0368, wR2 = 0.0898
R indices (all data)	R1 = 0.0461, wR2 = 0.0959
Extinction coefficient	0.069(7)
Largest diff. peak and hole	0.212 and -0.199 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and Equivalent isotropic displacement parameters [$Å^2$ x 10^3] for **6.**

ATOM	x	y	z	U(eq)
O(1)	7967(1)	-1829(2)	16083(2)	71(1)
O(2)	7139(1)	-606(2)	14541(2)	68(1)
N(1)	7933(1)	-1225(1)	14981(2)	41(1)
C(1)	8894(1)	-1195(2)	14194(2)	32(1)
C(2)	9798(2)	-1800(2)	14826(2)	44(1)
C(3)	10742(2)	-1774(2)	14187(2)	49(1)
C(4)	10784(2)	-1124(2)	12927(2)	46(1)
C(5)	9887(1)	-516(2)	12291(2)	38(1)
C(6)	8914(1)	-556(2)	12900(2)	30(1)
N(2)	8005(1)	61(1)	12238(1)	35(1)
C(7)	7778(1)	104(2)	10844(2)	30(1)
O(3)	8289(1)	-233(1)	9914(1)	48(1)
O(4)	6758(1)	675(1)	10626(1)	41(1)
N(3)	6365(1)	571(1)	9241(1)	36(1)
C(8)	6398(1)	1612(2)	8320(2)	34(1)
O(5)	6807(1)	2670(1)	8613(1)	53(1)
C(9)	5845(2)	1121(2)	6972(2)	46(1)
C(10)	5518(2)	-304(2)	7239(2)	47(1)
C(11)	5871(1)	-581(2)	8740(2)	41(1)
O(6)	5780(1)	-1549(2)	9452(2)	70(1)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3. Bond lengths [Å] and angles [°] for **6**.

O(1)-N(1)	1.215(2)	O(2)-N(1)	1.220(2)
N(1)-C(1)	1.470(2)	C(1)-C(2)	1.384(2)
C(1)-C(6)	1.398(2)	C(2)-C(3)	1.374(3)
C(3)-C(4)	1.377(3)	C(4)-C(5)	1.379(3)
C(5)-C(6)	1.393(2)	C(6)-N(2)	1.405(2)
N(2)-C(7)	1.342(2)	C(7)-O(3)	1.187(2)
C(7)-O(4)	1.403(2)	O(4)-N(3)	1.381(2)
N(3)-C(8)	1.373(2)	N(3)-C(11)	1.383(2)
C(8)-O(5)	1.206(2)	C(8)-C(9)	1.500(3)
C(9)-C(10)	1.521(3)	C(10)-C(11)	1.496(3)
C(11)-O(6)	1.201(2)		

O(1)-N(1)-O(2)	121.88(16)	O(1)-N(1)-C(1)	118.72(15)
O(2)-N(1)-C(1)	119.35(13)	C(2)-C(1)-C(6)	121.27(16)
C(2)-C(1)-N(1)	116.28(15)	C(6)-C(1)-N(1)	122.42(14)
C(3)-C(2)-C(1)	120.09(18)	C(2)-C(3)-C(4)	119.48(18)
C(3)-C(4)-C(5)	120.83(18)	C(4)-C(5)-C(6)	120.81(17)
C(5)-C(6)-C(1)	117.49(15)	C(5)-C(6)-N(2)	120.27(14)
C(1)-C(6)-N(2)	122.22(14)	C(7)-N(2)-C(6)	124.28(13)
O(3)-C(7)-N(2)	130.71(15)	O(3)-C(7)-O(4)	123.00(14)
N(2)-C(7)-O(4)	106.29(12)	N(3)-O(4)-C(7)	111.33(11)
C(8)-N(3)-O(4)	122.14(13)	C(8)-N(3)-C(11)	116.95(14)
O(4)-N(3)-C(11)	120.84(13)	O(5)-C(8)-N(3)	123.99(15)
O(5)-C(8)-C(9)	130.59(16)	N(3)-C(8)-C(9)	105.42(15)
C(8)-C(9)-C(10)	106.20(15)	C(11)-C(10)-C(9)	105.91(15)
O(6)-C(11)-N(3)	123.01(17)	O(6)-C(11)-C(10)	131.47(18)
N(3)-C(11)-C(10)	105.51(15)		

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for **6**.

ATOM	U11	U22	U33	U23	U13	U12
O(1)	83(1)	83(1)	49(1)	32(1)	14(1)	0(1)
O(2)	57(1)	86(1)	64(1)	33(1)	25(1)	24(1)
N(1)	53(1)	36(1)	36(1)	6(1)	6(1)	-3(1)
C(1)	41(1)	24(1)	30(1)	-3(1)	-1(1)	0(1)
C(2)	58(1)	30(1)	41(1)	3(1)	-11(1)	4(1)
C(3)	45(1)	43(1)	56(1)	-12(1)	-17(1)	15(1)
C(4)	34(1)	61(1)	42(1)	-20(1)	-4(1)	10(1)
C(5)	37(1)	51(1)	27(1)	-10(1)	1(1)	3(1)
C(6)	34(1)	29(1)	24(1)	-7(1)	-3(1)	4(1)
N(2)	34(1)	49(1)	22(1)	0(1)	1(1)	12(1)
C(7)	32(1)	31(1)	27(1)	1(1)	0(1)	2(1)
O(3)	44(1)	74(1)	26(1)	-4(1)	4(1)	12(1)
O(4)	40(1)	55(1)	26(1)	1(1)	-5(1)	12(1)
N(3)	38(1)	41(1)	27(1)	3(1)	-7(1)	1(1)
C(8)	30(1)	38(1)	33(1)	5(1)	1(1)	5(1)
O(5)	62(1)	42(1)	54(1)	6(1)	-4(1)	-8(1)
C(9)	48(1)	56(1)	34(1)	5(1)	-7(1)	8(1)
C(10)	38(1)	60(1)	43(1)	-7(1)	-5(1)	-7(1)
C(11)	30(1)	43(1)	48(1)	4(1)	-3(1)	-2(1)
O(6)	72(1)	54(1)	80(1)	23(1)	-17(1)	-21(1)

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(ha^*)^2 U11 + ... + 2hka^*b^*U_{12}]$

Table 5. Hydrogen coordinates [x 10^4] and isotropic displacement parameters [$Å^2$ x 10^3] for **6**.

ATOM	x	y	z	U(eq)
H(2)	9724(16)	-2200(2)	15710(2)	57
H(3)	11378(19)	-2160(2)	14620(2)	64
H(4)	11468(19)	-1080(2)	12480(2)	60
H(5)	9926(16)	-60(2)	11400(2)	50
H(21)	7409(11)	268(18)	12822(17)	46
H(9A)	6354(18)	1190(2)	6240(2)	61
H(9B)	5248(19)	1610(2)	6820(2)	61
H(10A)	4770(2)	-470(2)	7110(2)	61
H(10B)	5842(18)	-910(2)	6650(2)	61

Table 6. Selected torsion angles [°] for **6**.

O(1)-N(1)-C(1)-C(6)	178.16(16)
N(1)-C(1)-C(6)-N(2)	-2.4(2)
C(1)-C(6)-N(2)-C(7)	-145.72(16)
C(6)-N(2)-C(7)-O(4)	173.79(14)
N(2)-C(7)-O(4)-N(3)	-170.05(13)
C(7)-O(4)-N(3)-C(8)	-100.43(17)

Table 7. Hydrogen-bonds for **6** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)>
N(2)-H(21)...O(2)	0.989(9)	1.920(16)	2.6192(19)	125.4(14)
N(2)-H(21)...O(5)#1	0.989(9)	2.356(16)	3.0861(19)	130.0(14)

Symmetry transformations used to generate equivalent atoms: #1 x,-y+1/2,z+1/2