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Table 1. Crystal data and

SUPPORTING INFORMATION

Identification code	pipioxam
Empirical formula	$C_7H_{14}N_2O_3$
Formula weight	174.20
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 9.5230(10) Å α = 90° b = 7.0500(10) Å β = 96.730(10)° c = 13.747(2) Å γ = 90°
Volume	916.6(2) $Å^3$
Z	4
Density (calculated)	1.262 Mg/m^3
Absorption coefficient	0.099 mm^{-1}
F(000)	376
Crystal size	0.51 x 0.34 x 0.25 mm
θ range for data collection	2.47 to 25.00°
Index ranges	$-11 \le h \le 1$, $0 \le k \le 8$, $-16 \le \ell \le 16$
Reflections collected	1734
Independent reflections	1622 (R_{int} = 0.0088)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1622 / 0 / 109
Goodness-of-fit on F^2	1.050
Final R indices [I>2σ(I)]	R1 = 0.0347, wR2 = 0.0863
R indices (all data)	R1 = 0.0434, wR2 = 0.0925
Largest diff. peak and hole	0.199 and −0.206 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	825(1)	377(2)	1644(1)	29(1)
N(1)	2507(1)	-1419(2)	2496(1)	24(1)
C(1)	1174(2)	-981(2)	2187(1)	21(1)
C(2)	30(2)	-2263(2)	2561(1)	22(1)
O(21)	-1211(1)	-1649(2)	2391(1)	28(1)
O(22)	424(1)	-3752(2)	3002(1)	27(1)
N(3)	-2023(1)	1786(2)	1338(1)	24(1)
C(4)	-1317(2)	3590(2)	1106(1)	33(1)
C(5)	-2386(2)	4929(2)	565(1)	35(1)
C(6)	-3148(2)	3995(3)	-345(1)	37(1)
C(7)	-3816(2)	2129(2)	-93(1)	33(1)
C(8)	-2739(2)	823(2)	454(1)	29(1)

Table 3. Bond lengths [Å] and angles [°] for 1.

O(1)-C(1)	1.235(2)	N(1)-C(1)	1.327(2)
C(1)-C(2)	1.549(2)	C(2)-O(22)	1.247(2)
C(2)-O(21)	1.254(2)	N(3)-C(8)	1.487(2)
N(3)-C(4)	1.490(2)	C(4)-C(5)	1.518(2)
C(5)-C(6)	1.520(2)	C(6)-C(7)	1.519(2)
C(7)-C(8)	1.511(2)		

O(1)-C(1)-N(1)	123.58(13)	O(1)-C(1)-C(2)	120.22(12)
N(1)-C(1)-C(2)	116.20(13)	O(22)-C(2)-O(21)	127.21(13)
O(22)-C(2)-C(1)	117.93(12)	O(21)-C(2)-C(1)	114.85(13)
C(8)-N(3)-C(4)	112.93(12)	N(3)-C(4)-C(5)	110.03(13)
C(4)-C(5)-C(6)	111.20(14)	C(7)-C(6)-C(5)	111.10(13)
C(8)-C(7)-C(6)	111.35(13)	N(3)-C(8)-C(7)	110.35(13)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 1.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
O(1)	22(1)	27(1)	37(1)	7(1)	4(1)	-1(1)
N(1)	20(1)	21(1)	33(1)	1(1)	7(1)	-2(1)
C(1)	21(1)	19(1)	23(1)	-4(1)	5(1)	1(1)
C(2)	22(1)	21(1)	23(1)	-5(1)	5(1)	-1(1)
O(21)	17(1)	30(1)	38(1)	5(1)	7(1)	2(1)
O(22)	24(1)	23(1)	37(1)	5(1)	8(1)	2(1)
N(3)	22(1)	25(1)	27(1)	-1(1)	4(1)	5(1)
C(4)	27(1)	30(1)	42(1)	-4(1)	5(1)	-5(1)
C(5)	43(1)	23(1)	43(1)	0(1)	14(1)	1(1)
C(6)	47(1)	39(1)	27(1)	7(1)	9(1)	11(1)
C(7)	32(1)	41(1)	25(1)	-6(1)	1(1)	1(1)
C(8)	30(1)	24(1)	33(1)	-5(1)	7(1)	-2(1)

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

	x	y	z	U(eq)
H(12)	2536(1)	-2281(2)	2874(1)	29
H(11)	3186(1)	-646(2)	2272(1)	29
H(31)	-2548(1)	2060(2)	1788(1)	29
H(32)	-1393(1)	942(2)	1640(1)	29
H(41)	-804(2)	4062(2)	1752(1)	40
H(42)	-578(2)	3312(2)	679(1)	40
H(41)	-3001(2)	5297(2)	1025(1)	42
H(52)	-1806(2)	6051(2)	387(1)	42
H(61)	-2395(2)	3747(3)	-795(1)	45
H(62)	-3801(2)	4879(3)	-702(1)	45
H(71)	-4545(2)	2304(2)	292(1)	39
H(72)	-4164(2)	1507(2)	-716(1)	39
H(81)	-1995(2)	381(2)	65(1)	34
H(82)	-3195(2)	-268(2)	711(1)	34

erators for generating equivalent atoms for pipioxam: 1

-x+1/2, y+1/2, -z+1/2
-x+1/2, y-1/2, -z+1/2
-x-1/2, y+1/2, -z+1/2

lected torsion angles

171.02	(0.13)	O1 - C1 - C2 - O22
-10.10	(0.19)	N1 - C1 - C2 - O22
-9.87	(0.19)	O1 - C1 - C2 - O21
169.01	(0.13)	N1 - C1 - C2 - O21
57.33	(0.17)	C8 - N3 - C4 - C5
-55.11	(0.18)	N3 - C4 - C5 - C6
54.39	(0.19)	C4 - C5 - C6 - C7
-54.33	(0.18)	C5 - C6 - C7 - C8
-57.37	(0.16)	C4 - N3 - C8 - C7
55.07	(0.17)	C6 - C7 - C8 - N3

istance N-O

2.864	(0.002)	N1 - O22_$1
2.728	(0.002)	N1 - O22
2.930	(0.002)	N1 - O1_$2
2.790	(0.002)	N3 - O21_$3
2.873	(0.002)	N3 - O1
2.880	(0.002)	N3 - O21

istance NH-O

1.947	(0.002)	H11 - O22_$1
2.287	(0.002)	H12 - O22
2.315	(0.002)	H12 - O1_$2
1.952	(0.002)	H31 - O21_$3
2.149	(0.002)	H32 - O1
2.095	(0.002)	H32 - O21

ngle NHO

170.05	(0.05)	N1 - H11 - O22_$1
115.58	(0.04)	N1 - H12 - O22
134.47	(0.04)	N1 - H12 - O1_$2
163.95	(0.05)	N3 - H31 - O21_$3
135.88	(0.04)	N3 - H32 - O1
143.80	(0.04)	N3 - H32 - O21

Table 1. Crystal data and structure refinement for 2a

Identification code	2a5noxam
Empirical formula	$C_{12}H_{13}N_7O_7$
Formula weight	367.29
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 10.206(6) Å α = 90° b = 7.598(5) Å β = 94.86(5)° c = 19.78(2) Å γ = 90°
Volume	1529(2) $Å^3$
Z	4
Density (calculated)	1.596 Mg/m^3
Absorption coefficient	0.134 mm^{-1}
F(000)	760
Crystal size	0.56 x 0.35 x 0.19 mm
θ range for data collection	2.00 to 25.00°
Index ranges	$0 \le h \le 12$, $0 \le k \le 9$, $-23 \le \ell \le 23$
Reflections collected	2847
Independent reflections	2686 (R_{int} = 0.0281)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2686 / 0 / 235
Goodness-of-fit on F^2	1.057
Final R indices [$I>2\sigma(I)$]	R1 = 0.0420, wR2 = 0.0994
R indices (all data)	R1 = 0.0646, wR2 = 0.1117
Largest diff. peak and hole	0.211 and -0.263 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	4567(2)	-2061(2)	6652(1)	19(1)
N(1)	5212(2)	-197(3)	7506(1)	20(1)
C(1)	5025(2)	-617(3)	6856(1)	15(1)
C(2)	5417(2)	791(3)	6344(1)	14(1)
O(22)	5790(2)	2273(2)	6577(1)	20(1)
O(21)	5329(2)	325(2)	5741(1)	20(1)
N(3A)	3390(2)	-443(2)	9340(1)	14(1)
C(4A)	3549(2)	-741(3)	10025(1)	13(1)
N(4A)	4003(2)	-2277(2)	10242(1)	16(1)
C(5A)	3230(2)	660(3)	10464(1)	15(1)
C(6A)	2740(2)	2203(3)	10207(1)	16(1)
C(7A)	2550(2)	2393(3)	9495(1)	15(1)
N(7A)	1960(2)	3976(3)	9199(1)	19(1)
O(71A)	1572(2)	5103(2)	9584(1)	27(1)
O(72A)	1842(2)	4117(2)	8575(1)	25(1)
C(8A)	2900(2)	1087(3)	9078(1)	15(1)
N(3B)	576(2)	-3612(3)	5733(1)	20(1)
C(4B)	429(2)	-5057(3)	6127(1)	19(1)
N(4B)	-125(2)	-6470(3)	5807(1)	24(1)
C(5B)	828(2)	-5069(3)	6831(1)	22(1)
C(6B)	1313(2)	-3562(3)	7128(1)	21(1)
C(7B)	1412(2)	-2070(3)	6723(1)	18(1)
N(7B)	1872(2)	-416(3)	7020(1)	22(1)
O(71B)	2079(2)	-342(2)	7641(1)	30(1)
O(72B)	2023(2)	855(2)	6643(1)	33(1)
C(8B)	1062(2)	-2161(3)	6037(1)	18(1)

Table 3. Bond lengths [Å] and angles [°] for 1g 2

O(1)-C(1)	1.246(3)	N(1)-C(1)	1.323(3)
C(1)-C(2)	1.550(3)	C(2)-O(21)	1.240(3)
C(2)-O(22)	1.263(3)	N(3A)-C(8A)	1.351(3)
N(3A)-C(4A)	1.370(3)	C(4A)-N(4A)	1.314(3)
C(4A)-C(5A)	1.428(3)	C(5A)-C(6A)	1.357(3)
C(6A)-C(7A)	1.414(3)	C(7A)-C(8A)	1.357(3)
C(7A)-N(7A)	1.447(3)	N(7A)-O(71A)	1.233(3)
N(7A)-O(72A)	1.235(3)	N(3B)-C(8B)	1.331(3)
N(3B)-C(4B)	1.362(3)	C(4B)-N(4B)	1.347(3)
C(4B)-C(5B)	1.417(4)	C(5B)-C(6B)	1.361(3)
C(6B)-C(7B)	1.397(3)	C(7B)-C(8B)	1.375(3)
C(7B)-N(7B)	1.448(3)	N(7B)-O(71B)	1.230(3)
N(7B)-O(72B)	1.237(3)		

O(1)-C(1)-N(1)	123.1(2)	O(1)-C(1)-C(2)	120.4(2)
N(1)-C(1)-C(2)	116.5(2)	O(21)-C(2)-O(22)	126.9(2)
O(21)-C(2)-C(1)	115.5(2)	O(22)-C(2)-C(1)	117.6(2)
C(8A)-N(3A)-C(4A)	122.0(2)	N(4A)-C(4A)-N(3A)	118.5(2)
N(4A)-C(4A)-C(5A)	123.8(2)	N(3A)-C(4A)-C(5A)	117.7(2)
C(6A)-C(5A)-C(4A)	120.9(2)	C(5A)-C(6A)-C(7A)	118.4(2)
C(8A)-C(7A)-C(6A)	120.7(2)	C(8A)-C(7A)-N(7A)	119.0(2)
C(6A)-C(7A)-N(7A)	120.3(2)	O(71A)-N(7A)-O(72A)	123.2(2)
O(71A)-N(7A)-C(7A)	118.2(2)	O(72A)-N(7A)-C(7A)	118.6(2)
N(3A)-C(8A)-C(7A)	120.3(2)	C(8B)-N(3B)-C(4B)	117.6(2)
N(4B)-C(4B)-N(3B)	115.8(2)	N(4B)-C(4B)-C(5B)	122.1(2)
N(3B)-C(4B)-C(5B)	122.1(2)	C(6B)-C(5B)-C(4B)	118.8(2)
C(5B)-C(6B)-C(7B)	118.4(2)	C(8B)-C(7B)-C(6B)	120.0(2)
C(8B)-C(7B)-N(7B)	119.5(2)	C(6B)-C(7B)-N(7B)	120.5(2)
O(71B)-N(7B)-O(72B)	123.1(2)	O(71B)-N(7B)-C(7B)	117.9(2)
O(72B)-N(7B)-C(7B)	119.0(2)	N(3B)-C(8B)-C(7B)	122.9(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 2

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O(1)	28(1)	15(1)	15(1)	0(1)	1(1)	-5(1)
N(1)	34(1)	13(1)	12(1)	2(1)	3(1)	-5(1)
C(1)	15(1)	15(1)	16(1)	0(1)	1(1)	1(1)
C(2)	16(1)	15(1)	12(1)	-1(1)	0(1)	2(1)
O(22)	32(1)	13(1)	15(1)	-2(1)	6(1)	-5(1)
O(21)	29(1)	17(1)	13(1)	0(1)	1(1)	-4(1)
N(3A)	15(1)	13(1)	14(1)	-2(1)	1(1)	1(1)
C(4A)	9(1)	16(1)	14(1)	-1(1)	0(1)	-2(1)
N(4A)	20(1)	15(1)	13(1)	-1(1)	1(1)	2(1)
C(5A)	13(1)	20(1)	12(1)	-1(1)	0(1)	0(1)
C(6A)	14(1)	15(1)	18(1)	-5(1)	4(1)	-1(1)
C(7A)	13(1)	15(1)	18(1)	1(1)	0(1)	0(1)
N(7A)	16(1)	15(1)	24(1)	1(1)	-2(1)	1(1)
O(71A)	33(1)	17(1)	32(1)	-4(1)	2(1)	10(1)
O(72A)	30(1)	24(1)	21(1)	7(1)	-4(1)	2(1)
C(8A)	13(1)	18(1)	13(1)	1(1)	-1(1)	-3(1)
N(3B)	18(1)	19(1)	22(1)	-1(1)	-1(1)	1(1)
C(4B)	12(1)	20(1)	26(1)	0(1)	4(1)	2(1)
N(4B)	26(1)	20(1)	27(1)	-4(1)	0(1)	-4(1)
C(5B)	22(1)	19(1)	23(1)	4(1)	4(1)	1(1)
C(6B)	18(1)	26(1)	18(1)	1(1)	0(1)	3(1)
C(7B)	16(1)	19(1)	18(1)	-4(1)	0(1)	1(1)
N(7B)	21(1)	24(1)	19(1)	-3(1)	-3(1)	1(1)
O(71B)	37(1)	35(1)	17(1)	-7(1)	-2(1)	-4(1)
O(72B)	52(1)	19(1)	27(1)	2(1)	-5(1)	-5(1)
C(8B)	15(1)	18(1)	20(1)	2(1)	2(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for ~~4~~ 2

	x	y	z	U(eq)
H(12)	5429(2)	969(3)	7626(1)	23
H(11)	5004(2)	-1027(3)	7838(1)	23
H(3A)	3607(2)	-1415(2)	9039(1)	17
H(41A)	4156(2)	-2385(2)	10737(1)	19
H(42A)	4218(2)	-3195(2)	9952(1)	19
H(5A)	3414(2)	613(3)	10942(1)	18
H(6A)	2526(2)	3203(3)	10496(1)	19
H(8A)	2790(2)	1189(3)	8559(1)	18
H(41B)	-119(2)	-7609(3)	6077(1)	29
H(42B)	-322(2)	-6600(3)	5347(1)	29
H(5B)	703(2)	-6214(3)	7089(1)	26
H(6B)	1653(2)	-3619(3)	7610(1)	25
H(8B)	1146(2)	-1219(3)	5742(1)	21

EQIV $1 1-x,-.5+y,1.5-z
EQIV $2 1-x,.5+y,1.5-z
EQIV $3 x,-.5-y,.5+z
EQIV $4 -x,y-1.5,1.5-z
EQIV $5 x,y-1,z
EQIV $6 -x,-1-y,1-z
EQIV $7 x,.5-y,z+.5
EQIV $8 x,.5-y,z-.5

Selected torsion angles

-4.81	(0.30)	O1 - C1 - C2 - O21
174.74	(0.19)	N1 - C1 - C2 - O21
175.28	(0.20)	O1 - C1 - C2 - O22
-5.17	(0.30)	N1 - C1 - C2 - O22
178.40	(0.19)	C8A - N3A - C4A - N4A
-2.67	(0.29)	C8A - N3A - C4A - C5A
-178.65	(0.20)	N4A - C4A - C5A - C6A
2.47	(0.31)	N3A - C4A - C5A - C6A
0.08	(0.32)	C4A - C5A - C6A - C7A
-2.59	(0.32)	C5A - C6A - C7A - C8A
176.47	(0.20)	C5A - C6A - C7A - N7A
175.47	(0.20)	C8A - C7A - N7A - O71A
-3.60	(0.30)	C6A - C7A - N7A - O71A
-2.85	(0.30)	C8A - C7A - N7A - O72A
178.07	(0.20)	C6A - C7A - N7A - O72A
0.24	(0.31)	C4A - N3A - C8A - C7A
2.47	(0.32)	C6A - C7A - C8A - N3A
-176.60	(0.18)	N7A - C7A - C8A - N3A
176.91	(0.19)	C8B - N3B - C4B - N4B
-2.75	(0.33)	C8B - N3B - C4B - C5B
-176.35	(0.22)	N4B - C4B - C5B - C6B
3.30	(0.34)	N3B - C4B - C5B - C6B
-0.80	(0.33)	C4B - C5B - C6B - C7B
-2.04	(0.34)	C5B - C6B - C7B - C8B
177.53	(0.21)	C5B - C6B - C7B - N7B
174.45	(0.21)	C8B - C7B - N7B - O71B
-5.13	(0.32)	C6B - C7B - N7B - O71B
-4.65	(0.33)	C8B - C7B - N7B - O72B
175.78	(0.21)	C6B - C7B - N7B - O72B
-0.24	(0.33)	C4B - N3B - C8B - C7B
2.67	(0.35)	C6B - C7B - C8B - N3B
-176.90	(0.21)	N7B - C7B - C8B - N3B

Distance N-O

2.889	(0.003)	N1 - O22_$1
2.727	(0.003)	N1 - O22
2.904	(0.003)	N1 - O1_$2
2.694	(0.003)	N3A - O22_$1
2.847	(0.003)	N4A - O1_$3
2.790	(0.003)	N4A - O21_$1
3.060	(0.003)	N4B - O71A_$4
3.325	(0.003)	N4B - O72B_$5

Distance NH-O

1.956	(0.003)	H11 - O22_$1
2.357	(0.003)	H12 - O22

2.068 (0.003) H12 - O1_$2
1.727 (0.003) H3A - O22_$1
1.872 (0.003) H41A - O1_$3
1.861 (0.003) H42A - O21_$1
2.570 (0.003) H41B - O71A_$4
2.642 (0.003) H41B - O72B_$5

Angle NHO

168.07 (0.07) N1 - H11 - O22_$1
103.03 (0.07) N1 - H12 - O22
147.55 (0.07) N1 - H12 - O1_$2
166.01 (0.08) N3A - H3A - O22_$1
170.85 (0.07) N4A - H41A - O1_$3
169.18 (0.08) N4A - H42A - O21_$1
109.31 (0.08) N4B - H41B - O71A_$4
124.50 (0.07) N4B - H41B - O72B_$5

Distance N-N

3.043 (0.004) N4B - N3B_$6

Distance NH-N

2.137 (0.003) H42B - N3B_$6

Angle NHN

168.09 (0.08) N4B - H42B - N3B_$6

Distance C-O

3.336 (0.004) C6A - O72B_$7
3.092 (0.004) C8A - O71B
4.828 (0.005) C8A - O72B
3.366 (0.004) C6B - O72A_$5
3.352 (0.004) C8B - O71A_$8

Distance CH-O

2.475 (0.003) H6A - O72B_$7
2.227 (0.003) H8A - O71B
3.814 (0.004) H8A - O72B
2.564 (0.003) H6B - O72A_$5
2.517 (0.003) H8B - O71A_$8

Angle CHO

145.82 (0.07) C6A - H6A - O72B_$7
141.00 (0.08) C8A - H8A - O71B
170.11 (0.04) C8A - H8A - O72B
138.23 (0.07) C6B - H6B - O72A_$5
149.38 (0.07) C8B - H8B - O71A_$8

Table 1. Crystal data and structure refinement for 3.

Identification code	imidoxam
Empirical formula	$C_5H_7N_3O_3$
Formula weight	157.14
Temperature	123(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 6.162(3) Å α = 90° b = 12.801(2) Å β = 96.61° c = 8.7770(10) Å γ = 90°
Volume	687.7(4) $Å^3$
Z	4
Density (calculated)	1.518 Mg/m^3
Absorption coefficient	0.127 mm^{-1}
F(000)	328
Crystal size	0.68 x 0.18 x 0.12 mm
θ range for data collection	2.83 to 24.99°
Index ranges	$0 \le h \le 7$, $0 \le k \le 15$, $-10 \le \ell \le 10$
Reflections collected	1332
Independent reflections	1215 (R_{int} = 0.0518)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1215 / 0 / 100
Goodness-of-fit on F^2	1.035
Final R indices [$I>2\sigma(I)$]	R1 = 0.0770, wR2 = 0.1717
R indices (all data)	R1 = 0.1483, wR2 = 0.2162
Largest diff. peak and hole	0.408 and −0.483 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for $\frac{1}{3}$U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	5675(6)	6608(3)	3922(4)	27(1)
N(1)	3750(7)	5811(4)	1890(5)	20(1)
C(1)	5547(9)	6167(4)	2665(5)	19(1)
C(2)	7696(8)	6028(4)	1872(5)	16(1)
O(21)	9446(6)	6178(3)	2702(4)	20(1)
O(22)	7437(6)	5805(3)	466(4)	23(1)
N(3)	10048(8)	3663(3)	1777(4)	21(1)
C(4)	7932(9)	3479(4)	2039(6)	20(1)
C(5)	7933(8)	3402(4)	3576(6)	20(1)
N(6)	10010(8)	3553(4)	4220(4)	22(1)
C(7)	11289(9)	3704(4)	3103(6)	21(1)

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

O(1)-C(1)	1.234(6)	N(1)-C(1)	1.313(7)
C(1)-C(2)	1.576(7)	C(2)-O(21)	1.244(6)
C(2)-O(22)	1.259(6)	N(3)-C(7)	1.318(7)
N(3)-C(4)	1.370(7)	C(4)-C(5)	1.353(7)
C(5)-N(6)	1.352(7)	N(6)-C(7)	1.341(7)

O(1)-C(1)-N(1)	125.8(5)	O(1)-C(1)-C(2)	118.4(4)
N(1)-C(1)-C(2)	115.7(4)	O(21)-C(2)-O(22)	127.8(5)
O(21)-C(2)-C(1)	116.1(4)	O(22)-C(2)-C(1)	116.1(4)
C(7)-N(3)-C(4)	109.0(4)	C(5)-C(4)-N(3)	106.8(5)
N(6)-C(5)-C(4)	107.4(4)	C(7)-N(6)-C(5)	108.8(4)
N(3)-C(7)-N(6)	108.0(5)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 3

The anisotropic displacement factor exponent takes the form:

$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
O(1)	28(2)	42(2)	12(2)	-8(2)	10(2)	-5(2)
N(1)	19(2)	30(3)	12(2)	-1(2)	8(2)	-1(2)
C(1)	25(3)	19(3)	13(3)	2(2)	5(2)	-1(2)
C(2)	16(3)	23(3)	11(2)	1(2)	6(2)	-7(2)
O(21)	18(2)	31(2)	13(2)	-1(2)	7(2)	0(2)
O(22)	29(2)	34(2)	7(2)	-2(2)	8(2)	-5(2)
N(3)	29(3)	27(3)	7(2)	1(2)	5(2)	-1(2)
C(4)	20(3)	25(3)	16(3)	-2(2)	3(2)	-2(2)
C(5)	20(3)	25(3)	15(3)	2(2)	4(2)	-4(2)
N(6)	31(3)	25(3)	10(2)	-1(2)	7(2)	-3(2)
C(7)	16(3)	29(3)	18(3)	1(2)	8(2)	-2(2)

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

	x	y	z	U(eq)
H(11)	2390(7)	6023(4)	2284(5)	24
H(12)	3726(7)	5607(4)	947(5)	24
H(3)	10509(8)	3743(3)	855(4)	25
H(4)	6756(9)	3421(4)	1233(6)	24
H(5)	6711(8)	3218(4)	4164(6)	24
H(6)	10639(8)	3407(4)	5262(4)	26
H(7)	12766(9)	3820(4)	3409(6)	25

1 x-1, y, z
2 -x+1, -y+1, -z
3 -x+2, -y+1, -z
4 -x+2, -y+1, -z+1
5 -x+1, y-1/2, -z+1/2
6 -x+1, -y+1, -z+1

elected torsion angles

 14.26 (0.72) O1 - C1 - C2 - O21
166.93 (0.46) N1 - C1 - C2 - O21
-163.97 (0.50) O1 - C1 - C2 - O22
 14.84 (0.67) N1 - C1 - C2 - O22
 -0.41 (0.63) C7 - N3 - C4 - C5
  0.80 (0.63) N3 - C4 - C5 - N6
 -0.91 (0.64) C4 - C5 - N6 - C7
 -0.15 (0.61) C4 - N3 - C7 - N6
  0.66 (0.61) C5 - N6 - C7 - N3

istance N-O

   2.863 (0.006) N1 - O21_$1
   2.716 (0.006) N1 - O22
   2.957 (0.006) N1 - O22_$2
   2.729 (0.005) N3 - O22_$3
   2.962 (0.006) N6 - O1_$4
   2.705 (0.005) N6 - O21_$4

istance NH-O

   1.902 (0.006) H11 - O21_$1
   2.386 (0.006) H12 - O22
   2.262 (0.006) H12 - O22_$2
   1.903 (0.006) H3 - O22_$3
   2.302 (0.006) H6 - O1_$4
   1.870 (0.005) H6 - O21_$4

ngle NHO

165.76 (0.17) N1 - H11 - O21_$1
103.04 (0.13) N1 - H12 - O22
137.31 (0.13) N1 - H12 - O22_$2
152.88 (0.17) N3 - H3 - O22_$3
124.58 (0.13) N6 - H6 - O1_$4
142.58 (0.18) N6 - H6 - O21_$4

istance C-O

   3.310 (0.007) C4 - O1_$5
   3.299 (0.006) C5 - O1_$6
   3.058 (0.006) C7 - O1_$4

istance CH-O

   2.757 (0.007) H4 - O1_$5
   2.367 (0.006) H5 - O1_$6
   2.488 (0.006) H7 - O1_$4

ngle CHO

117.57	(0.14)	C4 - H4 - O1_$5
156.96	(0.16)	C5 - H5 - O1_$6
119.67	(0.14)	C7 - H7 - O1_$4

Table 1. Crystal data and structure refinement for 4

Identification code	4clboxam
Empirical formula	$C_9H_{11}ClN_2O_3$
Formula weight	230.65
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 15.6740(10) Å α = 90° b = 12.1290(10) Å β = 92.820(10)° c = 11.429(2) Å γ = 90°
Volume	2170.1(4) $Å^3$
Z	8
Density (calculated)	1.412 Mg/m^3
Absorption coefficient	0.341 mm^{-1}
F(000)	960
Crystal size	0.44 x 0.28 x 0.18 mm
θ range for data collection	2.12 to 22.50°
Index ranges	$-16 \le h \le 16$, $-13 \le k \le 0$, $0 \le \ell \le 12$
Reflections collected	3002
Independent reflections	2830 (R_{int} = 0.0176)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2829 / 0 / 271
Goodness-of-fit on F^2	1.054
Final R indices [$I>2\sigma(I)$]	R1 = 0.0471, wR2 = 0.0972
R indices (all data)	R1 = 0.0903, wR2 = 0.1171
Largest diff. peak and hole	0.267 and -0.244 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for ~~4~~ U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1A)	953(2)	-64(2)	4624(2)	52(1)
N(1A)	880(2)	-866(2)	2847(3)	45(1)
C(1A)	822(2)	-10(3)	3559(3)	35(1)
C(2A)	577(2)	1099(3)	2958(3)	31(1)
O(21A)	480(2)	1893(2)	3636(2)	45(1)
O(22A)	506(2)	1104(2)	1865(2)	35(1)
O(1B)	1325(2)	4869(2)	2575(2)	44(1)
N(1B)	831(2)	4229(2)	4280(2)	37(1)
C(1B)	1142(2)	5000(3)	3611(3)	32(1)
C(2B)	1299(2)	6132(3)	4197(3)	34(1)
O(21B)	1548(2)	6898(2)	3566(2)	41(1)
O(22B)	1177(2)	6183(2)	5268(2)	48(1)
N(3A)	1087(2)	3092(2)	1045(2)	35(1)
C(4A)	1997(2)	2875(3)	778(3)	45(1)
C(5A)	2499(2)	2374(3)	1787(3)	43(1)
C(6A)	2949(3)	3020(4)	2604(4)	56(1)
C(7A)	3428(3)	2561(5)	3526(4)	63(1)
C(8A)	3446(3)	1439(5)	3637(4)	59(1)
Cl(8A)	4037(1)	838(1)	4808(1)	97(1)
C(9A)	3007(3)	769(4)	2861(4)	65(1)
C(10A)	2541(3)	1235(4)	1924(4)	53(1)
N(3B)	1640(2)	8258(2)	6099(2)	36(1)
C(4B)	2522(3)	8571(3)	5784(4)	54(1)
C(5B)	3174(3)	7711(3)	6140(3)	46(1)
C(6B)	3335(3)	6850(4)	5407(4)	64(1)
C(7B)	3941(3)	6063(4)	5711(4)	69(1)
C(8B)	4397(3)	6154(4)	6766(4)	58(1)
Cl(8B)	5153(1)	5148(1)	7163(1)	86(1)
C(9B)	4250(3)	7000(4)	7513(4)	66(1)
C(10B)	3644(3)	7774(4)	7190(4)	62(1)

Table 3. Bond lengths [Å] and angles [°] for 4

O(1A)-C(1A)	1.226(4)	N(1A)-C(1A)	1.325(4)
C(1A)-C(2A)	1.551(5)	C(2A)-O(22A)	1.248(4)
C(2A)-O(21A)	1.250(4)	O(1B)-C(1B)	1.241(4)
N(1B)-C(1B)	1.317(4)	C(1B)-C(2B)	1.542(5)
C(2B)-O(22B)	1.249(4)	C(2B)-O(21B)	1.251(4)
N(3A)-C(4A)	1.497(4)	C(4A)-C(5A)	1.493(5)
C(5A)-C(6A)	1.385(5)	C(5A)-C(10A)	1.391(6)
C(6A)-C(7A)	1.380(6)	C(7A)-C(8A)	1.368(7)
C(8A)-C(9A)	1.363(6)	C(8A)-Cl(8A)	1.749(4)
C(9A)-C(10A)	1.386(6)	N(3B)-C(4B)	1.495(5)
C(4B)-C(5B)	1.502(5)	C(5B)-C(6B)	1.370(6)
C(5B)-C(10B)	1.379(6)	C(6B)-C(7B)	1.378(6)
C(7B)-C(8B)	1.375(6)	C(8B)-C(9B)	1.362(6)
C(8B)-Cl(8B)	1.745(5)	C(9B)-C(10B)	1.372(6)

O(1A)-C(1A)-N(1A)	123.7(3)	O(1A)-C(1A)-C(2A)	120.8(3)
N(1A)-C(1A)-C(2A)	115.5(3)	O(22A)-C(2A)-O(21A)	127.5(3)
O(22A)-C(2A)-C(1A)	117.1(3)	O(21A)-C(2A)-C(1A)	115.4(3)
O(1B)-C(1B)-N(1B)	124.9(3)	O(1B)-C(1B)-C(2B)	119.3(3)
N(1B)-C(1B)-C(2B)	115.8(3)	O(22B)-C(2B)-O(21B)	126.6(3)
O(22B)-C(2B)-C(1B)	116.2(3)	O(21B)-C(2B)-C(1B)	117.2(3)
C(5A)-C(4A)-N(3A)	112.7(3)	C(6A)-C(5A)-C(10A)	117.7(4)
C(6A)-C(5A)-C(4A)	121.5(4)	C(10A)-C(5A)-C(4A)	120.7(4)
C(7A)-C(6A)-C(5A)	121.8(4)	C(8A)-C(7A)-C(6A)	118.7(5)
C(9A)-C(8A)-C(7A)	121.7(4)	C(9A)-C(8A)-Cl(8A)	118.8(4)
C(7A)-C(8A)-Cl(8A)	119.5(4)	C(8A)-C(9A)-C(10A)	119.3(5)
C(9A)-C(10A)-C(5A)	120.8(4)	N(3B)-C(4B)-C(5B)	112.5(3)
C(6B)-C(5B)-C(10B)	117.9(4)	C(6B)-C(5B)-C(4B)	120.4(4)
C(10B)-C(5B)-C(4B)	121.6(4)	C(5B)-C(6B)-C(7B)	121.2(4)
C(8B)-C(7B)-C(6B)	119.2(4)	C(9B)-C(8B)-C(7B)	120.8(4)
C(9B)-C(8B)-Cl(8B)	119.9(4)	C(7B)-C(8B)-Cl(8B)	119.3(4)
C(8B)-C(9B)-C(10B)	118.9(4)	C(9B)-C(10B)-C(5B)	121.9(4)

Symmetry transformations used to generate equivalent atoms:

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

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O(1A)	95(2)	35(2)	25(2)	0(1)	-6(1)	12(2)
N(1A)	81(3)	25(2)	30(2)	-1(2)	-2(2)	10(2)
C(1A)	45(2)	25(2)	34(2)	-1(2)	2(2)	-2(2)
C(2A)	33(2)	27(2)	32(2)	-1(2)	-3(2)	-3(2)
O(21A)	76(2)	27(2)	33(1)	-5(1)	-4(1)	6(1)
O(22A)	52(2)	29(2)	24(1)	2(1)	-1(1)	-2(1)
O(1B)	73(2)	32(2)	28(1)	-4(1)	11(1)	-4(1)
N(1B)	60(2)	20(2)	29(2)	5(2)	3(2)	-3(2)
C(1B)	41(2)	28(2)	25(2)	-2(2)	-2(2)	7(2)
C(2B)	48(2)	29(2)	25(2)	1(2)	-1(2)	-1(2)
O(21B)	64(2)	27(2)	32(1)	2(1)	3(1)	-8(1)
O(22B)	81(2)	36(2)	26(2)	-6(1)	9(1)	-12(2)
N(3A)	50(2)	29(2)	26(2)	2(1)	1(1)	-1(2)
C(4A)	47(3)	54(3)	34(2)	3(2)	10(2)	-2(2)
C(5A)	38(2)	51(3)	39(2)	1(2)	1(2)	-2(2)
C(6A)	53(3)	58(3)	56(3)	8(3)	-5(2)	-8(2)
C(7A)	48(3)	91(4)	49(3)	5(3)	-7(2)	-1(3)
C(8A)	39(3)	91(4)	47(3)	13(3)	5(2)	23(3)
Cl(8A)	67(1)	153(2)	69(1)	35(1)	-4(1)	38(1)
C(9A)	61(3)	58(3)	75(3)	10(3)	8(3)	18(3)
C(10A)	42(3)	58(3)	57(3)	2(2)	2(2)	11(2)
N(3B)	57(2)	24(2)	28(2)	-2(1)	3(2)	2(2)
C(4B)	61(3)	46(3)	54(3)	9(2)	12(2)	-7(2)
C(5B)	45(3)	49(3)	45(2)	-1(2)	10(2)	-7(2)
C(6B)	62(3)	84(4)	46(3)	-10(3)	-2(2)	15(3)
C(7B)	67(3)	78(4)	64(3)	-21(3)	5(3)	19(3)
C(8B)	41(3)	70(3)	62(3)	8(3)	8(2)	4(2)
Cl(8B)	57(1)	96(1)	106(1)	16(1)	2(1)	18(1)
C(9B)	61(3)	81(4)	56(3)	-5(3)	-12(2)	2(3)
C(10B)	74(3)	59(3)	53(3)	-15(2)	-2(3)	0(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for ~~4~~ 4

	x	y	z	U(eq)
H(12A)	809(2)	-769(2)	2031(3)	55
H(11A)	1059(2)	-1573(2)	3121(3)	55
H(11B)	643(2)	3422(2)	4058(2)	44
H(12B)	680(2)	4411(2)	5155(2)	44
H(31A)	799(2)	2409(2)	1308(2)	42
H(32A)	835(2)	3401(2)	412(2)	42
H(33A)	1130(2)	3611(2)	1527(2)	42
H(41A)	1987(2)	2400(3)	85(3)	54
H(42A)	2229(2)	3605(3)	485(3)	54
H(6A)	2931(3)	3805(4)	2376(4)	67
H(7A)	3833(3)	2995(5)	4180(4)	75
H(9A)	3038(3)	30(4)	2866(4)	77
H(10A)	2110(3)	808(4)	1333(4)	63
H(31B)	1451(2)	7589(2)	5783(2)	44
H(32B)	1585(2)	8381(2)	6897(2)	44
H(33B)	1277(2)	8790(2)	5736(2)	44
H(41B)	2581(3)	9304(3)	6234(4)	64
H(42B)	2482(3)	8590(3)	4921(4)	64
H(6B)	2959(3)	6793(4)	4589(4)	77
H(7B)	4142(3)	5400(4)	5211(4)	83
H(9B)	4600(3)	6976(4)	8281(4)	79
H(10B)	3460(3)	8372(4)	7674(4)	75

Selected torsion angles

175.61	(0.34)	O1A - C1A - C2A - O22A
-3.98	(0.47)	N1A - C1A - C2A - O22A
-3.88	(0.51)	O1A - C1A - C2A - O21A
176.53	(0.32)	N1A - C1A - C2A - O21A
-173.61	(0.32)	O1B - C1B - C2B - O22B
5.14	(0.47)	N1B - C1B - C2B - O22B
5.21	(0.50)	O1B - C1B - C2B - O21B
-176.05	(0.31)	N1B - C1B - C2B - O21B
-91.40	(0.43)	N3A - C4A - C5A - C6A
89.54	(0.45)	N3A - C4A - C5A - C10A
0.32	(0.60)	C10A - C5A - C6A - C7A
-178.76	(0.38)	C4A - C5A - C6A - C7A
-0.90	(0.65)	C5A - C6A - C7A - C8A
0.21	(0.70)	C6A - C7A - C8A - C9A
-179.20	(0.30)	C6A - C7A - C8A - Cl8A
1.04	(0.67)	C7A - C8A - C9A - C10A
-179.55	(0.31)	Cl8A - C8A - C9A - C10A
-1.63	(0.63)	C8A - C9A - C10A - C5A
0.95	(0.61)	C6A - C5A - C10A - C9A
-179.96	(0.34)	C4A - C5A - C10A - C9A
87.15	(0.46)	N3B - C4B - C5B - C6B
-94.72	(0.45)	N3B - C4B - C5B - C10B
0.73	(0.66)	C10B - C5B - C6B - C7B
178.93	(0.41)	C4B - C5B - C6B - C7B
-0.73	(0.72)	C5B - C6B - C7B - C8B
0.79	(0.71)	C6B - C7B - C8B - C9B
179.03	(0.36)	C6B - C7B - C8B - Cl8B
-0.85	(0.70)	C7B - C8B - C9B - C10B
-179.07	(0.37)	Cl8B - C8B - C9B - C10B
0.86	(0.71)	C8B - C9B - C10B - C5B
-0.80	(0.67)	C6B - C5B - C10B - C9B
-178.97	(0.40)	C4B - C5B - C10B - C9B

Distance N-O

3.007	(0.004)	N1A - O21B_$1
2.692	(0.004)	N1A - O22A
3.031	(0.004)	N1A - O22B_$2
2.973	(0.004)	N1B - O21A
2.668	(0.004)	N1B - O22B
3.049	(0.004)	N1B - O22A_$3
2.758	(0.004)	N3A - O22A
2.893	(0.004)	N3A - O1A_$2
2.868	(0.004)	N3A - O21A_$2
2.790	(0.004)	N3A - O1B
2.774	(0.004)	N3B - O22B
2.887	(0.004)	N3B - O1B_$4
2.836	(0.003)	N3B - O21B_$4
2.822	(0.004)	N3B - O1A_$5

Distance NH-O

2.061	(0.004)	H11A - O21B_$1
2.327	(0.004)	H12A - O22A
2.181	(0.004)	H12A - O22B_$2
1.930	(0.004)	H11B - O21A
2.287	(0.004)	H12B - O22B
2.083	(0.004)	H12B - O22A_$3
1.774	(0.004)	H31A - O22A

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     2.221 (0.004)  H32A - O1A_$2
     2.109 (0.004)  H32A - O21A_$2
     1.955 (0.004)  H33A - O1B
     1.848 (0.004)  H31B - O22B
     2.302 (0.004)  H32B - O1B_$4
     1.941 (0.003)  H32B - O21B_$4
     1.934 (0.004)  H33B - O1A_$5


Angle NHO

  173.40 ( 0.10)  N1A - H11A - O21B_$1
  102.49 ( 0.09)  N1A - H12A - O22A
  149.63 ( 0.10)  N1A - H12A - O22B_$2
  171.21 ( 0.12)  N1B - H11B - O21A
   99.03 ( 0.09)  N1B - H12B - O22B
  150.07 ( 0.10)  N1B - H12B - O22A_$3
  168.11 ( 0.12)  N3A - H31A - O22A
  132.09 ( 0.10)  N3A - H32A - O1A_$2
  142.87 ( 0.10)  N3A - H32A - O21A_$2
  174.62 ( 0.10)  N3A - H33A - O1B
  173.09 ( 0.12)  N3B - H31B - O22B
  120.26 ( 0.09)  N3B - H32B - O1B_$4
  160.38 ( 0.11)  N3B - H32B - O21B_$4
  156.06 ( 0.12)  N3B - H33B - O1A_$5

EQIV $1 x,y-1,z
EQIV $2 x,.5-y,z-.5
EQIV $3 x,.5-y,.5+z
EQIV $4 x,1.5-y,.5+z
EQIV $5 x,y+1,z
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Table 5. Crystal data and structure refinement for 5.

Identification code	3cloxam
Empirical formula	$C_9H_{11}ClN_2O_3$
Formula weight	230.65
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P21/c
Unit cell dimensions	a = 8.800(2) Å α = 90° b = 11.727(2) Å β = 99.14(3)° c = 11.115(2) Å γ = 90°
Volume	1132.5(4) Å^3
Z	4
Density (calculated)	1.353 Mg/m^3
Absorption coefficient	0.327 mm^{-1}
F(000)	480
Crystal size	0.3 x 0.45 x 0.2 mm
θ range for data collection	2.34 to 19.99°
Index ranges	$-1 \le h \le 8$, $-1 \le k \le 11$, $-10 \le \ell \le 10$
Reflections collected	1506
Independent reflections	1062 (R_{int} = 0.0155)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1062 / 0 / 136
Goodness-of-fit on F^2	1.057
Final R indices [I>2σ(I)]	R1 = 0.0400, wR2 = 0.0916
R indices (all data)	R1 = 0.0563, wR2 = 0.1009
Largest diff. peak and hole	0.211 and -0.194 eÅ^{-3}

Table 6. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 5. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cl(13)	8576(2)	4782(2)	1309(1)	114(1)
O(1)	14163(3)	-317(2)	8430(2)	45(1)
O(22)	14087(3)	1131(2)	5683(2)	51(1)
N(17)	13659(3)	3416(2)	5021(2)	36(1)
O(21)	13861(3)	1834(2)	7507(2)	45(1)
N(1)	14946(4)	-902(2)	6696(2)	46(1)
C(13)	9121(6)	3972(5)	2598(4)	69(1)
C(17)	12255(4)	3974(3)	5324(3)	48(1)
C(1)	14406(4)	-139(3)	7381(3)	33(1)
C(2)	14084(4)	1049(3)	6803(3)	34(1)
C(11)	10854(5)	3651(4)	4455(4)	52(1)
C(12)	10425(5)	4299(4)	3405(3)	52(1)
C(16)	9993(6)	2716(5)	4675(5)	93(2)
C(14)	8260(6)	3050(6)	2806(6)	101(2)
C(15)	8697(7)	2441(6)	3848(7)	132(2)

Table 7. Bond lengths [Å] and angles [°] for 5.

Cl(13)-C(13)	1.723(5)	O(1)-C(1)	1.236(4)
O(22)-O(22)#1	0.000(9)	O(22)-C(2)	1.250(4)
N(17)-C(17)	1.484(4)	O(21)-C(2)	1.244(4)
N(1)-C(1)	1.312(4)	C(13)-C(14)	1.361(7)
C(13)-C(12)	1.394(6)	C(17)-C(11)	1.489(5)
C(1)-C(2)	1.541(5)	C(2)-O(22)#1	1.250(4)
C(11)-C(16)	1.376(6)	C(11)-C(12)	1.393(5)
C(16)-C(15)	1.385(7)	C(14)-C(15)	1.363(7)

O(22)#1-O(22)-C(2)	0(10)	C(14)-C(13)-C(12)	122.2(4)
C(14)-C(13)-Cl(13)	119.3(4)	C(12)-C(13)-Cl(13)	118.4(4)
N(17)-C(17)-C(11)	112.0(3)	O(1)-C(1)-N(1)	124.3(3)
O(1)-C(1)-C(2)	119.9(3)	N(1)-C(1)-C(2)	115.8(3)
O(21)-C(2)-O(22)#1	126.5(3)	O(21)-C(2)-O(22)	126.5(3)
O(22)#1-C(2)-O(22)	0.0(3)	O(21)-C(2)-C(1)	116.4(3)
O(22)#1-C(2)-C(1)	117.1(3)	O(22)-C(2)-C(1)	117.1(3)
C(16)-C(11)-C(12)	120.0(4)	C(16)-C(11)-C(17)	120.6(4)
C(12)-C(11)-C(17)	119.4(4)	C(11)-C(12)-C(13)	118.3(4)
C(11)-C(16)-C(15)	119.1(5)	C(13)-C(14)-C(15)	118.1(5)
C(14)-C(15)-C(16)	122.3(5)		

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z

Table 8. Anisotropic displacement parameters [$Å^2$ x 10^3] for 5.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Cl(13)	111(1)	152(2)	72(1)	7(1)	-10(1)	51(1)
O(1)	69(2)	42(2)	28(2)	6(1)	15(1)	13(1)
O(22)	94(2)	34(2)	28(2)	6(1)	15(1)	12(1)
N(17)	51(2)	31(2)	27(2)	-1(1)	7(1)	-3(2)
O(21)	76(2)	27(1)	34(1)	-4(1)	16(1)	1(1)
N(1)	81(2)	28(2)	31(2)	0(2)	18(2)	11(2)
C(13)	60(3)	87(4)	59(3)	-1(3)	6(3)	30(3)
C(17)	53(3)	50(2)	43(2)	-8(2)	14(2)	5(2)
C(1)	40(2)	31(2)	27(2)	-2(2)	3(2)	-1(2)
C(2)	43(2)	29(2)	30(2)	-3(2)	6(2)	-1(2)
C(11)	47(3)	52(3)	58(3)	-4(2)	13(2)	3(2)
C(12)	46(3)	63(3)	47(3)	-4(2)	11(2)	13(2)
C(16)	73(3)	89(4)	112(4)	26(3)	-6(3)	-26(3)
C(14)	68(4)	114(5)	110(5)	-1(4)	-16(3)	-9(4)
C(15)	101(5)	114(5)	170(7)	19(5)	-15(5)	-58(4)

Table 9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 5.

	x	y	z	U(eq)
H(17C)	13715(3)	3405(2)	4229(2)	43
H(17B)	13663(3)	2601(2)	5155(2)	43
H(17A)	14581(3)	3801(2)	5491(2)	43
H(1B)	15334(4)	-1604(2)	6991(2)	55
H(1A)	15019(4)	-797(2)	5862(2)	55
H(172)	12150(4)	3792(3)	6203(3)	57
H(171)	12437(4)	4999(3)	5293(3)	57
H(12)	11354(5)	5008(4)	3177(3)	62
H(16)	10384(6)	2202(5)	5574(5)	112
H(14)	7238(6)	2808(6)	2091(6)	121
H(15)	8259(7)	1807(6)	3916(7)	159

$1 -x+3, -y, -z+1
$2 -x+3, y-1/2, -z+3/2
$3 -x+3, y+1/2, -z+3/2
$4 x, y, z
$5 x, -y+1/2, z-1/2

Selected torsion angles

0.00	(99.99)	O22_$4 - O22 - C2 - O21
0.00	(1.31)	O22_$4 - O22 - C2 - O22_$4
0.00	(99.99)	O22_$4 - O22 - C2 - C1
12.96	(0.47)	O1 - C1 - C2 - O21
-166.59	(0.30)	N1 - C1 - C2 - O21
-167.70	(0.31)	O1 - C1 - C2 - O22_$4
12.75	(0.46)	N1 - C1 - C2 - O22_$4
-167.70	(0.31)	O1 - C1 - C2 - O22
12.75	(0.46)	N1 - C1 - C2 - O22
90.00	(0.45)	N17 - C17 - C11 - C16
-89.39	(0.40)	N17 - C17 - C11 - C12
-0.19	(0.58)	C16 - C11 - C12 - C13
179.20	(0.34)	C17 - C11 - C12 - C13
0.29	(0.62)	C14 - C13 - C12 - C11
179.23	(0.28)	Cl13 - C13 - C12 - C11
-0.68	(0.74)	C12 - C11 - C16 - C15
179.93	(0.49)	C17 - C11 - C16 - C15
0.51	(0.81)	C12 - C13 - C14 - C15
-178.42	(0.47)	Cl13 - C13 - C14 - C15
-1.44	(0.99)	C13 - C14 - C15 - C16
1.54	(0.96)	C11 - C16 - C15 - C14

Distance N-O

2.916	(0.004)	N1 - O22_$1
2.939	(0.004)	N1 - O21_$2
2.792	(0.004)	N17 - O1_$3
2.788	(0.003)	N17 - O22_$4
2.844	(0.003)	N17 - O21_$5
2.694	(0.004)	N1 - O22_$4

Distance H-O

2.037	(0.004)	H1A - O22_$1
2.010	(0.004)	H1B - O21_$2
1.818	(0.003)	H17A - O1_$3
1.840	(0.003)	H17B - O22_$4
1.959	(0.003)	H17C - O21_$5
2.403	(0.004)	H1A - O22_$4

Angle NHO

153.52	(0.10)	N1 - H1A - O22_$1
175.50	(0.10)	N1 - H1B - O21_$2
163.43	(0.11)	N17 - H17A - O1_$3
166.04	(0.11)	N17 - H17B - O22_$4
172.50	(0.10)	N17 - H17C - O21_$5
97.38	(0.09)	N1 - H1A - O22_$4

Table 1. Crystal data and structure refinement for 6.

Identification code	koxam1
Empirical formula	$C_2H_4KNO_4$
Formula weight	145.16
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P21/c
Unit cell dimensions	a = 3.8160(10) Å α = 90° b = 13.553(3) Å β = 90.18(3)° c = 10.506(2) Å γ = 90°
Volume	543.3(2) Å^3
Z	4
Density (calculated)	1.775 Mg/m^3
Absorption coefficient	0.902 mm^{-1}
F(000)	296
Crystal size	0.8 x 0.52 x 0.36 mm
θ range for data collection	2.45 to 25.00°
Index ranges	$0 \le h \le 4$, $0 \le k \le 16$, $-12 \le \ell \le 12$
Reflections collected	1114
Independent reflections	963 (R_{int} = 0.0167)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	963 / 0 / 73
Goodness-of-fit on F^2	1.167
Final R indices [I>2σ(I)]	R1 = 0.0347, wR2 = 0.0854
R indices (all data)	R1 = 0.0409, wR2 = 0.0897
Largest diff. peak and hole	0.311 and -0.781 eÅ^{-3}

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 6. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
K(1)	1266(1)	6251(1)	8968(1)	28(1)
O(22)	6075(5)	7055(1)	10605(2)	34(1)
C(2)	6675(5)	7738(1)	11370(2)	20(1)
O(21)	6280(4)	7733(1)	12541(1)	29(1)
C(1)	8086(6)	8711(1)	10785(2)	22(1)
N(1)	7832(6)	8790(1)	9536(2)	32(1)
O(1)	9396(5)	9353(1)	11475(2)	34(1)
O(1W)	3820(4)	5248(1)	11419(2)	38(1)

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

K(1)-O(22)#1	2.737(2)	K(1)-O(22)	2.737(2)
K(1)-O(21)#2	2.784(2)	K(1)-O(1W)#3	2.795(2)
K(1)-O(21)#4	2.797(2)	K(1)-O(1)#2	2.834(2)
K(1)-O(1W)#5	2.838(2)	K(1)-O(22)#6	2.844(2)
K(1)-O(1W)	3.068(2)	K(1)-C(2)#2	3.517(2)
K(1)-K(1)#7	3.8160(10)	K(1)-K(1)#6	3.8160(10)
O(22)-O(22)#1	0.000(5)	O(22)-C(2)	1.248(3)
O(22)-K(1)#7	2.844(2)	C(2)-O(21)	1.239(2)
C(2)-O(22)#1	1.248(3)	C(2)-C(1)	1.552(3)
C(2)-K(1)#8	3.517(2)	O(21)-K(1)#8	2.784(2)
O(21)-K(1)#9	2.797(2)	C(1)-O(1)	1.236(3)
C(1)-N(1)	1.320(3)	O(1)-K(1)#8	2.834(2)
O(1W)-K(1)#3	2.795(2)	O(1W)-K(1)#5	2.838(2)

O(22)#1-K(1)-O(22)	0.00(9)	O(22)#1-K(1)-O(21)#2	126.70(5)
O(22)-K(1)-O(21)#2	126.70(5)	O(22)#1-K(1)-O(1W)#3	86.10(6)
O(22)-K(1)-O(1W)#3	86.10(6)	O(21)#2-K(1)-O(1W)#3	137.61(5)
O(22)#1-K(1)-O(21)#4	71.50(5)	O(22)-K(1)-O(21)#4	71.50(5)
O(21)#2-K(1)-O(21)#4	86.28(5)	O(1W)#3-K(1)-O(21)#4	79.58(5)
O(22)#1-K(1)-O(1)#2	149.55(5)	O(22)-K(1)-O(1)#2	149.55(5)
O(21)#2-K(1)-O(1)#2	58.31(5)	O(1W)#3-K(1)-O(1)#2	79.78(5)
O(21)#4-K(1)-O(1)#2	79.45(5)	O(22)#1-K(1)-O(1W)#5	146.30(5)
O(22)-K(1)-O(1W)#5	146.30(5)	O(21)#2-K(1)-O(1W)#5	79.08(5)
O(1W)#3-K(1)-O(1W)#5	85.29(5)	O(21)#4-K(1)-O(1W)#5	138.06(5)
O(1)#2-K(1)-O(1W)#5	59.38(5)	O(22)#1-K(1)-O(22)#6	86.26(5)
O(22)-K(1)-O(22)#6	86.26(5)	O(21)#2-K(1)-O(22)#6	70.13(5)
O(1W)#3-K(1)-O(22)#6	146.65(5)	O(21)#4-K(1)-O(22)#6	127.92(5)
O(1)#2-K(1)-O(22)#6	119.71(5)	O(1W)#5-K(1)-O(22)#6	83.31(5)
O(22)#1-K(1)-O(1W)	55.85(5)	O(22)-K(1)-O(1W)	55.85(5)
O(21)#2-K(1)-O(1W)	152.41(5)	O(1W)#3-K(1)-O(1W)	65.71(6)
O(21)#4-K(1)-O(1W)	116.89(5)	O(1)#2-K(1)-O(1W)	136.58(5)
O(1W)#5-K(1)-O(1W)	91.07(6)	O(22)#6-K(1)-O(1W)	83.25(5)
O(22)#1-K(1)-C(2)#2	131.61(5)	O(22)-K(1)-C(2)#2	131.61(5)
O(21)#2-K(1)-C(2)#2	18.37(4)	O(1W)#3-K(1)-C(2)#2	120.19(5)
O(21)#4-K(1)-C(2)#2	74.45(5)	O(1)#2-K(1)-C(2)#2	43.23(5)
O(1W)#5-K(1)-C(2)#2	80.13(5)	O(22)#6-K(1)-C(2)#2	88.50(5)
O(1W)-K(1)-C(2)#2	168.59(5)	O(22)#1-K(1)-K(1)#7	48.04(4)
O(22)-K(1)-K(1)#7	48.04(4)	O(21)#2-K(1)-K(1)#7	132.99(4)
O(1W)#3-K(1)-K(1)#7	47.83(4)	O(21)#4-K(1)-K(1)#7	46.71(4)
O(1)#2-K(1)-K(1)#7	104.41(4)	O(1W)#5-K(1)-K(1)#7	133.12(4)
O(22)#6-K(1)-K(1)#7	134.30(4)	O(1W)-K(1)-K(1)#7	71.63(4)
C(2)#2-K(1)-K(1)#7	119.72(4)	O(22)#1-K(1)-K(1)#6	131.96(4)
O(22)-K(1)-K(1)#6	131.96(4)	O(21)#2-K(1)-K(1)#6	47.01(4)
O(1W)#3-K(1)-K(1)#6	132.17(4)	O(21)#4-K(1)-K(1)#6	133.29(4)
O(1)#2-K(1)-K(1)#6	75.59(4)	O(1W)#5-K(1)-K(1)#6	46.88(4)
O(22)#6-K(1)-K(1)#6	45.70(4)	O(1W)-K(1)-K(1)#6	108.36(4)
C(2)#2-K(1)-K(1)#6	60.28(4)	K(1)#7-K(1)-K(1)#6	180.00(4)
O(22)#1-O(22)-C(2)	0(10)	O(22)#1-O(22)-K(1)	0(10)
C(2)-O(22)-K(1)	145.2(2)	O(22)#1-O(22)-K(1)#7	0(10)
C(2)-O(22)-K(1)#7	123.20(14)	K(1)-O(22)-K(1)#7	86.26(5)
O(21)-C(2)-O(22)#1	127.8(2)	O(21)-C(2)-O(22)	127.8(2)
O(22)#1-C(2)-O(22)	0.0(2)	O(21)-C(2)-C(1)	116.2(2)
O(22)#1-C(2)-C(1)	116.0(2)	O(22)-C(2)-C(1)	116.0(2)
O(21)-C(2)-K(1)#8	45.08(11)	O(22)#1-C(2)-K(1)#8	151.57(14)
O(22)-C(2)-K(1)#8	151.57(14)	C(1)-C(2)-K(1)#8	78.69(11)
C(2)-O(21)-K(1)#8	116.55(13)	C(2)-O(21)-K(1)#9	127.96(13)
K(1)#8-O(21)-K(1)#9	86.28(5)	O(1)-C(1)-N(1)	123.6(2)
O(1)-C(1)-C(2)	120.4(2)	N(1)-C(1)-C(2)	116.0(2)
C(1)-O(1)-K(1)#8	116.03(13)	K(1)#3-O(1W)-K(1)#5	85.29(5)

K(1)#3-O(1W)-K(1)	114.28(6)	K(1)#5-O(1W)-K(1)	88.93(5)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z #2 x-1,-y+3/2,z-1/2 #3 -x+1,-y+1,-z+2

#4 x,-y+3/2,z-1/2 #5 -x,-y+1,-z+2 #6 x-1,y,z #7 x+1,y,z

#8 x+1,-y+3/2,z+1/2 #9 x,-y+3/2,z+1/2

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

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
K(1)	27(1)	31(1)	26(1)	-1(1)	-2(1)	-2(1)
O(22)	54(1)	24(1)	25(1)	-1(1)	0(1)	-14(1)
C(2)	20(1)	21(1)	20(1)	1(1)	1(1)	-1(1)
O(21)	42(1)	27(1)	18(1)	3(1)	3(1)	-4(1)
C(1)	27(1)	19(1)	21(1)	0(1)	1(1)	-1(1)
N(1)	54(1)	23(1)	19(1)	3(1)	-2(1)	-13(1)
O(1)	54(1)	25(1)	23(1)	-2(1)	-1(1)	-14(1)
O(1W)	51(1)	29(1)	34(1)	3(1)	6(1)	-9(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 6.

	x	y	z	U(eq)
H(1B)	8440(6)	9355(1)	9207(2)	38
H(1A)	7067(6)	8287(1)	8994(2)	38
H(2W)	2858(4)	5221(1)	12194(2)	45
H(1W)	4727(4)	5891(1)	11413(2)	45

6

```
$1   x, -y+3/2, z-1/2
 $2   -x+2, -y+2, -z+2
 $3   x, y, z
 $4   -x+1, y-1/2, -z+5/2
 $5   x-1, y, z
 $6   x+1, y, z
 $7   -x, -y+1, -z+2
 $8   -x+1, -y+1, -z+2
 $9   x, -y+3/2, z+1/2
 $10  x+1, -y+3/2, z+1/2
 $11  x-1, -y+3/2, z-1/2

Selected torsion angles

     0.00 ( 1.17)  O22_$3 - K1 - O22 - O22_$3
     0.00 (99.99)  O21_$11 - K1 - O22 - O22_$3
     0.00 (99.99)  O1W_$8 - K1 - O22 - O22_$3
     0.00 (99.99)  O21_$1 - K1 - O22 - O22_$3
     0.00 (99.99)  O1_$11 - K1 - O22 - O22_$3
     0.00 (99.99)  O1W_$7 - K1 - O22 - O22_$3
     0.00 (99.99)  O22_$5 - K1 - O22 - O22_$3
     0.00 (87.07)  O1W - K1 - O22 - O22_$3
     0.00 (80.39)  C2_$11 - K1 - O22 - O22_$3
     0.00 (99.99)  K1_$6 - K1 - O22 - O22_$3
     0.00 (99.99)  K1_$5 - K1 - O22 - O22_$3
     0.00 (99.99)  O22_$3 - K1 - O22 - C2
    32.02 ( 0.25)  O21_$11 - K1 - O22 - C2
  -177.24 ( 0.24)  O1W_$8 - K1 - O22 - C2
   102.45 ( 0.24)  O21_$1 - K1 - O22 - C2
   120.59 ( 0.23)  O1_$11 - K1 - O22 - C2
  -101.75 ( 0.24)  O1W_$7 - K1 - O22 - C2
   -29.72 ( 0.25)  O22_$5 - K1 - O22 - C2
  -114.10 ( 0.24)  O1W - K1 - O22 - C2
    54.93 ( 0.23)  C2_$11 - K1 - O22 - C2
   150.28 ( 0.25)  K1_$6 - K1 - O22 - C2
   -29.72 ( 0.25)  K1_$5 - K1 - O22 - C2
     0.00 (99.99)  O22_$3 - K1 - O22 - K1_$6
  -118.27 ( 0.05)  O21_$11 - K1 - O22 - K1_$6
    32.48 ( 0.05)  O1W_$8 - K1 - O22 - K1_$6
   -47.83 ( 0.04)  O21_$1 - K1 - O22 - K1_$6
   -29.69 ( 0.11)  O1_$11 - K1 - O22 - K1_$6
   107.97 ( 0.08)  O1W_$7 - K1 - O22 - K1_$6
   180.00  O22_$5 - K1 - O22 - K1_$6
    95.62 ( 0.06)  O1W - K1 - O22 - K1_$6
   -95.35 ( 0.06)  C2_$11 - K1 - O22 - K1_$6
     0.00  K1_$6 - K1 - O22 - K1_$6
   180.00  K1_$5 - K1 - O22 - K1_$6
     0.00 (99.99)  O22_$3 - O22 - C2 - O21
    94.35 ( 0.28)  K1 - O22 - C2 - O21
  -121.89 ( 0.20)  K1_$6 - O22 - C2 - O21
     0.00 ( 0.78)  O22_$3 - O22 - C2 - O22_$3
     0.00 (99.99)  K1 - O22 - C2 - O22_$3
     0.00 (99.99)  K1_$6 - O22 - C2 - O22_$3
     0.00 (99.99)  O22_$3 - O22 - C2 - C1
   -85.69 ( 0.27)  K1 - O22 - C2 - C1
    58.07 ( 0.22)  K1_$6 - O22 - C2 - C1
     0.00 (99.99)  O22_$3 - O22 - C2 - K1_$10
   157.95 ( 0.14)  K1 - O22 - C2 - K1_$10
   -58.29 ( 0.33)  K1_$6 - O22 - C2 - K1_$10
   142.97 ( 0.19)  O22_$3 - C2 - O21 - K1_$10
   142.97 ( 0.19)  O22 - C2 - O21 - K1_$10
   -36.99 ( 0.21)  C1 - C2 - O21 - K1_$10
     0.00  K1_$10 - C2 - O21 - K1_$10
  -109.70 ( 0.22)  O22_$3 - C2 - O21 - K1_$9
  -109.70 ( 0.22)  O22 - C2 - O21 - K1_$9
    70.34 ( 0.22)  C1 - C2 - O21 - K1_$9
```