Table. Crystal data and structure refinement for epoxide **13**.

Identification code	nik11t	
Empirical formula	C12 H11 N O3	
Formula weight	217.22	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.3176(5) Å	α= 84.1880(10)°.
	b = 7.8311(5) Å	β= 88.7440(10)°.
	c = 9.0991(6) Å	γ = 79.797(2)°.
Volume	510.53(6) $Å^3$	
Z	2	
Density (calculated)	1.413 Mg/m^3	
Absorption coefficient	0.103 mm^{-1}	
F(000)	228	
Crystal size	0.7 x 0.3 x 0.13 mm^3	
Theta range for data collection	2.25 to 27.69°.	
Index ranges	-5<=h<=9, -9<=k<=8, -11<=l<=11	
Reflections collected	3216	
Independent reflections	2061 [R(int) = 0.0311]	
Completeness to theta = 27.69°	86.3 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2061 / 0 / 145	
Goodness-of-fit on F2	1.053	
Final R indices [I>2sigma(I)]	R1 = 0.0390, wR2 = 0.1074	
R indices (all data)	R1 = 0.0422, wR2 = 0.1109	
Largest diff. peak and hole	0.241 and -0.218 e. $Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for epoxide 13. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)

O(2)	3271(1)	2522(1)	5510(1)	38(1)
O(3)	-871(1)	1980(1)	7606(1)	40(1)
O(1)	1826(2)	5801(1)	6797(1)	42(1)
N(1)	2823(1)	1282(1)	7994(1)	27(1)
C(1)	2106(2)	4373(2)	7493(1)	29(1)
C(6)	3075(2)	1253(2)	10730(1)	32(1)
C(2)	2467(2)	3898(2)	9060(1)	28(1)
C(5)	3071(2)	2299(2)	11870(1)	36(1)
C(7)	2782(2)	2078(2)	9305(1)	25(1)
C(3)	2474(2)	4927(2)	10222(2)	36(1)
C(11)	2178(2)	2636(2)	6797(1)	28(1)
C(4)	2782(2)	4110(2)	11630(2)	39(1)
C(10)	322(2)	2247(2)	6359(2)	34(1)
C(8)	1909(2)	-235(2)	7909(2)	36(1)
C(9)	208(2)	483(2)	7003(2)	38(1)
C(12)	5184(2)	2574(2)	5739(2)	46(1)

Table 3. Bond lengths [Å] and angles [°] for epoxide 13.

O(2)-C(11)	1.4052(15)
O(2)-C(12)	1.4282(18)
O(3)-C(10)	1.4378(17)
O(3)-C(9)	1.4430(17)
O(1)-C(1)	1.2141(16)
N(1)-C(7)	1.3983(15)
N(1)-C(11)	1.4640(15)
N(1)-C(8)	1.4719(17)
C(1)-C(2)	1.4538(17)
C(1)-C(11)	1.5503(18)
C(6)-C(5)	1.3842(19)
C(6)-C(7)	1.3921(17)
C(2)-C(3)	1.3940(17)
C(2)-C(7)	1.3988(17)
C(5)-C(4)	1.392(2)
C(3)-C(4)	1.378(2)
C(11)-C(10)	1.5135(18)
C(10)-C(9)	1.461(2)
C(8)-C(9)	1.499(2)
C(11)-O(2)-C(12)	114.01(10)
C(10)-O(3)-C(9)	60.95(9)
C(7)-N(1)-C(11)	108.05(9)
C(7)-N(1)-C(8)	120.55(10)
C(11)-N(1)-C(8)	110.26(10)
O(1)-C(1)-C(2)	129.92(12)
O(1)-C(1)-C(11)	124.00(12)

C(2)-C(1)-C(11)	106.07(10)
C(5)-C(6)-C(7)	117.54(12)
C(3)-C(2)-C(7)	121.17(11)
C(3)-C(2)-C(1)	130.97(12)
C(7)-C(2)-C(1)	107.82(11)
C(6)-C(5)-C(4)	122.37(12)
C(6)-C(7)-N(1)	127.12(11)
C(6)-C(7)-C(2)	120.37(11)
N(1)-C(7)-C(2)	112.48(10)
C(4)-C(3)-C(2)	118.41(12)
O(2)-C(11)-N(1)	114.04(10)
O(2)-C(11)-C(10)	104.86(10)
N(1)-C(11)-C(10)	104.39(10)
O(2)-C(11)-C(1)	113.42(10)
N(1)-C(11)-C(1)	104.46(9)
C(10)-C(11)-C(1)	115.59(11)
C(3)-C(4)-C(5)	120.13(12)
O(3)-C(10)-C(9)	59.70(9)
O(3)-C(10)-C(11)	112.72(10)
C(9)-C(10)-C(11)	107.31(11)
N(1)-C(8)-C(9)	103.96(10)
O(3)-C(9)-C(10)	59.35(9)
O(3)-C(9)-C(8)	111.29(11)
C(10)-C(9)-C(8)	109.33(11)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for epoxide 13. The anisotropic displacement factor exponent takes the form: -2 p 2[h2 a*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(2)	39(1)	56(1)	21(1)	-5(1)	3(1)	-14(1)
O(3)	34(1)	42(1)	46(1)	-11(1)	6(1)	-11(1)
O(1)	55(1)	31(1)	39(1)	9(1)	-9(1)	-11(1)
N(1)	34(1)	25(1)	22(1)	-3(1)	0(1)	-4(1)
C(1)	30(1)	29(1)	28(1)	1(1)	-3(1)	-7(1)
C(6)	36(1)	31(1)	26(1)	1(1)	0(1)	-2(1)
C(2)	30(1)	28(1)	26(1)	-3(1)	-2(1)	-6(1)
C(5)	38(1)	50(1)	21(1)	-2(1)	-2(1)	-7(1)
C(7)	25(1)	28(1)	23(1)	-4(1)	1(1)	-3(1)
C(3)	41(1)	31(1)	37(1)	-10(1)	-3(1)	-7(1)
C(11)	31(1)	31(1)	20(1)	-1(1)	-1(1)	-7(1)
C(4)	43(1)	47(1)	30(1)	-17(1)	-1(1)	-9(1)
C(10)	34(1)	41(1)	29(1)	-6(1)	-4(1)	-10(1)

C(8)	48(1)	26(1)	35(1)	-8(1)	3(1)	-9(1)
C(9)	42(1)	39(1)	37(1)	-14(1)	3(1)	-15(1)
C(12)	38(1)	62(1)	39(1)	-6(1)	10(1)	-16(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for epoxide 13.

	x	y	z	U(eq)
H(6A)	3265	45	10911	38
H(5A)	3269	1773	12829	44
H(3A)	2276	6137	10051	43
H(4A)	2797	4770	12423	47
H(10A)	-203	2682	5382	41
H(8A)	1579	-708	8885	43
H(8B)	2710	-1143	7431	43
H(9A)	-399	-286	6468	45
H(12A)	5844	2487	4819	69
H(12B)	5702	1617	6436	69
H(12C)	5292	3653	6117	69

Table 6. Torsion angles [°] for epoxide 13.

O(1)-C(1)-C(2)-C(3)	4.8(2)
C(11)-C(1)-C(2)-C(3)	-176.25(13)
O(1)-C(1)-C(2)-C(7)	-177.34(14)
C(11)-C(1)-C(2)-C(7)	1.59(13)
C(7)-C(6)-C(5)-C(4)	0.2(2)
C(5)-C(6)-C(7)-N(1)	176.51(12)
C(5)-C(6)-C(7)-C(2)	-1.08(19)
C(11)-N(1)-C(7)-C(6)	171.95(12)
C(8)-N(1)-C(7)-C(6)	43.97(18)
C(11)-N(1)-C(7)-C(2)	-10.30(14)
C(8)-N(1)-C(7)-C(2)	-138.28(12)
C(3)-C(2)-C(7)-C(6)	1.31(19)
C(1)-C(2)-C(7)-C(6)	-176.78(11)
C(3)-C(2)-C(7)-N(1)	-176.60(11)
C(1)-C(2)-C(7)-N(1)	5.30(14)
C(7)-C(2)-C(3)-C(4)	-0.7(2)
C(1)-C(2)-C(3)-C(4)	176.95(13)
C(12)-O(2)-C(11)-N(1)	-57.02(15)
C(12)-O(2)-C(11)-C(10)	-170.59(12)
C(12)-O(2)-C(11)-C(1)	62.40(15)

C(7)-N(1)-C(11)-O(2)	134.84(11)
C(8)-N(1)-C(11)-O(2)	-91.51(12)
C(7)-N(1)-C(11)-C(10)	-111.30(11)
C(8)-N(1)-C(11)-C(10)	22.34(13)
C(7)-N(1)-C(11)-C(1)	10.48(12)
C(8)-N(1)-C(11)-C(1)	144.13(10)
O(1)-C(1)-C(11)-O(2)	46.90(17)
C(2)-C(1)-C(11)-O(2)	-132.11(11)
O(1)-C(1)-C(11)-N(1)	171.66(12)
C(2)-C(1)-C(11)-N(1)	-7.35(13)
O(1)-C(1)-C(11)-C(10)	-74.26(16)
C(2)-C(1)-C(11)-C(10)	106.73(12)
C(2)-C(3)-C(4)-C(5)	-0.2(2)
C(6)-C(5)-C(4)-C(3)	0.4(2)
C(9)-O(3)-C(10)-C(11)	-97.41(12)
O(2)-C(11)-C(10)-O(3)	168.97(10)
N(1)-C(11)-C(10)-O(3)	48.76(14)
C(1)-C(11)-C(10)-O(3)	-65.36(14)
O(2)-C(11)-C(10)-C(9)	105.24(12)
N(1)-C(11)-C(10)-C(9)	-14.98(13)
C(1)-C(11)-C(10)-C(9)	-129.10(12)
C(7)-N(1)-C(8)-C(9)	106.41(12)
C(11)-N(1)-C(8)-C(9)	-20.57(13)
C(10)-O(3)-C(9)-C(8)	100.49(12)
C(11)-C(10)-C(9)-O(3)	106.64(11)
O(3)-C(10)-C(9)-C(8)	-103.85(12)
C(11)-C(10)-C(9)-C(8)	2.79(14)
N(1)-C(8)-C(9)-O(3)	-53.26(14)
N(1)-C(8)-C(9)-C(10)	10.44(14)

Symmetry transformations used to generate equivalent atoms: