MX114_11 (SLH033f2 Sarah Harding CSIRO)

3-(2,5-Dimethylphenyl)-5,5-dimethyl-4-methyleneoxazolidin-2-one, 3c

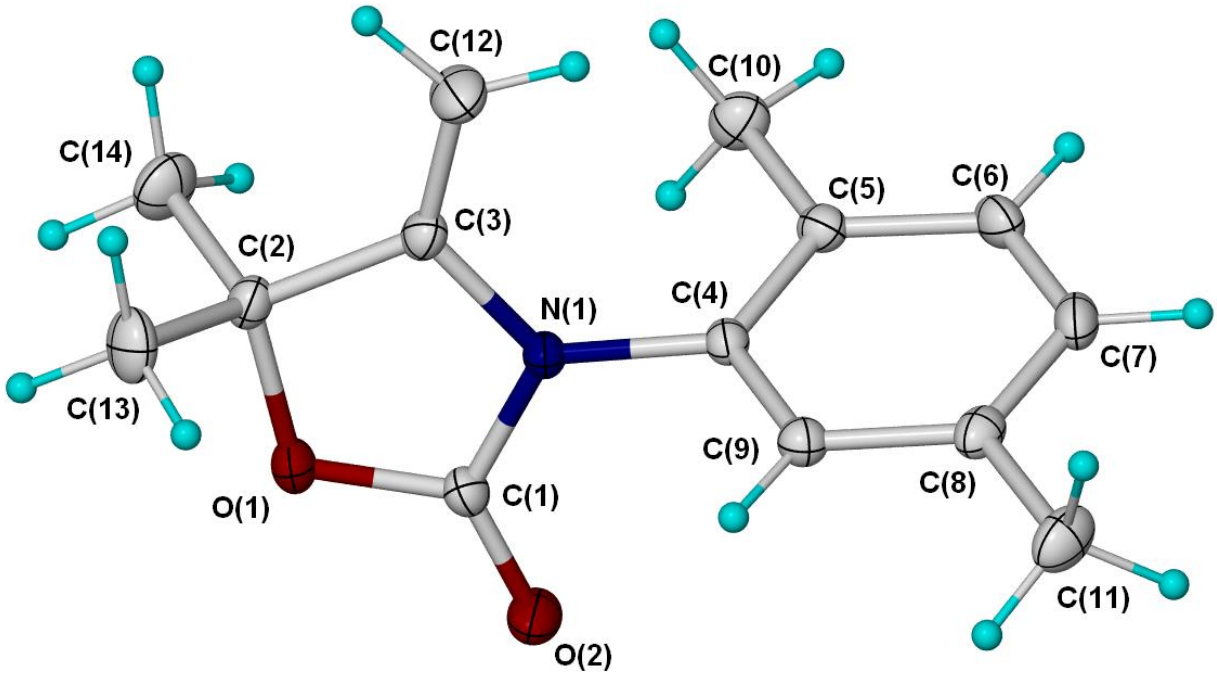

Figure 1. Molecular diagram with non-hydrogen atoms represented by 50% thermal ellipsoids and hydrogen atoms as spheres of arbitrary size.

Table 1. Crystal data and structure refinement for MX114_11.

Identification code	mx114_11
Empirical formula	C14 H17 N O2
Formula weight	231.29
Temperature	123(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 9.9538(3) A alpha = 90 deg. b = 14.0904(4) A beta = 105.647(3) deg. c = 9.3597(3) A gamma = 90 deg.
Volume	1264.08(7) A^3
Z, Calculated density	4, 1.215 Mg/m^3
Absorption coefficient	0.081 mm^-1
F(000)	496
Crystal size	0.25 x 0.15 x 0.08 mm
Theta range for data collection	2.12 to 32.19 deg.
Limiting indices	-14<=h<=14, -20<=k<=19, -13<=l<=13
Reflections collected / unique	15445 / 4197 [R(int) = 0.0249]
Completeness to theta = 27.50	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.72431
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4197 / 0 / 156
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	R1 = 0.0447, wR2 = 0.1184
R indices (all data)	R1 = 0.0574, wR2 = 0.1280
Largest diff. peak and hole	0.370 and -0.204 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for MX114_11.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	4524(1)	127(1)	2357(1)	22(1)
O(2)	6253(1)	-753(1)	3809(1)	30(1)
N(1)	6455(1)	871(1)	3581(1)	18(1)
C(1)	5802(1)	7(1)	3312(1)	19(1)
C(2)	4274(1)	1134(1)	1956(1)	20(1)
C(3)	5599(1)	1611(1)	2852(1)	19(1)
C(4)	7824(1)	1004(1)	4562(1)	17(1)
C(5)	8946(1)	1165(1)	3966(1)	19(1)
C(6)	10251(1)	1285(1)	4977(1)	24(1)
C(7)	10417(1)	1259(1)	6494(1)	24(1)
C(8)	9284(1)	1112(1)	7075(1)	21(1)
C(9)	7977(1)	979(1)	6082(1)	19(1)
C(10)	8769(1)	1189(1)	2321(1)	26(1)
C(11)	9459(1)	1101(1)	8726(1)	30(1)
C(12)	5903(1)	2525(1)	2947(1)	29(1)
C(13)	2997(1)	1444(1)	2424(1)	30(1)
C(14)	4080(1)	1216(1)	295(1)	33(1)

Table 3. Bond lengths [A] and angles [deg] for MX114_11.

O(1)-C(1)	1.3535(12)
O(1)-C(2)	1.4726(12)
O(2)-C(1)	1.2054(12)
N(1)-C(1)	1.3707(12)
N(1)-C(3)	1.4024(12)
N(1)-C(4)	1.4346(12)
C(2)-C(13)	1.5160(15)
C(2)-C(3)	1.5162(14)
C(2)-C(14)	1.5180(14)
C(3)-C(12)	1.3198(15)
C(4)-C(9)	1.3894(13)
C(4)-C(5)	1.3952(13)
C(5)-C(6)	1.3963(14)
C(5)-C(10)	1.5018(14)
C(6)-C(7)	1.3847(16)
C(7)-C(8)	1.3934(15)
C(8)-C(9)	1.3924(14)
C(8)-C(11)	1.5079(15)
C(1)-O(1)-C(2)	110.61(7)
C(1)-N(1)-C(3)	112.01(8)
C(1)-N(1)-C(4)	123.74(8)
C(3)-N(1)-C(4)	124.16(8)
O(2)-C(1)-O(1)	123.45(9)
O(2)-C(1)-N(1)	127.51(9)
O(1)-C(1)-N(1)	109.04(8)
O(1)-C(2)-C(13)	107.51(9)
O(1)-C(2)-C(3)	102.98(7)
C(13)-C(2)-C(3)	112.61(9)
O(1)-C(2)-C(14)	107.47(9)
C(13)-C(2)-C(14)	112.89(9)
C(3)-C(2)-C(14)	112.62(9)
C(12)-C(3)-N(1)	126.51(10)
C(12)-C(3)-C(2)	128.22(9)
N(1)-C(3)-C(2)	105.27(8)
C(9)-C(4)-C(5)	122.32(9)
C(9)-C(4)-N(1)	118.37(8)
C(5)-C(4)-N(1)	119.30(8)
C(4)-C(5)-C(6)	116.59(9)
C(4)-C(5)-C(10)	121.92(9)
C(6)-C(5)-C(10)	121.48(9)
C(7)-C(6)-C(5)	121.56(9)
C(6)-C(7)-C(8)	121.28(9)
C(9)-C(8)-C(7)	117.89(9)
C(9)-C(8)-C(11)	120.80(10)
C(7)-C(8)-C(11)	121.31(10)
C(4)-C(9)-C(8)	120.35(9)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for MX114_11.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	17(1)	23(1)	24(1)	1(1)	0(1)	-2(1)
O(2)	27(1)	18(1)	37(1)	4(1)	-3(1)	-3(1)
N(1)	14(1)	16(1)	21(1)	2(1)	1(1)	-1(1)
C(1)	17(1)	20(1)	19(1)	0(1)	3(1)	-3(1)
C(2)	17(1)	23(1)	18(1)	2(1)	3(1)	2(1)
C(3)	16(1)	21(1)	20(1)	3(1)	4(1)	3(1)
C(4)	15(1)	15(1)	19(1)	0(1)	2(1)	0(1)
C(5)	18(1)	18(1)	22(1)	2(1)	6(1)	1(1)
C(6)	16(1)	24(1)	32(1)	4(1)	7(1)	-1(1)
C(7)	17(1)	21(1)	29(1)	1(1)	-2(1)	-1(1)
C(8)	24(1)	16(1)	20(1)	0(1)	1(1)	1(1)
C(9)	19(1)	18(1)	20(1)	1(1)	5(1)	0(1)
C(10)	26(1)	31(1)	24(1)	3(1)	10(1)	3(1)
C(11)	36(1)	29(1)	20(1)	-1(1)	0(1)	4(1)
C(12)	23(1)	20(1)	40(1)	5(1)	4(1)	4(1)
C(13)	17(1)	40(1)	33(1)	-3(1)	6(1)	5(1)
C(14)	35(1)	42(1)	18(1)	4(1)	3(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for MX114_11.

	x	y	z	U(eq)
H(6)	11044	1387	4616	28
H(7)	11320	1344	7150	29
H(9)	7186	872	6445	23
H(10A)	8278	616	1866	39
H(10B)	9688	1217	2127	39
H(10C)	8226	1750	1897	39
H(11A)	9519	1754	9098	45
H(11B)	10316	758	9219	45
H(11C)	8657	783	8935	45
H(12A)	6777	2735	3557	34
H(12B)	5247	2972	2405	34
H(13A)	2171	1119	1812	45
H(13B)	2876	2132	2293	45
H(13C)	3120	1282	3470	45
H(14A)	3210	900	-233	49
H(14B)	4867	913	33	49
H(14C)	4035	1887	13	49

MX113_11 (SLH014f3 Sarah Harding CSIRO)

6-(3,4-Dichlorophenyl)-9,9-dimethyl-3-phenyl-1,8-dioxa-2,6-diazaspiro[4.4]non-2-en-7-one, 4b

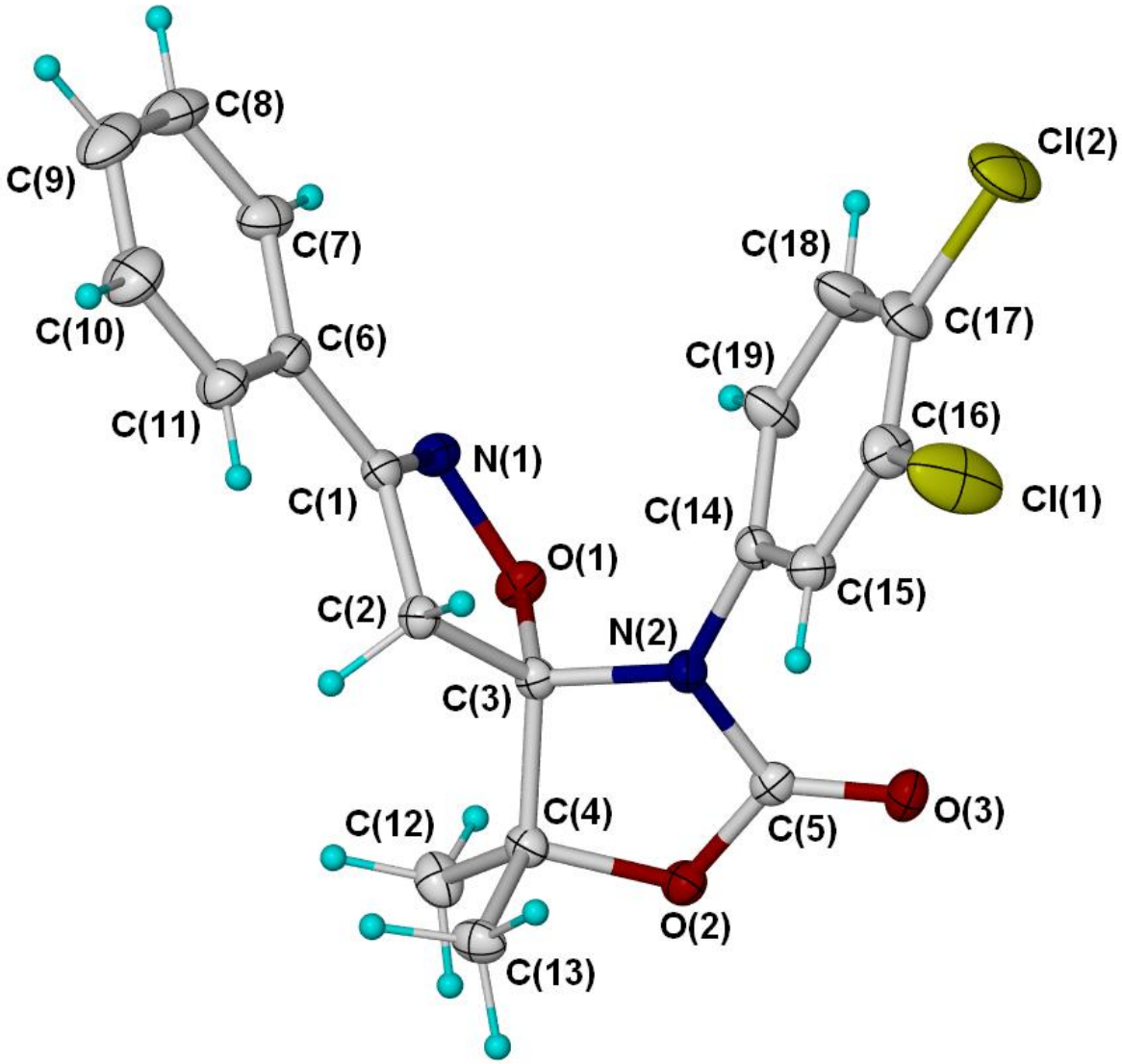

Figure 1. Molecular diagram with non-hydrogen atoms represented by 50% thermal ellipsoids and hydrogen atoms as spheres of arbitrary size.

Table 1. Crystal data and structure refinement for MX113_11.

Identification code	mx113_11
Empirical formula	C19 H16 Cl2 N2 O3
Formula weight	391.24
Temperature	123(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C 2/c
Unit cell dimensions	a = 29.5615(10) A alpha = 90 deg. b = 12.2972(3) A beta = 110.902(4) deg. c = 10.5852(4) A gamma = 90 deg.
Volume	3594.7(2) A^3
Z, Calculated density	8, 1.446 Mg/m^3
Absorption coefficient	0.383 mm^-1
F(000)	1616
Crystal size	0.25 x 0.25 x 0.25 mm
Theta range for data collection	2.54 to 32.45 deg.
Limiting indices	-42<=h<=42, -18<=k<=18, -15<=l<=14
Reflections collected / unique	22558 / 5930 [R(int) = 0.0229]
Completeness to theta = 27.50	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.88908
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5930 / 0 / 237
Goodness-of-fit on F^2	1.027
Final R indices [I>2sigma(I)]	R1 = 0.0385, wR2 = 0.0915
R indices (all data)	R1 = 0.0515, wR2 = 0.1002
Largest diff. peak and hole	0.470 and -0.663 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for MX113_11.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cl(1)	549(1)	-2460(1)	-977(1)	58(1)
Cl(2)	-149(1)	-1590(1)	463(1)	48(1)
O(1)	2048(1)	1378(1)	3582(1)	21(1)
O(2)	2694(1)	-623(1)	3640(1)	20(1)
O(3)	2163(1)	-1968(1)	3518(1)	23(1)
N(1)	1699(1)	2205(1)	2982(1)	22(1)
N(2)	1920(1)	-320(1)	2442(1)	18(1)
C(1)	1617(1)	2234(1)	1707(1)	19(1)
C(2)	1914(1)	1440(1)	1258(1)	18(1)
C(3)	2135(1)	750(1)	2524(1)	17(1)
C(4)	2678(1)	429(1)	2954(1)	18(1)
C(5)	2249(1)	-1058(1)	3225(1)	18(1)
C(6)	1271(1)	3004(1)	802(1)	21(1)
C(7)	987(1)	3685(1)	1277(1)	27(1)
C(8)	669(1)	4413(1)	402(2)	34(1)
C(9)	629(1)	4471(1)	-945(2)	37(1)
C(10)	907(1)	3795(1)	-1422(2)	35(1)
C(11)	1230(1)	3064(1)	-552(1)	27(1)
C(12)	3028(1)	1191(1)	3948(1)	25(1)
C(13)	2818(1)	202(1)	1731(1)	23(1)
C(14)	1416(1)	-566(1)	1928(1)	19(1)
C(15)	1242(1)	-1275(1)	841(1)	23(1)
C(16)	758(1)	-1582(1)	381(1)	27(1)
C(17)	449(1)	-1182(1)	995(2)	30(1)
C(18)	624(1)	-451(1)	2056(2)	36(1)
C(19)	1107(1)	-143(1)	2530(1)	29(1)

Table 3. Bond lengths [A] and angles [deg] for MX113_11.

Cl(1)-C(16)	1.7255(13)
Cl(2)-C(17)	1.7272(13)
O(1)-N(1)	1.4278(12)
O(1)-C(3)	1.4568(13)
O(2)-C(5)	1.3426(14)
O(2)-C(4)	1.4754(13)
O(3)-C(5)	1.2107(13)
N(1)-C(1)	1.2846(15)
N(2)-C(5)	1.3711(14)
N(2)-C(14)	1.4248(14)
N(2)-C(3)	1.4503(13)
C(1)-C(6)	1.4693(15)
C(1)-C(2)	1.5004(15)
C(2)-C(3)	1.5222(15)
C(3)-C(4)	1.5531(15)
C(4)-C(12)	1.5102(16)
C(4)-C(13)	1.5202(15)
C(6)-C(11)	1.3960(17)
C(6)-C(7)	1.4002(17)
C(7)-C(8)	1.3868(18)
C(8)-C(9)	1.390(2)
C(9)-C(10)	1.384(2)
C(10)-C(11)	1.3923(18)
C(14)-C(15)	1.3879(16)
C(14)-C(19)	1.3888(16)
C(15)-C(16)	1.3902(17)
C(16)-C(17)	1.3858(19)
C(17)-C(18)	1.387(2)
C(18)-C(19)	1.3860(18)

N(1)-O(1)-C(3)	109.50(8)
C(5)-O(2)-C(4)	109.40(8)
C(1)-N(1)-O(1)	108.78(9)
C(5)-N(2)-C(14)	120.60(9)
C(5)-N(2)-C(3)	111.34(9)
C(14)-N(2)-C(3)	126.29(9)
N(1)-C(1)-C(6)	121.97(10)
N(1)-C(1)-C(2)	113.78(10)
C(6)-C(1)-C(2)	124.23(10)
C(1)-C(2)-C(3)	101.52(8)
N(2)-C(3)-O(1)	109.42(8)
N(2)-C(3)-C(2)	114.31(9)
O(1)-C(3)-C(2)	104.12(8)
N(2)-C(3)-C(4)	99.89(8)
O(1)-C(3)-C(4)	110.83(8)
C(2)-C(3)-C(4)	118.27(9)
O(2)-C(4)-C(12)	107.87(9)
O(2)-C(4)-C(13)	106.63(9)
C(12)-C(4)-C(13)	112.30(9)
O(2)-C(4)-C(3)	102.53(8)
C(12)-C(4)-C(3)	115.26(9)
C(13)-C(4)-C(3)	111.36(9)
O(3)-C(5)-O(2)	123.68(10)
O(3)-C(5)-N(2)	126.81(11)

O(2)-C(5)-N(2)	109.52(9)
C(11)-C(6)-C(7)	119.50(11)
C(11)-C(6)-C(1)	119.30(10)
C(7)-C(6)-C(1)	121.19(11)
C(8)-C(7)-C(6)	119.81(13)
C(7)-C(8)-C(9)	120.46(13)
C(10)-C(9)-C(8)	119.98(13)
C(9)-C(10)-C(11)	120.12(14)
C(10)-C(11)-C(6)	120.12(12)
C(15)-C(14)-C(19)	120.41(11)
C(15)-C(14)-N(2)	118.55(10)
C(19)-C(14)-N(2)	120.98(10)
C(14)-C(15)-C(16)	119.47(11)
C(17)-C(16)-C(15)	120.46(11)
C(17)-C(16)-Cl(1)	120.92(10)
C(15)-C(16)-Cl(1)	118.61(10)
C(16)-C(17)-C(18)	119.53(11)
C(16)-C(17)-Cl(2)	120.80(10)
C(18)-C(17)-Cl(2)	119.67(10)
C(19)-C(18)-C(17)	120.57(12)
C(18)-C(19)-C(14)	119.51(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for MX113_11.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cl(1)	37(1)	72(1)	62(1)	-43(1)	12(1)	-19(1)
Cl(2)	23(1)	52(1)	70(1)	-13(1)	16(1)	-14(1)
O(1)	26(1)	22(1)	16(1)	-1(1)	8(1)	4(1)
O(2)	20(1)	21(1)	18(1)	3(1)	5(1)	2(1)
O(3)	30(1)	19(1)	23(1)	3(1)	10(1)	2(1)
N(1)	21(1)	21(1)	24(1)	0(1)	8(1)	3(1)
N(2)	17(1)	17(1)	20(1)	2(1)	6(1)	-1(1)
C(1)	17(1)	18(1)	22(1)	-1(1)	7(1)	-1(1)
C(2)	19(1)	19(1)	16(1)	1(1)	6(1)	1(1)
C(3)	18(1)	17(1)	15(1)	0(1)	7(1)	-1(1)
C(4)	17(1)	22(1)	16(1)	2(1)	5(1)	0(1)
C(5)	22(1)	20(1)	14(1)	0(1)	8(1)	2(1)
C(6)	16(1)	19(1)	26(1)	0(1)	5(1)	-1(1)
C(7)	20(1)	26(1)	32(1)	-5(1)	6(1)	2(1)
C(8)	22(1)	30(1)	43(1)	-6(1)	3(1)	7(1)
C(9)	28(1)	31(1)	40(1)	3(1)	-4(1)	9(1)
C(10)	34(1)	36(1)	30(1)	8(1)	3(1)	8(1)
C(11)	25(1)	27(1)	26(1)	4(1)	7(1)	4(1)
C(12)	23(1)	30(1)	19(1)	1(1)	3(1)	-6(1)
C(13)	21(1)	33(1)	18(1)	2(1)	9(1)	3(1)
C(14)	18(1)	19(1)	20(1)	2(1)	7(1)	-1(1)
C(15)	21(1)	22(1)	24(1)	-2(1)	7(1)	0(1)
C(16)	24(1)	25(1)	29(1)	-5(1)	5(1)	-4(1)
C(17)	20(1)	30(1)	40(1)	-2(1)	10(1)	-7(1)
C(18)	26(1)	40(1)	48(1)	-12(1)	22(1)	-8(1)
C(19)	26(1)	33(1)	32(1)	-9(1)	16(1)	-7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for MX113_11.

	x	y	z	U(eq)
H(2A)	2167	1813	1007	21
H(2B)	1709	997	484	21
H(7)	1013	3649	2196	32
H(8)	477	4876	725	41
H(9)	412	4973	-1538	45
H(10)	878	3830	-2345	42
H(11)	1422	2605	-881	32
H(12A)	3354	878	4248	38
H(12B)	2929	1295	4731	38
H(12C)	3028	1894	3512	38
H(13A)	2573	-266	1095	35
H(13B)	3133	-164	2024	35
H(13C)	2839	889	1286	35
H(15)	1452	-1548	415	27
H(18)	411	-158	2461	43
H(19)	1225	354	3262	34