ORGANOMETALLICS
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Table 1. Crystal data and structure refinement for 2.

Identification code	bomm4
Empirical formula	$C_9H_{14}Cl_2GaN$
Formula weight	276.83
Crystal colour, -habit	colourless, irregular
Crystal size	1.00 x 0.60 x 0.50 mm
Temperature	173(2) K
Wavelength	0.71073 Å (graphite monochromator)
Space group	$P2_12_12_1$
Unit cell dimensions	a = 8.733(6) Å α = 90° b = 9.738(7) Å β = 90° c = 13.381(8) Å γ = 90°
Volume	1137.9(13) $Å^3$
Z	4
Density (calculated)	1.616 Mg/m^3
Absorption coefficient	2.843 mm^{-1}
F(000)	560
θ range for data collection	2.59 to 29.99°
Index ranges	$0 \le h \le 12$, $0 \le k \le 13$, $0 \le \ell \le 18$
Reflections collected	1902
Independent reflections	1902 (R_{int} = 0.0000)
Absorption correction	None
Data / restraints / parameters	1900 / 0 / 120
Goodness-of-fit on F^2	1.146
Final R indices [$I>2\sigma(I)$]	R1 = 0.0597 for 1714 reflections, wR2 = 0.1465
R indices (all data)	R1 = 0.0663, wR2 = 0.1532
Largest and mean Δ/σ	0.000 and 0.000
Absolute structure parameter	0.00(3)
Largest diff. peak and hole	1.2 and -1.4 $eÅ^{-3}$

Table 2. Measurement and program parameters for 2.

Diffractometer used	Siemens P2(1) diffractometer
Scan type	Wyckhoff-scan
Scan range	1.2^{o} in ω arround $K\alpha_{1,2}$- maximum
Scan speed	3.9 - 29.3 ^{o}/min in ω
Standard reflections	3 of 100 measured reflections
Programs used	Siemens SHELXTL plus / SHELXL-93
Structure solution	direct
Structure refinement	Full-matrix least-squares on F^2
Structure factor source	International Tables Vol.C

Definition of R- values: $R1 = \sum||F_o|-|F_c||/\sum|F_o|$

$$wR2 = [\ \sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]\ \ ]^{1/2}$$

Definition of the weighting scheme

calc $w=1/[\sigma^2(Fo^2)+(0.0929P)^2+1.4398P]$ where $P=(Fo^2+2Fc^2)/3$

Table 3. Atomic coordinates (x 10^4) and isotropic displacement parameters U(iso) or U(eq)[a] [$Å^2$ x 10^3] for 2.

	x	y	z	U(eq)
Ga(1)	-1496(1)	-5494(1)	-6007(1)	22(1)
Cl(1)	-1999(2)	-5814(2)	-4439(1)	39(1)
Cl(2)	969(2)	-5632(2)	-6235(2)	40(1)
N(1)	-2263(7)	-7220(6)	-6685(4)	30(1)
C(1)	-2695(8)	-4023(7)	-6688(5)	28(1)
C(2)	-2693(10)	-2791(8)	-6052(6)	37(2)
C(3)	-4025(11)	-2742(9)	-5553(6)	41(2)
C(4)	-4967(9)	-3877(9)	-5831(5)	38(2)
C(5)	-4228(7)	-4648(8)	-6537(4)	30(1)
C(6)	-4745(9)	-5933(9)	-7029(6)	42(2)
C(7)	-3970(10)	-7224(9)	-6605(7)	41(2)
C(8)	-1664(11)	-8487(8)	-6200(6)	45(2)
C(9)	-1793(9)	-7220(8)	-7738(5)	36(2)

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

Table 4. Selected bond lengths [Å] and angles [°] for 2.

Ga(1)-C(1)	1.995(7)	Ga(1)-N(1)	2.025(6)
Ga(1)-Cl(1)	2.166(2)	Ga(1)-Cl(2)	2.178(2)
N(1)-C(9)	1.467(8)	N(1)-C(8)	1.489(10)
N(1)-C(7)	1.494(11)	C(1)-C(2)	1.471(10)
C(1)-C(5)	1.485(10)	C(2)-C(3)	1.342(12)
C(3)-C(4)	1.427(13)	C(4)-C(5)	1.369(10)
C(5)-C(6)	1.484(11)	C(6)-C(7)	1.537(13)

C(1)-Ga(1)-N(1)	102.6(3)	C(1)-Ga(1)-Cl(1)	116.1(2)
N(1)-Ga(1)-Cl(1)	104.4(2)	C(1)-Ga(1)-Cl(2)	119.9(2)
N(1)-Ga(1)-Cl(2)	102.3(2)	Cl(1)-Ga(1)-Cl(2)	109.09(8)
C(9)-N(1)-C(8)	108.7(6)	C(9)-N(1)-C(7)	110.4(7)
C(8)-N(1)-C(7)	108.5(7)	C(9)-N(1)-Ga(1)	109.7(5)
C(8)-N(1)-Ga(1)	112.1(5)	C(7)-N(1)-Ga(1)	107.4(5)
C(2)-C(1)-C(5)	104.9(6)	C(2)-C(1)-Ga(1)	108.7(5)
C(5)-C(1)-Ga(1)	96.7(4)	C(3)-C(2)-C(1)	108.4(8)
C(2)-C(3)-C(4)	110.0(7)	C(5)-C(4)-C(3)	109.5(7)
C(4)-C(5)-C(6)	128.7(7)	C(4)-C(5)-C(1)	107.1(7)
C(6)-C(5)-C(1)	124.0(6)	C(5)-C(6)-C(7)	113.1(6)
N(1)-C(7)-C(6)	114.3(7)		

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement [a)] parameters [$Å^2 \times 10^3$] for 2.

	U11	U22	U33	U23	U13	U12
Ga(1)	20(1)	25(1)	22(1)	0(1)	0(1)	1(1)
Cl(1)	44(1)	52(1)	20(1)	1(1)	0(1)	10(1)
Cl(2)	21(1)	44(1)	54(1)	9(1)	2(1)	1(1)
N(1)	32(3)	30(3)	27(3)	-1(2)	8(2)	-3(2)
C(1)	26(3)	32(3)	26(3)	-2(3)	-2(2)	8(3)
C(2)	41(4)	30(3)	40(4)	-4(3)	-9(3)	11(3)
C(3)	50(4)	42(4)	31(3)	-9(3)	-3(3)	23(4)
C(4)	26(3)	58(5)	30(3)	0(3)	1(3)	13(3)
C(5)	25(3)	45(4)	19(2)	-7(3)	-2(2)	5(3)
C(6)	25(3)	62(5)	37(4)	-17(4)	-2(3)	-4(3)
C(7)	35(4)	48(4)	40(4)	-13(3)	4(3)	-19(4)
C(8)	59(5)	30(3)	46(4)	4(3)	7(4)	-2(4)
C(9)	43(4)	40(4)	24(3)	-10(3)	11(3)	-4(3)

a) The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

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

	x	y	z	U(eq)
H(1)	-2408(8)	-3858(7)	-7401(5)	34
H(2)	-1886(10)	-2140(8)	-6003(6)	45
H(3)	-4300(11)	-2052(9)	-5084(6)	49
H(4)	-5953(9)	-4068(9)	-5566(5)	45
H(6A)	-4526(9)	-5872(9)	-7754(6)	50
H(6B)	-5868(9)	-6021(9)	-6947(6)	50
H(7A)	-4255(10)	-7318(9)	-5892(7)	49
H(7B)	-4371(10)	-8038(9)	-6963(7)	49
H(8A)	-2155(62)	-9294(9)	-6497(38)	68
H(8B)	-1887(73)	-8459(35)	-5483(11)	68
H(8C)	-554(17)	-8543(38)	-6301(46)	68
H(9A)	-2074(67)	-6342(28)	-8046(13)	54
H(9B)	-2309(58)	-7971(43)	-8091(12)	54
H(9C)	-681(14)	-7347(65)	-7781(5)	54

Table 1. Crystal data and structure refinement for 3.

Identification code	bomm8
Empirical formula	$C_9H_{14}Br_2GaN$
Formula weight	365.75
Crystal colour	colourless
Crystal size	0.60 x 0.60 x 0.50 mm
Temperature	173(2) K
Wavelength	0.71073 Å (graphite monochromator)
Space group	$P2_1/n$
Unit cell dimensions	a = 7.330(2) Å α = 90° b = 14.743(5) Å β = 91.10(3)° c = 11.047(3) Å γ = 90°
Volume	1193.6(6) $Å^3$
Z	4
Density (calculated)	2.035 Mg/m^3
Absorption coefficient	8.958 mm^{-1}
F(000)	704
θ range for data collection	2.30 to 27.57°
Index ranges	$0 \le h \le 9$, $0 \le k \le 19$, $-14 \le \ell \le 14$
Reflections collected	2928
Independent reflections	2730 (R_{int} = 0.1293)
Absorption correction	Semi-empirical from ψ-scans
Data / restraints / parameters	2715 / 0 / 120
Goodness-of-fit on F^2	1.293
Final R indices [$I>2\sigma(I)$]	R1 = 0.0781 for 1965 reflections, wR2 = 0.2151
R indices (all data)	R1 = 0.1052, wR2 = 0.2738
Largest and mean Δ/σ	0.000 and 0.000
Largest diff. peak and hole	1.5 and -1.0 $eÅ^{-3}$

Table 2. Measurement and program parameters for 3.

Diffractometer used	Siemens P2(1) diffractometer
Scan type	Omega-scan
Scan range	1.2^{o} in ω arround $K\alpha_{1,2}$- m
Scan speed	3.9 - 29.3 ^{o}/min in ω
Standard reflections	3 of 100 measured reflections
Programs used	Siemens SHELXTL plus / SHELXL-93
Structure solution	direct
Structure refinement	Full-matrix least-squares on F^2
Structure factor source	International Tables Vol.C

Definition of R- values: $R1 = \sum||F_o|-|F_c||/\sum|F_o|$

$$wR2 = (\sum w(F_o^2-F_c^2)^2/\sum wF_o^2)^{1/2}$$

Definition of the weighting scheme (CIF format):

calc w=1/[\s^2^(Fo^2^)+(0.1312P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3

Table 3. Atomic coordinates (x 10^4) and isotropic displacement parameters U(iso) or U(eq)[a] [$Å^2$ x 10^3] for 3.

	x	y	z	U(eq)
Ga(1)	782(1)	3282(1)	2068(1)	46(1)
Br(1)	-137(2)	4356(1)	3457(1)	65(1)
Br(2)	-601(2)	3569(1)	200(1)	60(1)
N(1)	3475(11)	3536(6)	1816(7)	49(2)
C(1)	792(13)	1998(7)	2660(9)	51(2)
C(2)	-989(14)	1605(8)	2396(10)	55(2)
C(3)	-940(15)	1081(8)	1416(11)	61(3)
C(4)	910(14)	1101(8)	975(10)	57(2)
C(5)	1970(13)	1589(8)	1734(9)	51(2)
C(6)	3952(13)	1829(7)	1597(10)	51(2)
C(7)	4236(13)	2777(8)	1083(9)	53(2)
C(8)	4420(14)	3586(8)	3008(10)	55(2)
C(9)	3752(16)	4414(8)	1162(12)	61(3)

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

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

Ga(1)-C(1)	2.003(11)	Ga(1)-N(1)	2.034(8)
Ga(1)-Br(1)	2.314(2)	Ga(1)-Br(2)	2.321(2)
N(1)-C(8)	1.478(13)	N(1)-C(9)	1.497(14)
N(1)-C(7)	1.495(14)	C(1)-C(2)	1.453(13)
C(1)-C(5)	1.48(2)	C(2)-C(3)	1.33(2)
C(3)-C(4)	1.45(2)	C(4)-C(5)	1.34(2)
C(5)-C(6)	1.506(13)	C(6)-C(7)	1.52(2)

C(1)-Ga(1)-N(1)	102.8(4)	C(1)-Ga(1)-Br(1)	115.5(3)
N(1)-Ga(1)-Br(1)	105.1(2)	C(1)-Ga(1)-Br(2)	117.5(3)
N(1)-Ga(1)-Br(2)	104.7(2)	Br(1)-Ga(1)-Br(2)	109.72(7)
C(8)-N(1)-C(9)	108.8(9)	C(8)-N(1)-C(7)	110.2(8)
C(9)-N(1)-C(7)	109.3(8)	C(8)-N(1)-Ga(1)	109.0(6)
C(9)-N(1)-Ga(1)	111.5(7)	C(7)-N(1)-Ga(1)	108.0(6)
C(2)-C(1)-C(5)	103.4(9)	C(2)-C(1)-Ga(1)	108.3(7)
C(5)-C(1)-Ga(1)	99.1(7)	C(3)-C(2)-C(1)	110.9(10)
C(2)-C(3)-C(4)	107.6(9)	C(5)-C(4)-C(3)	109.5(10)
C(4)-C(5)-C(1)	108.2(9)	C(4)-C(5)-C(6)	127.7(10)
C(1)-C(5)-C(6)	123.4(9)	C(5)-C(6)-C(7)	113.0(8)
N(1)-C(7)-C(6)	115.5(8)		

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement [a)] parameters [$Å^2 \times 10^3$] for 3.

	U11	U22	U33	U23	U13	U12
Ga(1)	43(1)	52(1)	43(1)	-2(1)	-2(1)	-1(1)
Br(1)	67(1)	65(1)	65(1)	-15(1)	9(1)	2(1)
Br(2)	61(1)	67(1)	53(1)	4(1)	-16(1)	0(1)
N(1)	50(4)	58(5)	39(4)	0(3)	0(3)	4(4)
C(1)	48(5)	52(5)	52(5)	-3(4)	-7(4)	2(4)
C(2)	51(5)	57(6)	58(6)	12(5)	-1(4)	-6(4)
C(3)	53(5)	59(6)	69(7)	13(6)	-12(5)	-14(5)
C(4)	56(5)	59(6)	56(6)	4(5)	-10(4)	-2(5)
C(5)	45(5)	64(6)	44(5)	6(4)	-2(4)	7(4)
C(6)	44(5)	57(6)	53(5)	3(5)	-3(4)	3(4)
C(7)	42(5)	74(7)	43(5)	-2(5)	12(4)	-3(4)
C(8)	56(6)	61(6)	48(5)	-2(5)	-14(4)	-1(5)
C(9)	68(6)	56(6)	61(6)	7(5)	4(5)	5(5)

a) The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + \ldots + 2hka^*b^* U_{12}]$

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

	x	y	z	U(eq)
H(1)	1239(13)	1918(7)	3514(9)	61
H(2)	-2047	1708	2860	66
H(3)	-1936	754	1069	73
H(4)	1310	813	258	69
H(6A)	4525(13)	1380(7)	1056(10)	62
H(6B)	4574(13)	1787(7)	2399(10)	62
H(7A)	5562(13)	2879(8)	997(9)	64
H(7B)	3672(13)	2801(8)	262(9)	64
H(8A)	4002(96)	4123(35)	3445(36)	83
H(8B)	5739(17)	3626(65)	2893(10)	83
H(8C)	4144(104)	3040(30)	3478(34)	83
H(9A)	2991(99)	4885(17)	1522(56)	92
H(9B)	3410(123)	4339(19)	306(20)	92
H(9C)	5038(31)	4592(34)	1231(74)	92

Table 1. Crystal data and structure refinement for 4.

Identification code	bomm9
Empirical formula	$C_9H_{14}GaI_2N$
Formula weight	459.73
Crystal colour	colourless
Crystal size	0.30 x 0.15 x 0.10 mm
Temperature	173(2) K
Wavelength	0.71073 Å (graphite monochromator)
Space group	$P2_12_12_1$
Unit cell dimensions	a = 7.3560(10) Å α = 90° b = 11.711(2) Å β = 90° c = 14.610(2) Å γ = 90°
Volume	1258.6(3) $Å^3$
Z	4
Density (calculated)	2.426 Mg/m^3
Absorption coefficient	7.053 mm^{-1}
F(000)	848
θ range for data collection	2 to 27.5°
Index ranges	$0 \le h \le 9$, $0 \le k \le 15$, $0 \le \ell \le 19$ $-9 \le h \le 0$, $-15 \le k \le 0$, $-19 \le \ell \le 0$
Reflections collected	3347
Independent reflections	2895 (R_{int} = 0.0236)
Absorption correction	Semi-empirical from ψ-scans
Data / restraints / parameters	2894 / 0 / 120
Goodness-of-fit on F^2	1.056
Final R indices [$I>2\sigma(I)$]	R1 = 0.0336 for 2560 reflections, wR2 = 0.0704
R indices (all data)	R1 = 0.0432, wR2 = 0.0748
Largest and mean Δ/σ	0.000 and 0.000
Absolute structure parameter	-0.03(4)
Largest diff. peak and hole	0.5 and -0.6 $eÅ^{-3}$

Table 2. Measurement and program parameters for 4.

Diffractometer used	Siemens P2(1) diffractometer
Scan type	Omega-scan
Scan range	1.2° in ω arround $K\alpha_{1,2}$- maximum
Scan speed	3.9 - 29.3 $^{\circ}$/min in ω
Standard reflections	3 of 100 measured reflections
Programs used	Siemens SHELXTL plus / SHELXL-93
Structure solution	direct
Structure refinement	Full-matrix least-squares on F^2
Structure factor source	International Tables Vol.C

Definition of R- values: $R1 = \sum||F_o|-|F_c||/\sum|F_o|$

$$wR2 = [\ \sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]\ ]^{1/2}$$

Definition of the weighting scheme (CIF format):

calc w=1/[\s^2^(Fo^2^)+(0.0333P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3

Table 3. Atomic coordinates (x 10^4) and isotropic displacement parameters U(iso) or U(eq)[a] [$Å^2$ x 10^3] for 4.

	x	y	z	U(eq)
I(1)	7737(1)	2380(1)	3239(1)	36(1)
I(2)	7830(1)	-1168(1)	3061(1)	36(1)
Ga(1)	6592(1)	522(1)	3938(1)	26(1)
N(1)	3819(7)	517(5)	3728(4)	26(1)
C(1)	6683(10)	394(6)	5312(5)	31(2)
C(2)	8442(11)	1(7)	5555(4)	34(2)
C(3)	8412(11)	-1135(7)	5742(5)	38(2)
C(4)	6532(11)	-1485(6)	5649(5)	35(2)
C(5)	5477(9)	-593(7)	5425(4)	31(1)
C(6)	3487(10)	-580(7)	5227(5)	37(2)
C(7)	3067(9)	-509(6)	4191(4)	31(2)
C(8)	3035(11)	1590(6)	4095(5)	38(2)
C(9)	3370(10)	460(7)	2729(4)	36(2)

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

Table 4. Selected bond lengths [Å] and angles [°] for 4.

I(1)-Ga(1)	2.5465(9)	I(2)-Ga(1)	2.5277(9)
Ga(1)-C(1)	2.013(7)	Ga(1)-N(1)	2.062(5)
Ga(1)-C(5)	2.664(7)	Ga(1)-C(2)	2.794(7)
Ga(1)-C(4)	3.431(7)	Ga(1)-C(3)	3.536(7)
N(1)-C(8)	1.483(9)	N(1)-C(7)	1.485(8)
N(1)-C(9)	1.499(8)	C(1)-C(2)	1.419(10)
C(1)-C(5)	1.467(10)	C(2)-C(3)	1.358(11)
C(3)-C(4)	1.449(12)	C(4)-C(5)	1.341(10)
C(5)-C(6)	1.492(10)	C(6)-C(7)	1.547(9)
C(1)-Ga(1)-N(1)	100.4(3)	C(1)-Ga(1)-I(2)	115.8(2)
N(1)-Ga(1)-I(2)	106.2(2)	C(1)-Ga(1)-I(1)	116.9(2)
N(1)-Ga(1)-I(1)	105.7(2)	I(2)-Ga(1)-I(1)	110.26(3)
C(1)-Ga(1)-C(5)	33.0(2)	N(1)-Ga(1)-C(5)	79.4(2)
I(2)-Ga(1)-C(5)	98.1(2)	I(1)-Ga(1)-C(5)	148.0(2)
C(1)-Ga(1)-C(2)	28.9(3)	N(1)-Ga(1)-C(2)	127.4(2)
I(2)-Ga(1)-C(2)	94.7(2)	I(1)-Ga(1)-C(2)	111.4(2)
C(5)-Ga(1)-C(2)	49.7(2)	C(1)-Ga(1)-C(4)	39.1(2)
N(1)-Ga(1)-C(4)	95.4(2)	I(2)-Ga(1)-C(4)	80.66(13)
I(1)-Ga(1)-C(4)	151.82(14)	C(5)-Ga(1)-C(4)	21.0(2)
C(2)-Ga(1)-C(4)	40.6(2)	C(1)-Ga(1)-C(3)	37.2(2)
N(1)-Ga(1)-C(3)	118.9(2)	I(2)-Ga(1)-C(3)	79.13(13)
I(1)-Ga(1)-C(3)	129.97(14)	C(5)-Ga(1)-C(3)	40.5(2)
C(2)-Ga(1)-C(3)	20.8(2)	C(4)-Ga(1)-C(3)	23.9(2)
C(8)-N(1)-C(7)	112.1(5)	C(8)-N(1)-C(9)	107.7(6)
C(7)-N(1)-C(9)	109.0(5)	C(8)-N(1)-Ga(1)	109.2(4)
C(7)-N(1)-Ga(1)	107.7(4)	C(9)-N(1)-Ga(1)	111.3(4)
C(2)-C(1)-C(5)	105.5(6)	C(2)-C(1)-Ga(1)	107.7(5)
C(5)-C(1)-Ga(1)	98.7(4)	C(3)-C(2)-C(1)	110.7(7)
C(3)-C(2)-Ga(1)	112.1(5)	C(1)-C(2)-Ga(1)	43.3(3)
C(2)-C(3)-C(4)	105.8(7)	C(2)-C(3)-Ga(1)	47.1(4)
C(4)-C(3)-Ga(1)	74.0(4)	C(5)-C(4)-C(3)	110.8(7)
C(5)-C(4)-Ga(1)	45.3(4)	C(3)-C(4)-Ga(1)	82.1(5)
C(4)-C(5)-C(1)	106.9(6)	C(4)-C(5)-C(6)	128.5(8)
C(1)-C(5)-C(6)	124.3(7)	C(4)-C(5)-Ga(1)	113.7(5)
C(1)-C(5)-Ga(1)	48.3(3)	C(6)-C(5)-Ga(1)	98.0(4)
C(5)-C(6)-C(7)	112.7(5)	N(1)-C(7)-C(6)	114.5(6)

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement [a] parameters [$Å^2 \times 10^3$] for 4.

	U11	U22	U33	U23	U13	U12
I(1)	41(1)	33(1)	33(1)	5(1)	-1(1)	-7(1)
I(2)	37(1)	36(1)	36(1)	-9(1)	-1(1)	8(1)
Ga(1)	25(1)	27(1)	24(1)	-1(1)	-1(1)	0(1)
N(1)	30(3)	24(3)	24(3)	-1(2)	0(2)	3(3)
C(1)	36(4)	27(4)	30(3)	-6(3)	1(3)	-3(3)
C(2)	43(4)	41(4)	17(3)	4(3)	-6(3)	-6(4)
C(3)	36(4)	46(4)	31(4)	4(3)	-5(3)	12(4)
C(4)	43(4)	30(4)	33(4)	3(3)	1(3)	0(3)
C(5)	35(4)	35(4)	22(3)	5(3)	1(3)	3(4)
C(6)	29(3)	43(4)	38(4)	4(4)	6(3)	-3(4)
C(7)	26(4)	28(3)	41(4)	-2(3)	0(3)	-6(3)
C(8)	39(5)	36(4)	39(4)	0(3)	3(3)	7(4)
C(9)	39(4)	42(4)	28(3)	0(3)	-11(3)	-3(4)

[a] The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + \ldots + 2hka^*b^* U_{12}]$

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

	x	y	z	U(eq)
H(1)	6281(10)	1096(6)	5645(5)	38
H(2)	9496(11)	468(7)	5584(4)	40
H(3)	9418(11)	-1604(7)	5900(5)	46
H(4)	6104(11)	-2242(6)	5736(5)	42
H(6A)	2928(10)	83(7)	5539(5)	44
H(6B)	2928(10)	-1281(7)	5479(5)	44
H(7A)	3561(9)	-1198(6)	3888(4)	38
H(7B)	1732(9)	-516(6)	4106(4)	38
H(8A)	3298(63)	1647(23)	4751(10)	57
H(8B)	1716(14)	1589(20)	4001(32)	57
H(8C)	3572(54)	2244(6)	3776(26)	57
H(9A)	3913(64)	1115(28)	2413(8)	54
H(9B)	2047(10)	477(47)	2649(5)	54
H(9C)	3855(66)	-249(25)	2470(9)	54

Table 1. Crystal data and structure refinement for 5.

Identification code	bomm5
Empirical formula	$C_{11}H_{20}GaN$
Formula weight	236.00
Crystal colour, -habit	colorless, plate
Crystal size	0.80 x 0.30 x 0.05 mm
Temperature	173(2) K
Wavelength	0.71073 Å (graphite monochromator)
Space group	$P2_1/n$
Unit cell dimensions	a = 7.411(2) Å α = 90° b = 14.352(4) Å β = 90.21(2)° c = 11.204(3) Å γ = 90°
Volume	1191.7(6) $Å^3$
Z	4
Density (calculated)	1.315 Mg/m^3
Absorption coefficient	2.269 mm^{-1}
F(000)	496
θ range for data collection	2.31 to 27.55°
Index ranges	$0 \le h \le 9$, $0 \le k \le 18$, $-14 \le l \le 14$
Reflections collected	2970
Independent reflections	2765 (R_{int} = 0.0367)
Absorption correction	None
Data / restraints / parameters	2758 / 0 / 122
Goodness-of-fit on F^2	1.059
Final R indices [$I>2\sigma(I)$]	R1 = 0.0620 for 1722 reflections, wR2 = 0.1369
R indices (all data)	R1 = 0.1188, wR2 = 0.1850
Largest and mean Δ/σ	-0.017 and 0.000
Largest diff. peak and hole	0.8 and -1.5 $eÅ^{-3}$

Table 2. Measurement and program parameters for 5.

Diffractometer used	Siemens P2(1) diffractometer
Scan type	Omega-scan
Scan range	1.6° in ω arround $K\alpha_{1,2}$- maximum
Scan speed	3.9 - 29.3 °/min in ω
Standard reflections	3 of 100 measured reflections
Programs used	Siemens SHELXTL plus / SHELXL-93
Structure solution	direct
Structure refinement	Full-matrix least-squares on F^2
Structure factor source	International Tables Vol.C

Definition of R- values: $R1 = \sum||F_o|-|F_c||/\sum|F_o|$

$$wR2 = (\sum w(F_o^2-F_c^2)^2/\sum wF_o^2)^{1/2}$$

Definition of the weighting scheme (CIF format):

calc w=1/[\s^2^(Fo^2^)+(0.0869P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3

Table 3. Atomic coordinates (x 10^4) and isotropic displacement parameters U(iso) or U(eq)[a] [$Å^2$ x 10^3] for 5.

	x	y	z	U(eq)
Ga(1)	5656(1)	8359(1)	7989(1)	26(1)
N(1)	8486(7)	8548(3)	8181(4)	26(1)
C(1)	5768(8)	7001(4)	7344(5)	26(1)
C(2)	3983(8)	6628(4)	7558(6)	35(1)
C(3)	4035(9)	6124(4)	8585(6)	37(2)
C(4)	5839(8)	6105(4)	9016(5)	30(1)
C(5)	6921(7)	6600(4)	8261(5)	27(1)
C(6)	8874(8)	6802(4)	8401(6)	31(1)
C(7)	9275(8)	7773(4)	8901(5)	30(1)
C(8)	9356(9)	8589(4)	6992(5)	36(1)
C(9)	8845(10)	9438(5)	8799(6)	44(2)
C(10)	4924(10)	9254(5)	6745(7)	48(2)
C(11)	4710(10)	8481(5)	9625(6)	41(2)

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

Table 4. Selected bond lengths [Å] and angles [°] for 5.

Ga(1)-C(10)	1.970(7)	Ga(1)-C(11)	1.972(6)
Ga(1)-C(1)	2.081(6)	Ga(1)-N(1)	2.125(5)
N(1)-C(9)	1.476(7)	N(1)-C(8)	1.483(7)
N(1)-C(7)	1.493(7)	C(1)-C(2)	1.448(8)
C(1)-C(5)	1.453(8)	C(2)-C(3)	1.359(9)
C(3)-C(4)	1.420(9)	C(4)-C(5)	1.367(8)
C(5)-C(6)	1.483(8)	C(6)-C(7)	1.531(8)

C(10)-Ga(1)-C(11)	120.1(3)	C(10)-Ga(1)-C(1)	112.1(3)
C(11)-Ga(1)-C(1)	114.9(2)	C(10)-Ga(1)-N(1)	104.9(3)
C(11)-Ga(1)-N(1)	104.4(2)	C(1)-Ga(1)-N(1)	96.5(2)
C(9)-N(1)-C(8)	108.0(5)	C(9)-N(1)-C(7)	108.8(5)
C(8)-N(1)-C(7)	110.1(4)	C(9)-N(1)-Ga(1)	109.5(4)
C(8)-N(1)-Ga(1)	110.3(4)	C(7)-N(1)-Ga(1)	110.1(3)
C(2)-C(1)-C(5)	105.8(5)	C(2)-C(1)-Ga(1)	104.5(4)
C(5)-C(1)-Ga(1)	98.6(4)	C(3)-C(2)-C(1)	108.3(5)
C(2)-C(3)-C(4)	108.8(5)	C(5)-C(4)-C(3)	109.5(5)
C(4)-C(5)-C(1)	107.3(5)	C(4)-C(5)-C(6)	127.7(5)
C(1)-C(5)-C(6)	124.6(5)	C(5)-C(6)-C(7)	113.8(5)
N(1)-C(7)-C(6)	113.9(5)		

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement [a] parameters [$Å^2 \times 10^3$] for 5.

	U11	U22	U33	U23	U13	U12
Ga(1)	24(1)	30(1)	23(1)	2(1)	0(1)	-1(1)
N(1)	32(3)	27(3)	19(2)	-3(2)	3(2)	-4(2)
C(1)	26(3)	32(3)	19(3)	-2(2)	-3(2)	-2(2)
C(2)	30(3)	38(3)	36(3)	-1(3)	-6(3)	-3(3)
C(3)	31(3)	35(4)	43(4)	1(3)	13(3)	-4(3)
C(4)	38(3)	25(3)	27(3)	2(2)	1(3)	0(3)
C(5)	29(3)	27(3)	25(3)	0(3)	3(2)	1(3)
C(6)	21(3)	38(4)	35(3)	3(3)	-2(2)	7(2)
C(7)	21(3)	42(4)	27(3)	-5(3)	-2(2)	-1(3)
C(8)	35(3)	43(4)	30(3)	5(3)	11(3)	-7(3)
C(9)	49(4)	41(4)	40(4)	-10(3)	1(3)	-12(3)
C(10)	40(4)	50(4)	53(5)	12(4)	-1(3)	4(3)
C(11)	43(4)	43(4)	39(4)	-2(3)	12(3)	4(3)

a) The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + \ldots + 2hka^*b^*U_{12}]$

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

	x	y	z	U(eq)
H(1)	6218(8)	6935(4)	6508(5)	31
H(2)	2953(8)	6719(4)	7065(6)	42
H(3)	3030(9)	5833(4)	8954(6)	44
H(4)	6232(8)	5796(4)	9720(5)	36
H(6A)	9463(8)	6740(4)	7613(6)	37
H(6B)	9414(8)	6330(4)	8939(6)	37
H(7A)	8798(8)	7810(4)	9724(5)	36
H(7B)	10599(8)	7858(4)	8946(5)	36
H(8A)	9013(48)	8038(16)	6526(16)	54
H(8B)	10670(9)	8602(31)	7093(6)	54
H(8C)	8961(47)	9153(16)	6573(17)	54
H(9A)	8343(54)	9413(13)	9607(15)	65
H(9B)	8280(53)	9949(6)	8355(23)	65
H(9C)	10150(10)	9542(16)	8847(36)	65
H(10A)	4013(49)	8967(12)	6226(27)	71
H(10B)	5978(16)	9428(26)	6269(28)	71
H(10C)	4417(60)	9811(15)	7121(7)	71
H(11A)	5659(21)	8318(31)	10200(6)	62
H(11B)	3681(39)	8060(24)	9727(14)	62
H(11C)	4322(57)	9125(9)	9760(15)	62