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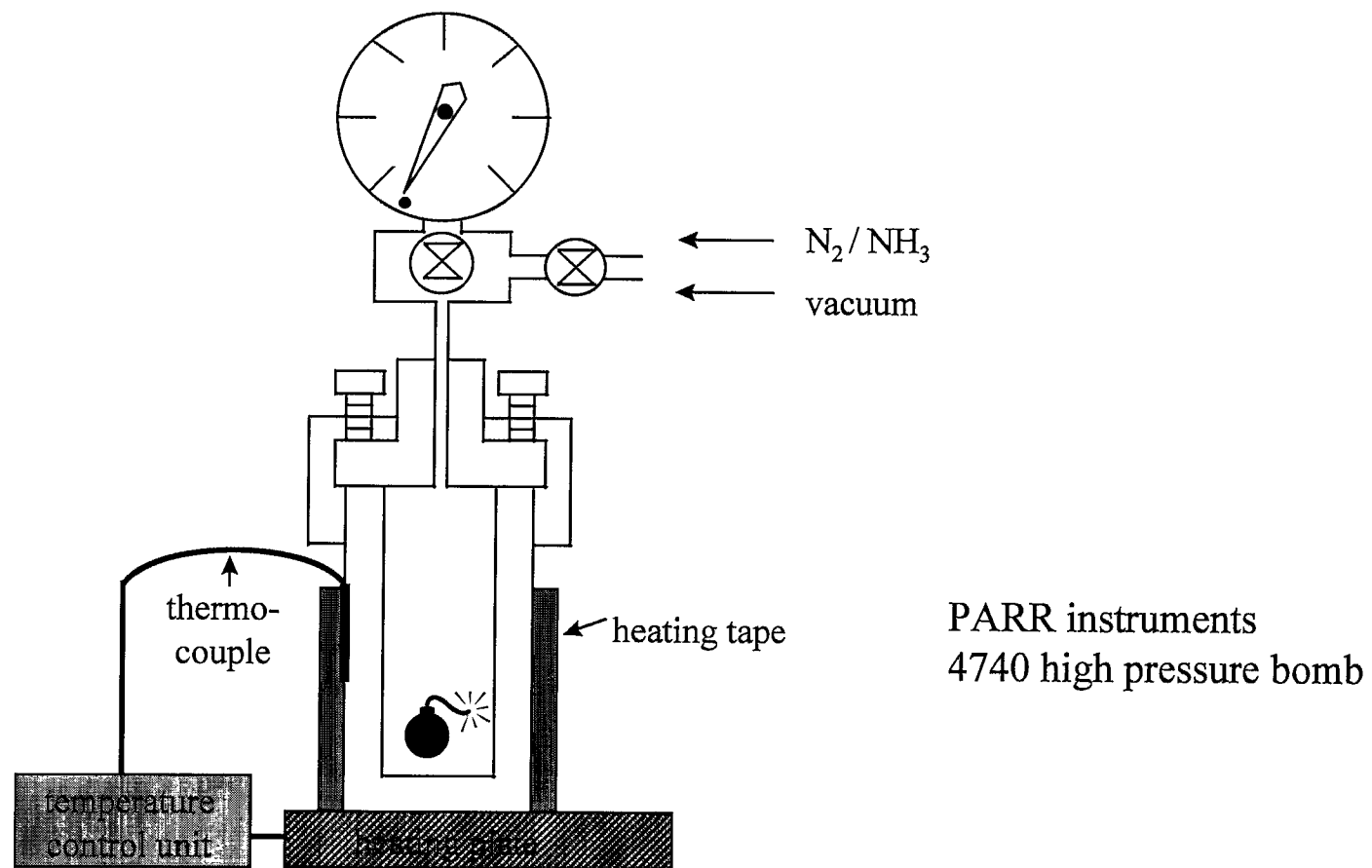


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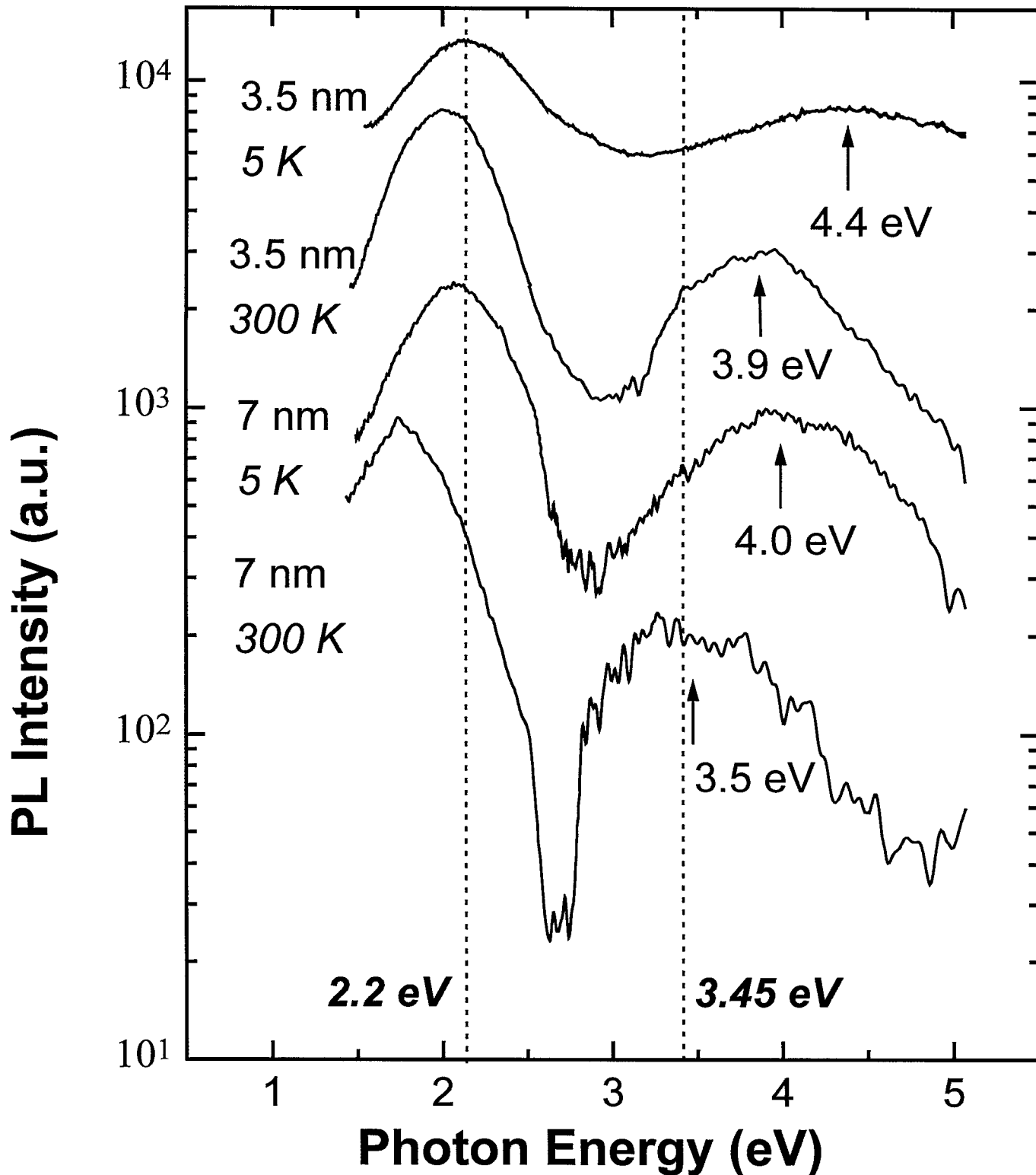
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Experimental Setup for Controlled Explosions of Galliumazides



Photoluminescence of GaN Nanocrystals



2.2 eV: typical donor-acceptor recombination of GaN
3.45 eV: band gap of the bulk phase of GaN at 300 K

Table 1. Crystal data and structure refinement for Na[Ga(N₃)₄].

Empirical formula	Ga N ₁₂ Na
Formula weight	260.83
Temperature	203(2) K
Wavelength	0.71070 Å
Crystal system, space group	Orthorhombic, P 2(1) 2(1) 2(1)
Unit cell dimensions	a = 7.011(4) Å alpha = 90 deg. b = 9.666(5) Å beta = 90 deg. c = 12.320(6) Å gamma = 90 deg.
Volume	834.9(8) Å ³
Z	4
Calculated density	2.075 mg/m ³
Absorption coefficient	3.330 mm ⁻¹
F(000)	504
Crystal size	0.45 x 0.25 x 0.20 mm
Theta range for data collection	2.68 to 34.99 deg.
Index ranges	0 ≤ h ≤ 11, 0 ≤ k ≤ 15, 0 ≤ l ≤ 19
Reflections collected / unique	2107 / 2107 [R(int) = 0.0000]
Absorption correction	Experimental
Max. and min. transmission	0.998 and 0.766
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2106 / 0 / 128
Goodness-of-fit on F ²	1.065
Final R indices [I > 2σ(I)]	R ₁ = 0.0275, R _w = 0.0683
R indices (all data)	R ₁ = 0.0368, R _w = 0.0721
Absolute structure parameter	-0.01(2)
Extinction coefficient	0.0205(15)
Largest diff. peak and hole	0.353 and -0.794 e Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Na}[\text{Ga}(\text{N}_3)_4]$:

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

	x	y	z	$U(\text{eq})$
Na(1)	2491(2)	5902(1)	3082(1)	24(1)
Ga(1)	2548(1)	9562(1)	3008(1)	20(1)
N(1)	901(3)	11019(2)	2583(2)	25(1)
N(2)	1491(3)	12209(2)	2685(2)	25(1)
N(3)	1930(4)	13337(3)	2746(3)	37(1)
N(4)	4999(3)	10281(2)	3376(2)	26(1)
N(5)	5680(4)	9997(2)	4258(2)	28(1)
N(6)	6398(6)	9783(3)	5062(3)	49(1)
N(7)	1612(4)	8342(2)	4104(2)	31(1)
N(8)	1067(4)	8564(2)	5013(2)	26(1)
N(9)	539(5)	8667(3)	5884(2)	37(1)
N(10)	2721(4)	8148(2)	1945(2)	27(1)
N(11)	2969(5)	8315(2)	988(2)	36(1)
N(12)	3223(9)	8375(4)	80(3)	72(2)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for $\text{Na}[\text{Ga}(\text{N}_3)_4]$.

Na(1)-N(6)#1	2.500(3)
Na(1)-N(1)#2	2.518(3)
Na(1)-N(9)#3	2.523(3)
Na(1)-N(3)#4	2.546(3)
Na(1)-N(4)#5	2.585(3)
Na(1)-N(10)	2.589(3)
Na(1)-N(7)	2.744(3)
Ga(1)-N(1)	1.896(2)
Ga(1)-N(10)	1.897(2)
Ga(1)-N(4)	1.909(3)
Ga(1)-N(7)	1.909(2)
N(1)-N(2)	1.229(3)
N(2)-N(3)	1.136(3)
N(4)-N(5)	1.218(3)
N(5)-N(6)	1.131(4)
N(7)-N(8)	1.202(3)
N(8)-N(9)	1.139(4)
N(10)-N(11)	1.203(3)
N(11)-N(12)	1.133(4)
N(6)#1-Na(1)-N(1)#2	91.13(12)
N(6)#1-Na(1)-N(9)#3	80.90(13)
N(1)#2-Na(1)-N(9)#3	163.14(10)
N(6)#1-Na(1)-N(3)#4	80.97(11)
N(1)#2-Na(1)-N(3)#4	81.09(9)
N(9)#3-Na(1)-N(3)#4	111.96(10)
N(6)#1-Na(1)-N(4)#5	141.45(11)
N(1)#2-Na(1)-N(4)#5	115.33(9)
N(9)#3-Na(1)-N(4)#5	79.17(10)
N(3)#4-Na(1)-N(4)#5	76.46(9)
N(6)#1-Na(1)-N(10)	137.37(10)
N(1)#2-Na(1)-N(10)	81.09(8)
N(9)#3-Na(1)-N(10)	94.69(10)
N(3)#4-Na(1)-N(10)	137.66(10)
N(4)#5-Na(1)-N(10)	77.11(8)
N(6)#1-Na(1)-N(7)	74.90(10)
N(1)#2-Na(1)-N(7)	84.17(9)
N(9)#3-Na(1)-N(7)	79.43(10)
N(3)#4-Na(1)-N(7)	151.36(10)
N(4)#5-Na(1)-N(7)	132.17(9)
N(10)-Na(1)-N(7)	62.68(8)
N(1)-Ga(1)-N(10)	112.58(10)
N(1)-Ga(1)-N(4)	110.08(10)
N(10)-Ga(1)-N(4)	111.62(11)
N(1)-Ga(1)-N(7)	116.47(12)

N(10)-Ga(1)-N(7)	93.69(11)
N(4)-Ga(1)-N(7)	111.53(12)
N(2)-N(1)-Ga(1)	117.5(2)
N(2)-N(1)-Na(1)#6	113.2(2)
Ga(1)-N(1)-Na(1)#6	129.18(11)
N(3)-N(2)-N(1)	175.5(3)
N(2)-N(3)-Na(1)#7	171.3(3)
N(5)-N(4)-Ga(1)	18.8(2)
N(5)-N(4)-Na(1)#8	113.9(2)
Ga(1)-N(4)-Na(1)#8	122.24(12)
N(6)-N(5)-N(4)	175.9(3)
N(5)-N(6)-Na(1)#3	170.5(3)
N(8)-N(7)-Ga(1)	131.1(2)
N(8)-N(7)-Na(1)	130.7(2)
Ga(1)-N(7)-Na(1)	97.47(11)
N(9)-N(8)-N(7)	174.7(3)
N(8)-N(9)-Na(1)#1	139.9(3)
N(11)-N(10)-Ga(1)	126.1(2)
N(11)-N(10)-Na(1)	130.7(2)
Ga(1)-N(10)-Na(1)	103.14(10)
N(12)-N(11)-N(10)	175.2(3)

Symmetry transformations used to generate equivalent atoms:

#1 $x-1/2, -y+3/2, -z+1$	#2 $-x, y-1/2, -z+1/2$	
#3 $x+1/2, -y+3/2, -z+1$	#4 $x, y-1, z$	#5 $-x+1, y-1/2, -z+1/2$
#6 $-x, y+1/2, -z+1/2$	#7 $x, y+1, z$	#8 $-x+1, y+1/2, -z+1/2$

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Na}[\text{Ga}(\text{N}_3)_4]$.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Na(1)	24(1)	23(1)	26(1)	1(1)	0(1)	-1(1)
Ga(1)	21(1)	16(1)	22(1)	1(1)	0(1)	(1)
N(1)	24(1)	18(1)	32(1)	-1(1)	-4(1)	1(1)
N(2)	24(1)	19(1)	32(1)	0(1)	-2(1)	2(1)
N(3)	37(1)	21(1)	54(2)	-2(1)	-1(1)	-1(1)
N(4)	25(1)	27(1)	26(1)	6(1)	-4(1)	-4(1)
N(5)	31(1)	23(1)	29(1)	1(1)	-5(1)	-3(1)
N(6)	62(2)	43(2)	41(2)	9(1)	-22(2)	-7(2)
N(7)	45(1)	22(1)	26(1)	2(1)	7(1)	-2(1)
N(8)	24(1)	26(1)	30(1)	4(1)	1(1)	-1(1)
N(9)	39(1)	43(1)	29(1)	-1(1)	8(1)	-3(1)
N(10)	36(1)	19(1)	26(1)	-1(1)	3(1)	1(1)
N(11)	55(2)	22(1)	31(1)	-3(1)	0(1)	-2(1)
N(12)	148(5)	39(2)	30(1)	3(1)	14(2)	-12(2)

Table 5. Crystal data and structure refinement for $\text{NEt}_3\text{Ga}(\text{N}_3)_3$ (2)

Identification code	raf07
Empirical formula	$\text{C}_6 \text{H}_{15} \text{Ga} \text{N}_{10}$
Formula weight	297.00
Temperature	203(2) K
Wavelength	0.71070 Å
Crystal system	Monoclinic
Space group	$P 2(1)/n$
Unit cell dimensions	$a = 8.394(5) \text{ \AA}$ $\alpha = 90^\circ$. $b = 13.059(8) \text{ \AA}$ $\beta = 95.93(5)^\circ$. $c = 11.939(7) \text{ \AA}$ $\gamma = 90^\circ$.
Volume	$1301.7(13) \text{ \AA}^3$
Z	4
Density (calculated)	1.515 Mg m^{-3}
Absorption coefficient	2.112 mm^{-1}
F(000)	608
Crystal size	0.6 x 0.6 x 0.4 mm
Theta range for data collection	2.32 to 33.01° .
Index ranges	$-12 \leq h \leq 12$, $0 \leq k \leq 20$, $0 \leq l \leq 18$
Reflections collected	4906
Independent reflections	4906 [$R(\text{int}) = 0.0000$]
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.835 and 0.672
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4905 / 0 / 244
Goodness-of-fit on F^2	1.042
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0326$, $R_w = 0.0690$
R indices (all data)	$R_1 = 0.0572$, $R_w = 0.0784$
Extinction coefficient	0.0081(6)
Largest diff. peak and hole	0.389 and -0.325 e\AA^{-3}

Table 6. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{NEt}_3\text{Ga}(\text{N}_3)_3$.

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

	x	y	z	$U(\text{eq})$
Ga(1)	5536(1)	3889(1)	2713(1)	38(1)
N(1)	5891(2)	5163(1)	2006(1)	48(1)
N(2)	5318(2)	5938(1)	2311(2)	49(1)
N(3)	4828(3)	6719(2)	2540(2)	76(1)
N(4)	3763(2)	3846(2)	3548(2)	70(1)
N(5)	3594(2)	4244(1)	4419(1)	45(1)
N(6)	3324(3)	4567(2)	5246(2)	84(1)
N(7)	7428(2)	3325(1)	3445(1)	51(1)
N(8)	8663(2)	3815(1)	3521(2)	53(1)
N(9)	9868(2)	4214(2)	3640(2)	82(1)
N(10)	4887(2)	2924(1)	1438(1)	40(1)
C(1)	3101(3)	2916(2)	1166(2)	54(1)
C(3)	5452(4)	1844(2)	1757(2)	54(1)
C(5)	5659(4)	3232(2)	400(2)	50(1)
C(1A)	3786(12)	3463(7)	510(7)	50(2)
C(3A)	3947(11)	2011(7)	1835(8)	50(2)
C(5A)	6314(10)	2500(7)	938(8)	47(2)
C(2)	2339(3)	3916(2)	808(3)	70(1)
C(4)	4808(4)	1421(2)	2797(2)	64(1)
C(6)	7439(3)	3313(2)	526(2)	60(1)

Table 7. Bond lengths [Å] and angles [°] for $\text{NEt}_3\text{Ga}(\text{N}_3)_3$.

Ga(1) -N(4)	1.875(2)	Ga(1) -N(7)	1.882(2)	Ga(1) -N(1)	1.904(2)
Ga(1) -N(10)	2.008(2)	N(1) -N(2)	1.194(2)	N(2) -N(3)	1.143(3)
N(4) -N(5)	1.184(2)	N(5) -N(6)	1.119(2)	N(7) -N(8)	1.214(2)
N(8) -N(9)	1.133(3)	N(10) -C(5A)	1.499(8)	N(10) -C(1)	1.500(3)
N(10) -C(5)	1.511(3)	N(10) -C(3)	1.525(3)	N(10) -C(3A)	1.533(8)
N(10) -C(1A)	1.538(9)	C(1) -C(2)	1.497(4)	C(1) -H(1A)	0.93(3)
C(1) -H(1B)	0.98(4)	C(3) -C(4)	1.509(4)	C(3) -H(3A)	1.00(3)
C(3) -H(3B)	1.00(3)	C(5) -C(6)	1.490(4)	C(5) -H(5A)	1.02(3)
C(5) -H(5B)	0.94(3)	C(1A) -C(2)	1.428(10)	C(1A) -H(1A1)	0.98
C(1A) -H(1A2)	0.98	C(1A) -H(2C)	1.50(4)	C(3A) -C(4)	1.504(10)
C(3A) -H(3A1)	0.98	C(3A) -H(3A2)	0.98	C(3A) -H(4C)	1.50(3)
C(5A) -C(6)	1.534(9)	C(5A) -H(5A1)	0.98	C(5A) -H(5A2)	0.98
C(5A) -H(6A)	1.50(3)	C(2) -H(2A)	1.00(3)	C(2) -H(2B)	0.88(4)
C(2) -H(2C)	0.92(4)	C(4) -H(4A)	0.86(4)	C(4) -H(4B)	0.94(3)
C(4) -H(4C)	0.95(3)	C(6) -H(6A)	0.86(4)	C(6) -H(6B)	0.94(3)
C(6) -H(6C)	1.00(3)				
N(4) -Ga(1)-N(7)	114.78(10)	N(4) -Ga(1)-N(1)	115.55(9)		
N(7) -Ga(1)-N(1)	112.62(8)	N(4) -Ga(1)-N(10)	102.50(8)		
N(7) -Ga(1)-N(10)	104.88(8)	N(1) -Ga(1)-N(10)	104.75(8)		
N(2) -N(1)-Ga(1)	121.3(2)	N(3) -N(2)-N(1)	174.6(2)		
N(5) -N(4)-Ga(1)	128.9(2)	N(6) -N(5)-N(4)	174.1(2)		
N(8) -N(7)-Ga(1)	120.13(14)	N(9) -N(8)-N(7)	174.8(2)		
C(1) -N(10)-C(5)	109.2(2)	C(1) -N(10)-C(3)	109.0(2)		
C(5) -N(10)-C(3)	107.6(2)	C(5A) -N(10)-C(3A)	107.1(5)		
C(5A) -N(10)-C(1A)	109.1(5)	C(3A) -N(10)-C(1A)	106.8(5)		
C(5A) -N(10)-Ga(1)	111.6(3)	C(1) -N(10)-Ga(1)	110.83(14)		
C(5) -N(10)-Ga(1)	110.43(14)	C(3) -N(10)-Ga(1)	109.7(2)		
C(3A) -N(10)-Ga(1)	111.2(4)	C(1A) -N(10)-Ga(1)	110.8(3)		
C(2) -C(1)-N(10)	116.3(2)	C(2) -C(1)-H(1A)	107(2)		
N(10) -C(1)-H(1A)	105(2)	C(2) -C(1)-H(1B)	109(2)		
N(10) -C(1)-H(1B)	107(2)	H(1A) -C(1)-H(1B)	112(3)		
C(4) -C(3)-N(10)	114.5(2)	C(4) -C(3)-H(3A)	111(2)		
N(10) -C(3)-H(3A)	108(2)	C(4) -C(3)-H(3B)	107(2)		
N(10) -C(3)-H(3B)	107(2)	H(3A) -C(3)-H(3B)	111(3)		
C(6) -C(5)-N(10)	116.5(2)	C(6) -C(5)-H(5A)	108(2)		
N(10) -C(5)-H(5A)	109(2)	C(6) -C(5)-H(5B)	112(2)		
N(10) -C(5)-H(5B)	107(2)	H(5A) -C(5)-H(5B)	105(3)		
C(2) -C(1A)-N(10)	118.2(6)	C(2) -C(1A)-H(1B)	85.0(13)		
N(10) -C(1A)-H(1B)	80.4(13)	C(2) -C(1A)-H(5A)	131.1(14)		
N(10) -C(1A)-H(5A)	87.9(13)	H(1B) -C(1A)-H(5A)	143(2)		
C(2) -C(1A)-H(1A1)	107.8	N(10) -C(1A)-H(1A1)	107.8		
C(2) -C(1A)-H(1A2)	107.8	N(10) -C(1A)-H(1A2)	107.8		
H(1A1) -C(1A)-H(1A2)	107.1	C(2) -C(1A)-H(2C)	36(2)		
N(10) -C(1A)-H(2C)	152(2)	H(1B) -C(1A)-H(2C)	102(2)		

H(5A) -C(1A)-H(2C)	104(2)	H(1A1) -C(1A)-H(2C)	80(2)
H(1A2) -C(1A)-H(2C)	94(2)	C(4) -C(3A)-N(10)	114.4(6)
C(4) -C(3A)-H(1A)	129.9(14)	N(10) -C(3A)-H(1A)	83.5(13)
C(4) -C(3A)-H(3A1)	108.7	N(10) -C(3A)-H(3A1)	108.7
C(4) -C(3A)-H(3A2)	108.7	N(10) -C(3A)-H(3A2)	108.7
H(3A1) -C(3A)-H(3A2)	107.6	C(4) -C(3A)-H(4C)	37.0(13)
N(10) -C(3A)-H(4C)	148.2(14)	H(1A) -C(3A)-H(4C)	106(2)
H(3A1) -C(3A)-H(4C)	79.6(13)	H(3A2) -C(3A)-H(4C)	97.2(12)
N(10) -C(5A)-C(6)	114.6(6)	N(10) -C(5A)-H(3B)	88.5(14)
C(6) -C(5A)-H(3B)	126(2)	N(10) -C(5A)-H(5B)	82.0(12)
C(6) -C(5A)-H(5B)	82.8(12)	H(3B) -C(5A)-H(5B)	151(2)
N(10) -C(5A)-H(5A1)	108.6	C(6) -C(5A)-H(5A1)	108.6
N(10) -C(5A)-H(5A2)	108.6	C(6) -C(5A)-H(5A2)	108.6
H(5A1) -C(5A)-H(5A2)	107.6	N(10) -C(5A)-H(6A)	145(2)
C(6) -C(5A)-H(6A)	32.9(14)	H(3B) -C(5A)-H(6A)	103(2)
H(5B) -C(5A)-H(6A)	100(2)	H(5A1) -C(5A)-H(6A)	99.2(14)
H(5A2) -C(5A)-H(6A)	82.4(14)	C(1A) -C(2)-H(2A)	108(2)
C(1) -C(2)-H(2A)	106(2)	C(1A) -C(2)-H(2B)	144(2)
C(1) -C(2)-H(2B)	106(2)	H(2A) -C(2)-H(2B)	106(3)
C(1A) -C(2)-H(2C)	76(3)	C(1) -C(2)-H(2C)	121(3)
H(2A) -C(2)-H(2C)	113(3)	H(2B) -C(2)-H(2C)	104(3)
C(3A) -C(4)-H(4A)	137(3)	C(3) -C(4)-H(4A)	108(3)
C(3A) -C(4)-H(4B)	109(2)	C(3) -C(4)-H(4B)	113(2)
H(4A) -C(4)-H(4B)	114(3)	C(3A) -C(4)-H(4C)	71(2)
C(3) -C(4)-H(4C)	118(2)	H(4A) -C(4)-H(4C)	98(3)
H(4B) -C(4)-H(4C)	104(2)	C(5) -C(6)-H(6A)	116(2)
C(5A) -C(6)-H(6A)	71(2)	C(5) -C(6)-H(6B)	108(2)
C(5A) -C(6)-H(6B)	137(2)	H(6A) -C(6)-H(6B)	100(3)
C(5) -C(6)-H(6C)	108(2)	C(5A) -C(6)-H(6C)	117(2)
H(6A) -C(6)-H(6C)	118(3)	H(6B) -C(6)-H(6C)	105(2)

Table 8. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{NEt}_3\text{Ga}(\text{N}_3)_3$.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Ga(1)	6(1)	47(1)	32(1)	-4(1)	7(1)	-1(1)
N(1)	57(1)	44(1)	43(1)	-4(1)	9(1)	4(1)
N(2)	42(1)	54(1)	51(1)	-8(1)	6(1)	-2(1)
N(3)	73(1)	57(1)	101(2)	-15(1)	22(1)	13(1)
N(4)	49(1)	108(2)	57(1)	-41(1)	22(1)	-22(1)
N(5)	39(1)	57(1)	39(1)	-8(1)	11(1)	-10(1)
N(6)	67(1)	133(2)	57(1)	-42(1)	30(1)	-38(1)
N(7)	43(1)	59(1)	51(1)	14(1)	-1(1)	-3(1)
N(8)	45(1)	58(1)	54(1)	12(1)	-2(1)	4(1)
N(9)	46(1)	80(2)	117(2)	19(1)	-9(1)	-6(1)
N(10)	44(1)	43(1)	34(1)	-4(1)	8(1)	-1(1)
C(1)	51(1)	64(2)	47(1)	-9(1)	3(1)	-11(1)
C(3)	74(2)	45(1)	48(1)	1(1)	20(1)	2(1)
C(5)	68(2)	53(2)	31(1)	-6(1)	13(1)	-6(1)
C(1A)	65(6)	45(5)	36(4)	-11(3)	-8(4)	-2(4)
C(3A)	52(5)	42(4)	56(5)	-7(4)	5(4)	-18(4)
C(5A)	46(4)	44(5)	52(5)	-15(4)	14(4)	-2(3)
C(2)	53(1)	85(2)	68(2)	-4(2)	-9(1)	9(1)
C(4)	81(2)	54(1)	60(1)	10(1)	20(1)	-3(1)
C(6)	66(1)	61(1)	57(1)	2(1)	33(1)	5(1)

Table 9. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{NEt}_3\text{Ga}(\text{N}_3)_3$.

	x	y	z	U(eq)
H(1A)	2695(33)	2732(22)	1833(25)	53(8)
H(1B)	2854(40)	2408(27)	568(31)	81(11)
H(3A)	5154(36)	1387(24)	1093(27)	62(9)
H(3B)	6640(39)	1877(23)	1927(26)	64(9)
H(5A)	5208(37)	3920(22)	125(26)	58(9)
H(5B)	5294(35)	2767(23)	-170(26)	62(9)
H(1A1)	4412	4002	187	42
H(1A2)	3497	2963	-89	42
H(3A1)	2928	2260	2065	42
H(3A2)	3698	1543	1199	42
H(5A1)	5938	2058	302	42
H(5A2)	6926	2073	1504	42
H(2A)	2632(32)	4404(22)	1441(26)	81(8)
H(2B)	1301(47)	3824(25)	790(31)	112(13)
H(2C)	2469(47)	4193(33)	118(39)	142(16)
H(4A)	5179(48)	815(34)	2909(33)	136(15)
H(4B)	4983(30)	1857(20)	3425(23)	74(8)
H(4C)	3695(42)	1260(21)	2753(27)	93(10)
H(6A)	7951(40)	2744(28)	620(29)	111(12)
H(6B)	7771(34)	3515(23)	-169(26)	90(9)
H(6C)	7754(34)	3891(20)	1058(25)	78(9)