

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

	x	y	z	U(eq)
Ga(11)	2191(1)	5987(1)	1328(1)	37(1)
Ga(12)	2098(1)	8627(1)	1050(1)	28(1)
Cl(11)	2515(1)	5085(2)	1505(1)	62(1)
Cl(12)	1957(1)	4477(2)	1400(1)	61(1)
N(11)	2123(1)	7569(5)	1645(2)	30(1)
N(12)	1805(1)	9040(5)	1053(2)	34(1)
N(13)	2162(1)	6964(5)	742(2)	34(1)
N(14)	2350(1)	9399(5)	920(2)	39(1)
C(11)	1888(1)	7525(6)	1670(2)	35(2)
C(12)	1746(1)	8262(7)	1388(2)	39(2)
C(13)	2391(1)	7262(7)	673(3)	43(2)
C(14)	2467(1)	8433(7)	756(3)	45(2)
C(111)	2268(1)	7971(6)	2103(2)	37(2)
C(112)	2503(1)	8199(7)	2028(3)	51(2)
C(113)	2176(1)	9221(7)	2269(2)	49(2)
C(114)	2269(1)	6943(7)	2472(2)	54(2)
C(121)	1651(1)	10028(7)	828(3)	45(2)
C(122)	1639(1)	11121(8)	1160(3)	67(2)
C(123)	1728(1)	10498(8)	403(3)	65(2)
C(124)	1416(1)	9454(9)	669(3)	70(3)
C(131)	2017(1)	6445(7)	297(2)	45(2)
C(132)	1778(1)	6357(7)	369(2)	51(2)
C(133)	2029(1)	7370(8)	-96(3)	61(2)
C(134)	2101(2)	5119(8)	190(3)	69(2)
C(141)	2425(1)	10736(7)	909(3)	47(2)
C(142)	2380(2)	11238(9)	409(3)	73(3)
C(143)	2676(1)	10856(8)	1115(3)	75(3)
C(144)	2301(1)	11517(7)	1208(3)	55(2)
Ga(21)	1458(1)	3796(1)	3342(1)	50(1)
Ga(22)	1468(1)	1087(1)	3141(1)	33(1)
Cl(21)	1634(1)	4754(2)	3968(1)	76(1)
Cl(22)	1277(1)	5329(2)	2935(1)	90(1)
N(21)	1655(1)	2665(6)	3059(2)	62(2)
N(22)	1687(1)	296(6)	3567(3)	76(2)
N(23)	1276(1)	2320(5)	3418(2)	50(2)
N(24)	1260(1)	679(5)	2621(2)	47(2)
C(21)	1874(2)	2412(8)	3453(3)	69(3)
C(22)	1870(2)	1189(9)	3651(3)	77(3)
C(23)	1081(2)	2428(9)	2983(3)	82(3)
C(24)	1085(2)	1620(10)	2628(4)	80(3)
C(211)	1752(2)	3043(8)	2672(4)	72(3)
C(212)	1530(2)	3191(11)	2270(3)	100(4)
C(213)	1868(1)	4301(8)	2728(3)	64(2)
C(214)	1891(1)	1988(8)	2525(3)	62(2)
C(221)	1744(1)	-995(7)	3718(3)	61(2)
C(222)	1866(2)	-1699(9)	3384(3)	81(3)
C(223)	1521(2)	-1679(9)	3679(4)	104(4)
C(224)	1876(2)	-1031(12)	4196(3)	154(7)

Table 1. Crystal Data, Data Collection and Structure Refinement for 1.

<i>Crystal data</i>	
empirical formula	C ₂₀ H ₄₀ Cl ₂ Ga ₂ N ₄
formula weight	546.90
crystal system	monoclinic
space group	C2/c (no. 15)
<i>a</i> , Å	61.445(13)
<i>b</i> , Å	10.441(1)
<i>c</i> , Å	29.371(1)
β , deg	101.45(1)
<i>V</i> , Å ³	18468(8)
ρ_{calcd} , g cm ⁻³	1.377
<i>Z</i>	28
F(000)	7952
μ (Mo <i>K</i> α), cm ⁻¹	22.57
crystal dimensions, mm	0.25 × 0.35 × 0.50
<i>Data collection</i>	
temperature, K	193
scan mode	ω
<i>hkl</i> range	-72→71; 0→12; 0→34
$\sin(\theta/\lambda)_{\text{max}}$, Å ⁻¹	0.64
measured reflns	16523
unique reflns	16188 (<i>R</i> _{int} = 0.0288)
reflns used for refinement	16188
absorption correction	empirical
<i>T</i> _{min} / <i>T</i> _{max}	0.8010/0.9999
<i>Refinement</i>	
least-squares parameters	911
final <i>R</i> values [<i>I</i> > 2 σ (<i>I</i>)]:	
<i>R</i> 1 ^a	0.0615
<i>wR</i> 2 ^b	0.1286
goodness-of-fit on <i>F</i> ²	1.056
ρ_{fin} (max/min), e Å ⁻³	1.300/-0.887

^a $R1 = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|$; ^b $wR2 = \{[\Sigma w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (ap)^2 + bp]$; $p = (F_o^2 + 2F_c^2)/3$; $a = 0.0464$; $b = 152.3001$.

C(231)	1178(2)	2104(9)	3817(4)	100(4)
C(232)	1012(2)	959(8)	3751(3)	75(3)
C(233)	1390(2)	1818(9)	4188(4)	92(3)
C(234)	1048(2)	3290(11)	3920(4)	98(3)
C(241)	1204(1)	-434(8)	2314(3)	61(2)
C(242)	1412(1)	-1171(9)	2298(3)	78(3)
C(243)	1044(2)	-1263(11)	2464(6)	173(8)
C(244)	1115(2)	98(12)	1805(3)	112(4)
Ga(31)	750(1)	6794(1)	460(1)	39(1)
Ga(32)	739(1)	4082(1)	243(1)	35(1)
Cl(31)	640(1)	7744(2)	1032(1)	57(1)
Cl(32)	874(1)	8326(2)	79(1)	56(1)
N(31)	965(1)	5362(5)	590(2)	38(1)
N(32)	919(1)	3749(5)	-185(2)	41(1)
N(33)	524(1)	5590(5)	129(2)	36(1)
N(34)	558(1)	3218(5)	578(2)	47(2)
C(31)	1113(1)	5448(7)	255(3)	44(2)
C(32)	1088(1)	4635(7)	-97(3)	46(2)
C(33)	379(1)	5246(7)	450(3)	45(2)
C(34)	399(1)	4088(7)	649(3)	47(2)
C(311)	1096(1)	5114(7)	1078(3)	49(2)
C(312)	933(1)	4853(8)	1396(3)	58(2)
C(313)	1244(1)	3931(7)	1059(3)	61(2)
C(314)	1240(1)	6256(8)	1254(3)	69(2)
C(321)	935(1)	2691(7)	-507(2)	45(2)
C(322)	724(1)	1922(8)	-578(3)	61(2)
C(323)	967(2)	3183(8)	-974(3)	72(3)
C(324)	1132(1)	1828(8)	-298(3)	65(2)
C(331)	387(1)	5931(7)	-347(2)	44(2)
C(332)	544(1)	6133(8)	-680(3)	54(2)
C(333)	233(1)	4815(8)	-514(3)	59(2)
C(334)	253(1)	7147(8)	-323(3)	65(2)
C(341)	547(1)	1889(7)	735(3)	56(2)
C(342)	773(1)	1264(7)	741(3)	58(2)
C(343)	368(1)	1151(8)	394(4)	79(3)
C(344)	497(2)	1804(8)	1223(3)	79(3)
Ga(41)	0	4383(1)	2500	56(1)
Ga(42)	0	7144(1)	2500	44(1)
Cl(4)	50(1)	3131(3)	3101(1)	122(1)
N(41)	229(1)	5711(5)	2576(2)	48(2)
N(42)	100(1)	7758(6)	3092(2)	69(2)
C(41)	322(1)	5840(8)	3088(3)	62(2)
C(42)	257(2)	6851(9)	3303(3)	78(3)
C(411)	417(2)	5618(10)	2323(4)	86(3)
C(412)	310(2)	5700(12)	1795(3)	103(4)
C(413)	543(2)	4335(10)	2440(4)	106(4)
C(414)	579(2)	6702(11)	2459(4)	109(4)
C(421)	70(2)	8954(9)	3343(4)	88(3)
C(422)	-133(2)	9623(10)	3081(5)	127(5)
C(424)	277(2)	9809(10)	3363(5)	125(5)
C(423)	46(2)	8706(13)	3841(4)	131(5)

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

Ga(11)-N(13)	1.979(5)	Ga(11)-N(11)	1.979(5)
Ga(11)-Cl(12)	2.171(2)	Ga(11)-Cl(11)	2.1731(19)
Ga(11)-Ga(12)	2.8992(10)	Ga(12)-N(14)	1.846(5)
Ga(12)-N(12)	1.857(5)	Ga(12)-N(13)	2.031(5)
Ga(12)-N(11)	2.047(5)	N(11)-C(11)	1.462(8)
N(11)-C(111)	1.518(8)	N(12)-C(12)	1.380(8)
N(12)-C(121)	1.466(8)	N(13)-C(13)	1.495(8)
N(13)-C(131)	1.527(8)	N(14)-C(14)	1.381(9)
N(14)-C(141)	1.473(8)	C(11)-C(12)	1.325(9)
C(11)-H(11)	0.92(5)	C(12)-H(12)	0.94(6)
C(13)-C(14)	1.314(10)	C(13)-H(13)	0.95(6)
C(14)-H(14)	0.85(8)	C(111)-C(112)	1.523(9)
C(111)-C(114)	1.524(9)	C(111)-C(113)	1.538(9)
C(112)-H(11A)	0.9800	C(112)-H(11B)	0.9800
C(112)-H(11C)	0.9800	C(113)-H(11D)	0.9800
C(113)-H(11E)	0.9800	C(113)-H(11F)	0.9800
C(114)-H(11G)	0.9800	C(114)-H(11H)	0.9800
C(114)-H(11I)	0.9800	C(121)-C(123)	1.502(10)
C(121)-C(122)	1.513(10)	C(121)-C(124)	1.547(10)
C(122)-H(12A)	0.9800	C(122)-H(12B)	0.9800
C(122)-H(12C)	0.9800	C(123)-H(12D)	0.9800
C(123)-H(12E)	0.9800	C(123)-H(12F)	0.9800
C(124)-H(12G)	0.9800	C(124)-H(12H)	0.9800
C(124)-H(12I)	0.9800	C(131)-C(133)	1.520(10)
C(131)-C(132)	1.523(9)	C(131)-C(134)	1.533(10)
C(132)-H(13A)	0.9800	C(132)-H(13B)	0.9800
C(132)-H(13C)	0.9800	C(133)-H(13D)	0.9800
C(133)-H(13E)	0.9800	C(133)-H(13F)	0.9800
C(134)-H(13G)	0.9800	C(134)-H(13H)	0.9800
C(134)-H(13I)	0.9800	C(141)-C(144)	1.509(10)
C(141)-C(142)	1.530(10)	C(141)-C(143)	1.548(10)
C(142)-H(14A)	0.9800	C(142)-H(14B)	0.9800
C(142)-H(14C)	0.9800	C(143)-H(14D)	0.9800
C(143)-H(14E)	0.9800	C(143)-H(14F)	0.9800
C(144)-H(14G)	0.9800	C(144)-H(14H)	0.9800
C(144)-H(14I)	0.9800	Ga(21)-N(23)	1.943(6)
Ga(21)-N(21)	1.991(6)	Ga(21)-Cl(22)	2.168(2)
Ga(21)-Cl(21)	2.182(2)	Ga(21)-Ga(22)	2.8938(10)
Ga(22)-N(24)	1.837(5)	Ga(22)-N(22)	1.842(6)
Ga(22)-N(23)	2.026(6)	Ga(22)-N(21)	2.051(6)
N(21)-C(211)	1.439(10)	N(21)-C(21)	1.612(10)
N(22)-C(221)	1.441(9)	N(22)-C(22)	1.442(11)
N(23)-C(231)	1.438(11)	N(23)-C(23)	1.571(11)
N(24)-C(24)	1.461(11)	N(24)-C(241)	1.469(9)
C(21)-C(22)	1.405(12)	C(21)-H(21)	0.9500
C(22)-H(22)	0.9500	C(23)-C(24)	1.343(12)
C(23)-H(23)	0.9500	C(24)-H(24)	0.9500
C(211)-C(213)	1.488(10)	C(211)-C(214)	1.508(11)
C(211)-C(212)	1.627(12)	C(212)-H(21A)	0.9800
C(212)-H(21B)	0.9800	C(212)-H(21C)	0.9800
C(213)-H(21D)	0.9800	C(213)-H(21E)	0.9800
C(213)-H(21F)	0.9800	C(214)-H(21G)	0.9800
C(214)-H(21H)	0.9800	C(214)-H(21I)	0.9800
C(221)-C(224)	1.474(12)	C(221)-C(223)	1.530(12)
C(221)-C(222)	1.536(12)	C(222)-H(22A)	0.9800

C(222)-H(22B)	0.9800	C(222)-H(22C)	0.9800
C(223)-H(22D)	0.9800	C(223)-H(22E)	0.9800
C(223)-H(22F)	0.9800	C(224)-H(22G)	0.9800
C(224)-H(22H)	0.9800	C(224)-H(22I)	0.9800
C(231)-C(234)	1.534(13)	C(231)-C(233)	1.553(15)
C(231)-C(232)	1.555(13)	C(232)-H(23A)	0.9800
C(232)-H(23B)	0.9800	C(232)-H(23C)	0.9800
C(233)-H(23D)	0.9800	C(233)-H(23E)	0.9800
C(233)-H(23F)	0.9800	C(234)-H(23G)	0.9800
C(234)-H(23H)	0.9800	C(234)-H(23I)	0.9800
C(241)-C(243)	1.444(13)	C(241)-C(242)	1.499(11)
C(241)-C(244)	1.588(13)	C(242)-H(24A)	0.9800
C(242)-H(24B)	0.9800	C(242)-H(24C)	0.9800
C(243)-H(24D)	0.9800	C(243)-H(24E)	0.9800
C(243)-H(24F)	0.9800	C(244)-H(24G)	0.9800
C(244)-H(24H)	0.9800	C(244)-H(24I)	0.9800
Ga(31)-N(31)	1.978(5)	Ga(31)-N(33)	1.981(5)
Ga(31)-Cl(31)	2.172(2)	Ga(31)-Cl(32)	2.175(2)
Ga(31)-Ga(32)	2.8995(10)	Ga(32)-N(34)	1.858(5)
Ga(32)-N(32)	1.865(5)	Ga(32)-N(33)	2.040(5)
Ga(32)-N(31)	2.046(5)	N(31)-C(31)	1.468(9)
N(31)-C(311)	1.521(9)	N(32)-C(32)	1.375(9)
N(32)-C(321)	1.471(8)	N(33)-C(33)	1.463(9)
N(33)-C(331)	1.524(8)	N(34)-C(34)	1.383(9)
N(34)-C(341)	1.468(9)	C(31)-C(32)	1.324(10)
C(31)-H(31)	0.90(8)	C(32)-H(32)	0.97(6)
C(33)-C(34)	1.339(10)	C(33)-H(33)	0.90(8)
C(34)-H(34)	0.91(7)	C(311)-C(314)	1.513(10)
C(311)-C(312)	1.521(10)	C(311)-C(313)	1.541(10)
C(312)-H(31A)	0.9800	C(312)-H(31B)	0.9800
C(312)-H(31C)	0.9800	C(313)-H(31D)	0.9800
C(313)-H(31E)	0.9800	C(313)-H(31F)	0.9800
C(314)-H(31G)	0.9800	C(314)-H(31H)	0.9800
C(314)-H(31I)	0.9800	C(321)-C(322)	1.506(10)
C(321)-C(323)	1.512(11)	C(321)-C(324)	1.536(9)
C(322)-H(32A)	0.9800	C(322)-H(32B)	0.9800
C(322)-H(32C)	0.9800	C(323)-H(32D)	0.9800
C(323)-H(32E)	0.9800	C(323)-H(32F)	0.9800
C(324)-H(32G)	0.9800	C(324)-H(32H)	0.9800
C(324)-H(32I)	0.9800	C(331)-C(332)	1.517(9)
C(331)-C(333)	1.520(10)	C(331)-C(334)	1.522(9)
C(332)-H(33A)	0.9800	C(332)-H(33B)	0.9800
C(332)-H(33C)	0.9800	C(333)-H(33D)	0.9800
C(333)-H(33E)	0.9800	C(333)-H(33F)	0.9800
C(334)-H(33G)	0.9800	C(334)-H(33H)	0.9800
C(334)-H(33I)	0.9800	C(341)-C(344)	1.524(11)
C(341)-C(342)	1.531(10)	C(341)-C(343)	1.540(11)
C(342)-H(34A)	0.9800	C(342)-H(34B)	0.9800
C(342)-H(34C)	0.9800	C(343)-H(34D)	0.9800
C(343)-H(34E)	0.9800	C(343)-H(34F)	0.9800
C(344)-H(34G)	0.9800	C(344)-H(34H)	0.9800
C(344)-H(34I)	0.9800	Ga(41)-N(41)	1.958(6)
Ga(41)-N(41)#1	1.958(6)	Ga(41)-Cl(4)#1	2.168(3)
Ga(41)-Cl(4)	2.168(3)	Ga(41)-Ga(42)	2.8829(16)
Ga(42)-N(42)	1.842(6)	Ga(42)-N(42)#1	1.842(6)
Ga(42)-N(41)	2.037(6)	Ga(42)-N(41)#1	2.037(6)
N(41)-C(411)	1.493(10)	N(41)-C(41)	1.506(10)
N(42)-C(42)	1.404(10)	N(42)-C(421)	1.479(11)
C(41)-C(42)	1.330(11)	C(41)-H(41)	0.9500

C(42)-H(42)	0.9500	C(411)-C(414)	1.509(13)
C(411)-C(413)	1.551(13)	C(411)-C(412)	1.563(14)
C(412)-H(41A)	0.9800	C(412)-H(41B)	0.9800
C(412)-H(41C)	0.9800	C(413)-H(41D)	0.9800
C(413)-H(41E)	0.9800	C(413)-H(41F)	0.9800
C(414)-H(41G)	0.9800	C(414)-H(41H)	0.9800
C(414)-H(41I)	0.9800	C(421)-C(422)	1.501(13)
C(421)-C(423)	1.523(15)	C(421)-C(424)	1.545(15)
C(422)-H(42A)	0.9800	C(422)-H(42B)	0.9800
C(422)-H(42C)	0.9800	C(424)-H(42D)	0.9800
C(424)-H(42E)	0.9800	C(424)-H(42F)	0.9800
C(423)-H(42G)	0.9800	C(423)-H(42H)	0.9800
C(423)-H(42I)	0.9800		
N(13)-Ga(11)-N(11)	89.3(2)	N(13)-Ga(11)-Cl(12)	120.83(16)
N(11)-Ga(11)-Cl(12)	110.86(16)	N(13)-Ga(11)-Cl(11)	110.55(16)
N(11)-Ga(11)-Cl(11)	121.15(15)	Cl(12)-Ga(11)-Cl(11)	104.80(9)
N(13)-Ga(11)-Ga(12)	44.41(15)	N(11)-Ga(11)-Ga(12)	44.87(14)
Cl(12)-Ga(11)-Ga(12)	128.46(7)	Cl(11)-Ga(11)-Ga(12)	126.75(7)
N(14)-Ga(12)-N(12)	138.8(2)	N(14)-Ga(12)-N(13)	92.2(2)
N(12)-Ga(12)-N(13)	118.2(2)	N(14)-Ga(12)-N(11)	119.2(2)
N(12)-Ga(12)-N(11)	91.7(2)	N(13)-Ga(12)-N(11)	86.0(2)
N(14)-Ga(12)-Ga(11)	110.39(17)	N(12)-Ga(12)-Ga(11)	110.80(16)
N(13)-Ga(12)-Ga(11)	42.98(14)	N(11)-Ga(12)-Ga(11)	43.02(14)
C(11)-N(11)-C(111)	111.9(5)	C(11)-N(11)-Ga(11)	107.4(4)
C(111)-N(11)-Ga(11)	120.5(4)	C(11)-N(11)-Ga(12)	98.9(4)
C(111)-N(11)-Ga(12)	122.7(4)	Ga(11)-N(11)-Ga(12)	92.1(2)
C(12)-N(12)-C(121)	119.9(5)	C(12)-N(12)-Ga(12)	105.1(4)
C(121)-N(12)-Ga(12)	134.6(4)	C(13)-N(13)-C(131)	111.3(5)
C(13)-N(13)-Ga(11)	107.6(4)	C(131)-N(13)-Ga(11)	119.8(4)
C(13)-N(13)-Ga(12)	98.7(4)	C(131)-N(13)-Ga(12)	123.6(4)
Ga(11)-N(13)-Ga(12)	92.6(2)	C(14)-N(14)-C(141)	119.8(6)
C(14)-N(14)-Ga(12)	105.6(4)	C(141)-N(14)-Ga(12)	134.1(4)
C(12)-C(11)-N(11)	119.1(6)	C(12)-C(11)-H(11)	126(3)
N(11)-C(11)-H(11)	115(3)	C(11)-C(12)-N(12)	123.6(6)
C(11)-C(12)-H(12)	121(4)	N(12)-C(12)-H(12)	115(4)
C(14)-C(13)-N(13)	118.5(6)	C(14)-C(13)-H(13)	129(3)
N(13)-C(13)-H(13)	112(3)	C(13)-C(14)-N(14)	123.7(7)
C(13)-C(14)-H(14)	121(6)	N(14)-C(14)-H(14)	115(6)
N(11)-C(111)-C(112)	108.6(5)	N(11)-C(111)-C(114)	110.8(5)
C(112)-C(111)-C(114)	110.1(6)	N(11)-C(111)-C(113)	109.2(5)
C(112)-C(111)-C(113)	109.3(6)	C(114)-C(111)-C(113)	108.9(6)
C(111)-C(112)-H(11A)	109.5	C(111)-C(112)-H(11B)	109.5
H(11A)-C(112)-H(11B)	109.5	C(111)-C(112)-H(11C)	109.5
H(11A)-C(112)-H(11C)	109.5	H(11B)-C(112)-H(11C)	109.5
C(111)-C(113)-H(11D)	109.5	C(111)-C(113)-H(11E)	109.5
H(11D)-C(113)-H(11E)	109.5	C(111)-C(113)-H(11F)	109.5
H(11D)-C(113)-H(11F)	109.5	H(11E)-C(113)-H(11F)	109.5
C(111)-C(114)-H(11G)	109.5	C(111)-C(114)-H(11H)	109.5
H(11G)-C(114)-H(11H)	109.5	C(111)-C(114)-H(11I)	109.5
H(11G)-C(114)-H(11I)	109.5	H(11H)-C(114)-H(11I)	109.5
N(12)-C(121)-C(122)	108.8(5)	N(12)-C(121)-C(122)	110.3(6)
C(123)-C(121)-C(122)	110.6(7)	N(12)-C(121)-C(124)	110.1(6)
C(123)-C(121)-C(124)	107.8(7)	C(122)-C(121)-C(124)	109.1(6)
C(121)-C(122)-H(12A)	109.5	C(121)-C(122)-H(12B)	109.5
H(12A)-C(122)-H(12B)	109.5	C(121)-C(122)-H(12C)	109.5
H(12A)-C(122)-H(12C)	109.5	H(12B)-C(122)-H(12C)	109.5
C(121)-C(123)-H(12D)	109.5	C(121)-C(123)-H(12E)	109.5
H(12D)-C(123)-H(12E)	109.5	C(121)-C(123)-H(12F)	109.5

H(12D)-C(123)-H(12F)	109.5	H(12E)-C(123)-H(12F)	109.5
C(121)-C(124)-H(12G)	109.5	C(121)-C(124)-H(12H)	109.5
H(12G)-C(124)-H(12H)	109.5	C(121)-C(124)-H(12I)	109.5
H(12G)-C(124)-H(12I)	109.5	H(12H)-C(124)-H(12I)	109.5
C(133)-C(131)-C(132)	109.7(6)	C(133)-C(131)-N(13)	108.5(6)
C(132)-C(131)-N(13)	108.5(5)	C(133)-C(131)-C(134)	110.3(6)
C(132)-C(131)-C(134)	110.4(6)	N(13)-C(131)-C(134)	109.4(6)
C(131)-C(132)-H(13A)	109.5	C(131)-C(132)-H(13B)	109.5
H(13A)-C(132)-H(13B)	109.5	C(131)-C(132)-H(13C)	109.5
H(13A)-C(132)-H(13C)	109.5	H(13B)-C(132)-H(13C)	109.5
C(131)-C(133)-H(13D)	109.5	C(131)-C(133)-H(13E)	109.5
H(13D)-C(133)-H(13E)	109.5	C(131)-C(133)-H(13F)	109.5
H(13D)-C(133)-H(13F)	109.5	H(13E)-C(133)-H(13F)	109.5
C(131)-C(134)-H(13G)	109.5	C(131)-C(134)-H(13H)	109.5
H(13G)-C(134)-H(13H)	109.5	C(131)-C(134)-H(13I)	109.5
H(13G)-C(134)-H(13I)	109.5	H(13H)-C(134)-H(13I)	109.5
N(14)-C(141)-C(144)	107.7(5)	N(14)-C(141)-C(142)	110.4(6)
C(144)-C(141)-C(142)	111.0(7)	N(14)-C(141)-C(143)	111.1(6)
C(144)-C(141)-C(143)	107.8(7)	C(142)-C(141)-C(143)	108.8(6)
C(141)-C(142)-H(14A)	109.5	C(141)-C(142)-H(14B)	109.5
H(14A)-C(142)-H(14B)	109.5	C(141)-C(142)-H(14C)	109.5
H(14A)-C(142)-H(14C)	109.5	H(14B)-C(142)-H(14C)	109.5
C(141)-C(143)-H(14D)	109.5	C(141)-C(143)-H(14E)	109.5
H(14D)-C(143)-H(14E)	109.5	C(141)-C(143)-H(14F)	109.5
H(14D)-C(143)-H(14F)	109.5	H(14E)-C(143)-H(14F)	109.5
C(141)-C(144)-H(14G)	109.5	C(141)-C(144)-H(14H)	109.5
H(14G)-C(144)-H(14H)	109.5	C(141)-C(144)-H(14I)	109.5
H(14G)-C(144)-H(14I)	109.5	H(14H)-C(144)-H(14I)	109.5
N(23)-Ga(21)-N(21)	89.4(2)	N(23)-Ga(21)-Cl(22)	113.9(2)
N(21)-Ga(21)-Cl(22)	119.7(2)	N(23)-Ga(21)-Cl(21)	117.9(2)
N(21)-Ga(21)-Cl(21)	112.5(2)	Cl(22)-Ga(21)-Cl(21)	103.94(10)
N(23)-Ga(21)-Ga(22)	44.33(16)	N(21)-Ga(21)-Ga(22)	45.10(18)
Cl(22)-Ga(21)-Ga(22)	129.67(8)	Cl(21)-Ga(21)-Ga(22)	126.38(7)
N(24)-Ga(22)-N(22)	139.1(3)	N(24)-Ga(22)-N(23)	96.6(3)
N(22)-Ga(22)-N(23)	114.6(3)	N(24)-Ga(22)-N(21)	113.8(3)
N(22)-Ga(22)-N(21)	95.1(3)	N(23)-Ga(22)-N(21)	85.5(2)
N(24)-Ga(22)-Ga(21)	110.89(19)	N(22)-Ga(22)-Ga(21)	110.0(2)
N(23)-Ga(22)-Ga(21)	42.08(17)	N(21)-Ga(22)-Ga(21)	43.46(18)
C(211)-N(21)-C(21)	101.2(7)	C(211)-N(21)-Ga(21)	123.4(5)
C(21)-N(21)-Ga(21)	106.7(5)	C(211)-N(21)-Ga(22)	130.0(5)
C(21)-N(21)-Ga(22)	101.0(5)	Ga(21)-N(21)-Ga(22)	91.4(3)
C(221)-N(22)-C(22)	114.8(6)	C(221)-N(22)-Ga(22)	136.8(5)
C(22)-N(22)-Ga(22)	105.3(5)	C(231)-N(23)-C(23)	107.5(8)
C(231)-N(23)-Ga(21)	124.2(6)	C(23)-N(23)-Ga(21)	102.3(5)
C(231)-N(23)-Ga(22)	126.9(6)	C(23)-N(23)-Ga(22)	97.4(5)
Ga(21)-N(23)-Ga(22)	93.6(3)	C(24)-N(24)-C(241)	117.3(6)
C(24)-N(24)-Ga(22)	103.0(5)	C(241)-N(24)-Ga(22)	137.1(5)
C(22)-C(21)-N(21)	111.3(8)	C(22)-C(21)-H(21)	124.3
N(21)-C(21)-H(21)	124.3	C(21)-C(22)-N(22)	126.6(8)
C(21)-C(22)-H(22)	116.7	N(22)-C(22)-H(22)	116.7
C(24)-C(23)-N(23)	117.3(8)	C(24)-C(23)-H(23)	121.3
N(23)-C(23)-H(23)	121.3	C(23)-C(24)-N(24)	124.0(9)
C(23)-C(24)-H(24)	118.0	N(24)-C(24)-H(24)	118.0
N(21)-C(211)-C(213)	114.7(8)	N(21)-C(211)-C(214)	111.9(7)
C(213)-C(211)-C(214)	113.0(7)	N(21)-C(211)-C(212)	100.3(7)
C(213)-C(211)-C(212)	108.2(8)	C(214)-C(211)-C(212)	107.7(8)
C(211)-C(212)-H(21A)	109.5	C(211)-C(212)-H(21B)	109.5
H(21A)-C(212)-H(21B)	109.5	C(211)-C(212)-H(21C)	109.5
H(21A)-C(212)-H(21C)	109.5	H(21B)-C(212)-H(21C)	109.5

C(211)-C(213)-H(21D)	109.5	C(211)-C(213)-H(21E)	109.5
H(21D)-C(213)-H(21E)	109.5	C(211)-C(213)-H(21F)	109.5
H(21D)-C(213)-H(21F)	109.5	H(21E)-C(213)-H(21F)	109.5
C(211)-C(214)-H(21G)	109.5	C(211)-C(214)-H(21H)	109.5
H(21G)-C(214)-H(21H)	109.5	C(211)-C(214)-H(21I)	109.5
H(21G)-C(214)-H(21I)	109.5	H(21H)-C(214)-H(21I)	109.5
N(22)-C(221)-C(224)	111.8(8)	N(22)-C(221)-C(223)	104.7(7)
C(224)-C(221)-C(223)	112.0(10)	N(22)-C(221)-C(222)	111.8(8)
C(224)-C(221)-C(222)	110.5(8)	C(223)-C(221)-C(222)	105.8(7)
C(221)-C(222)-H(22A)	109.5	C(221)-C(222)-H(22B)	109.5
H(22A)-C(222)-H(22B)	109.5	C(221)-C(222)-H(22C)	109.5
H(22A)-C(222)-H(22C)	109.5	H(22B)-C(222)-H(22C)	109.5
C(221)-C(223)-H(22D)	109.5	C(221)-C(223)-H(22E)	109.5
H(22D)-C(223)-H(22E)	109.5	C(221)-C(223)-H(22F)	109.5
H(22D)-C(223)-H(22F)	109.5	H(22E)-C(223)-H(22F)	109.5
C(221)-C(224)-H(22G)	109.5	C(221)-C(224)-H(22H)	109.5
H(22G)-C(224)-H(22H)	109.5	C(221)-C(224)-H(22I)	109.5
H(22G)-C(224)-H(22I)	109.5	H(22H)-C(224)-H(22I)	109.5
N(23)-C(231)-C(234)	110.6(8)	N(23)-C(231)-C(233)	100.0(8)
C(234)-C(231)-C(233)	114.3(10)	N(23)-C(231)-C(232)	112.8(9)
C(234)-C(231)-C(232)	107.1(8)	C(233)-C(231)-C(232)	112.1(9)
C(231)-C(232)-H(23A)	109.5	C(231)-C(232)-H(23B)	109.5
H(23A)-C(232)-H(23B)	109.5	C(231)-C(232)-H(23C)	109.5
H(23A)-C(232)-H(23C)	109.5	H(23B)-C(232)-H(23C)	109.5
C(231)-C(233)-H(23D)	109.5	C(231)-C(233)-H(23E)	109.5
H(23D)-C(233)-H(23E)	109.5	C(231)-C(233)-H(23F)	109.5
H(23D)-C(233)-H(23F)	109.5	H(23E)-C(233)-H(23F)	109.5
C(231)-C(234)-H(23G)	109.5	C(231)-C(234)-H(23H)	109.5
H(23G)-C(234)-H(23H)	109.5	C(231)-C(234)-H(23I)	109.5
H(23G)-C(234)-H(23I)	109.5	H(23H)-C(234)-H(23I)	109.5
C(243)-C(241)-N(24)	112.1(8)	C(243)-C(241)-C(242)	109.8(9)
N(24)-C(241)-C(242)	109.2(7)	C(243)-C(241)-C(244)	111.7(10)
N(24)-C(241)-C(244)	107.2(7)	C(242)-C(241)-C(244)	106.6(8)
C(241)-C(242)-H(24A)	109.5	C(241)-C(242)-H(24B)	109.5
H(24A)-C(242)-H(24B)	109.5	C(241)-C(242)-H(24C)	109.5
H(24A)-C(242)-H(24C)	109.5	H(24B)-C(242)-H(24C)	109.5
C(241)-C(243)-H(24D)	109.5	C(241)-C(243)-H(24E)	109.5
H(24D)-C(243)-H(24E)	109.5	C(241)-C(243)-H(24F)	109.5
H(24D)-C(243)-H(24F)	109.5	H(24E)-C(243)-H(24F)	109.5
C(241)-C(244)-H(24G)	109.5	C(241)-C(244)-H(24H)	109.5
H(24G)-C(244)-H(24H)	109.5	C(241)-C(244)-H(24I)	109.5
H(24G)-C(244)-H(24I)	109.5	H(24H)-C(244)-H(24I)	109.5
N(31)-Ga(31)-N(33)	89.5(2)	N(31)-Ga(31)-Cl(31)	119.58(17)
N(33)-Ga(31)-Cl(31)	111.91(16)	N(31)-Ga(31)-Cl(32)	111.55(17)
N(33)-Ga(31)-Cl(32)	119.83(17)	Cl(31)-Ga(31)-Cl(32)	104.89(8)
N(31)-Ga(31)-Ga(32)	44.84(15)	N(33)-Ga(31)-Ga(32)	44.68(15)
Cl(31)-Ga(31)-Ga(32)	128.19(6)	Cl(32)-Ga(31)-Ga(32)	126.93(6)
N(34)-Ga(32)-N(32)	139.8(2)	N(34)-Ga(32)-N(33)	91.5(2)
N(32)-Ga(32)-N(33)	119.0(2)	N(34)-Ga(32)-N(31)	118.1(2)
N(32)-Ga(32)-N(31)	91.3(2)	N(33)-Ga(32)-N(31)	86.0(2)
N(34)-Ga(32)-Ga(31)	110.41(18)	N(32)-Ga(32)-Ga(31)	109.77(17)
N(33)-Ga(32)-Ga(31)	43.04(14)	N(31)-Ga(32)-Ga(31)	42.98(15)
C(31)-N(31)-C(311)	111.1(5)	C(31)-N(31)-Ga(31)	107.6(4)
C(311)-N(31)-Ga(31)	121.2(4)	C(31)-N(31)-Ga(32)	99.0(4)
C(311)-N(31)-Ga(32)	122.5(4)	Ga(31)-N(31)-Ga(32)	92.2(2)
C(32)-N(32)-C(321)	118.8(6)	C(32)-N(32)-Ga(32)	106.0(5)
C(321)-N(32)-Ga(32)	134.2(5)	C(33)-N(33)-C(331)	110.7(5)
C(33)-N(33)-Ga(31)	107.3(4)	C(331)-N(33)-Ga(31)	120.6(4)
C(33)-N(33)-Ga(32)	99.3(4)	C(331)-N(33)-Ga(32)	123.5(4)

Ga(31)-N(33)-Ga(32)	92.3(2)	C(34)-N(34)-C(341)	119.6(6)
C(34)-N(34)-Ga(32)	106.1(5)	C(341)-N(34)-Ga(32)	134.1(5)
C(32)-C(31)-N(31)	119.7(7)	C(32)-C(31)-H(31)	121(5)
N(31)-C(31)-H(31)	120(5)	C(31)-C(32)-N(32)	122.8(7)
C(31)-C(32)-H(32)	120(4)	N(32)-C(32)-H(32)	117(4)
C(34)-C(33)-N(33)	119.4(7)	C(34)-C(33)-H(33)	112(5)
N(33)-C(33)-H(33)	128(5)	C(33)-C(34)-N(34)	122.1(7)
C(33)-C(34)-H(34)	120(4)	N(34)-C(34)-H(34)	117(4)
C(314)-C(311)-C(312)	110.0(7)	C(314)-C(311)-N(31)	110.6(6)
C(312)-C(311)-N(31)	108.7(5)	C(314)-C(311)-C(313)	109.6(6)
C(312)-C(311)-C(313)	110.0(7)	N(31)-C(311)-C(313)	107.9(6)
C(311)-C(312)-H(31A)	109.5	C(311)-C(312)-H(31B)	109.5
H(31A)-C(312)-H(31B)	109.5	C(311)-C(312)-H(31C)	109.5
H(31A)-C(312)-H(31C)	109.5	H(31B)-C(312)-H(31C)	109.5
C(311)-C(313)-H(31D)	109.5	C(311)-C(313)-H(31E)	109.5
H(31D)-C(313)-H(31E)	109.5	C(311)-C(313)-H(31F)	109.5
H(31D)-C(313)-H(31F)	109.5	H(31E)-C(313)-H(31F)	109.5
C(311)-C(314)-H(31G)	109.5	C(311)-C(314)-H(31H)	109.5
H(31G)-C(314)-H(31H)	109.5	C(311)-C(314)-H(31I)	109.5
H(31G)-C(314)-H(31I)	109.5	H(31H)-C(314)-H(31I)	109.5
N(32)-C(321)-C(322)	108.9(6)	N(32)-C(321)-C(323)	111.5(6)
C(322)-C(321)-C(323)	108.7(7)	N(32)-C(321)-C(324)	109.2(6)
C(322)-C(321)-C(324)	109.3(6)	C(323)-C(321)-C(324)	109.2(7)
C(321)-C(322)-H(32A)	109.5	C(321)-C(322)-H(32B)	109.5
H(32A)-C(322)-H(32B)	109.5	C(321)-C(322)-H(32C)	109.5
H(32A)-C(322)-H(32C)	109.5	H(32B)-C(322)-H(32C)	109.5
C(321)-C(323)-H(32D)	109.5	C(321)-C(323)-H(32E)	109.5
H(32D)-C(323)-H(32E)	109.5	C(321)-C(323)-H(32F)	109.5
H(32D)-C(323)-H(32F)	109.5	H(32E)-C(323)-H(32F)	109.5
C(321)-C(324)-H(32G)	109.5	C(321)-C(324)-H(32H)	109.5
H(32G)-C(324)-H(32H)	109.5	C(321)-C(324)-H(32I)	109.5
H(32G)-C(324)-H(32I)	109.5	H(32H)-C(324)-H(32I)	109.5
C(332)-C(331)-C(333)	109.5(6)	C(332)-C(331)-C(334)	109.4(6)
C(333)-C(331)-C(334)	110.4(6)	C(332)-C(331)-N(33)	108.5(5)
C(333)-C(331)-N(33)	108.2(6)	C(334)-C(331)-N(33)	110.9(6)
C(331)-C(332)-H(33A)	109.5	C(331)-C(332)-H(33B)	109.5
H(33A)-C(332)-H(33B)	109.5	C(331)-C(332)-H(33C)	109.5
H(33A)-C(332)-H(33C)	109.5	H(33B)-C(332)-H(33C)	109.5
C(331)-C(333)-H(33D)	109.5	C(331)-C(333)-H(33E)	109.5
H(33D)-C(333)-H(33E)	109.5	C(331)-C(333)-H(33F)	109.5
H(33D)-C(333)-H(33F)	109.5	H(33E)-C(333)-H(33F)	109.5
C(331)-C(334)-H(33G)	109.5	C(331)-C(334)-H(33H)	109.5
H(33G)-C(334)-H(33H)	109.5	C(331)-C(334)-H(33I)	109.5
H(33G)-C(334)-H(33I)	109.5	H(33H)-C(334)-H(33I)	109.5
N(34)-C(341)-C(344)	112.4(7)	N(34)-C(341)-C(342)	107.9(6)
C(344)-C(341)-C(342)	108.4(7)	N(34)-C(341)-C(343)	109.9(7)
C(344)-C(341)-C(343)	109.4(7)	C(342)-C(341)-C(343)	108.8(7)
C(341)-C(342)-H(34A)	109.5	C(341)-C(342)-H(34B)	109.5
H(34A)-C(342)-H(34B)	109.5	C(341)-C(342)-H(34C)	109.5
H(34A)-C(342)-H(34C)	109.5	H(34B)-C(342)-H(34C)	109.5
C(341)-C(343)-H(34D)	109.5	C(341)-C(343)-H(34E)	109.5
H(34D)-C(343)-H(34E)	109.5	C(341)-C(343)-H(34F)	109.5
H(34D)-C(343)-H(34F)	109.5	H(34E)-C(343)-H(34F)	109.5
C(341)-C(344)-H(34G)	109.5	C(341)-C(344)-H(34H)	109.5
H(34G)-C(344)-H(34H)	109.5	C(341)-C(344)-H(34I)	109.5
H(34G)-C(344)-H(34I)	109.5	H(34H)-C(344)-H(34I)	109.5
N(41)-Ga(41)-N(41)#1	89.8(3)	N(41)-Ga(41)-Cl(4)#1	120.2(2)
N(41)#1-Ga(41)-Cl(4)#1	110.6(2)	N(41)-Ga(41)-Cl(4)	110.6(2)
N(41)#1-Ga(41)-Cl(4)	120.2(2)	Cl(4)#1-Ga(41)-Cl(4)	105.8(2)

N(41)-Ga(41)-Ga(42)	44.92(16)	N(41)#1-Ga(41)-Ga(42)	44.92(16)
Cl(4)#1-Ga(41)-Ga(42)	127.08(10)	Cl(4)-Ga(41)-Ga(42)	127.08(10)
N(42)-Ga(42)-N(42)#1	139.3(4)	N(42)-Ga(42)-N(41)	93.3(3)
N(42)#1-Ga(42)-N(41)	116.9(3)	N(42)-Ga(42)-N(41)#1	116.9(3)
N(42)#1-Ga(42)-N(41)#1	93.3(3)	N(41)-Ga(42)-N(41)#1	85.4(3)
N(42)-Ga(42)-Ga(41)	110.4(2)	N(42)#1-Ga(42)-Ga(41)	110.4(2)
N(41)-Ga(42)-Ga(41)	42.72(16)	N(41)#1-Ga(42)-Ga(41)	42.72(16)
C(411)-N(41)-C(41)	109.1(7)	C(411)-N(41)-Ga(41)	120.5(5)
C(41)-N(41)-Ga(41)	107.3(5)	C(411)-N(41)-Ga(42)	125.4(5)
C(41)-N(41)-Ga(42)	99.1(4)	Ga(41)-N(41)-Ga(42)	92.4(2)
C(42)-N(42)-C(421)	119.6(7)	C(42)-N(42)-Ga(42)	104.6(6)
C(421)-N(42)-Ga(42)	135.4(6)	C(42)-C(41)-N(41)	117.1(7)
C(42)-C(41)-H(41)	121.5	N(41)-C(41)-H(41)	121.5
C(41)-C(42)-N(42)	124.8(8)	C(41)-C(42)-H(42)	117.6
N(42)-C(42)-H(42)	117.6	N(41)-C(411)-C(414)	110.8(9)
N(41)-C(411)-C(413)	110.2(8)	C(414)-C(411)-C(413)	108.3(8)
N(41)-C(411)-C(412)	106.0(8)	C(414)-C(411)-C(412)	110.4(9)
C(413)-C(411)-C(412)	111.1(10)	C(411)-C(412)-H(41A)	109.5
C(411)-C(412)-H(41B)	109.5	H(41A)-C(412)-H(41B)	109.5
C(411)-C(412)-H(41C)	109.5	H(41A)-C(412)-H(41C)	109.5
H(41B)-C(412)-H(41C)	109.5	C(411)-C(413)-H(41D)	109.5
C(411)-C(413)-H(41E)	109.5	H(41D)-C(413)-H(41E)	109.5
C(411)-C(413)-H(41F)	109.5	H(41D)-C(413)-H(41F)	109.5
H(41E)-C(413)-H(41F)	109.5	C(411)-C(414)-H(41G)	109.5
C(411)-C(414)-H(41H)	109.5	H(41G)-C(414)-H(41H)	109.5
C(411)-C(414)-H(41I)	109.5	H(41G)-C(414)-H(41I)	109.5
H(41H)-C(414)-H(41I)	109.5	N(42)-C(421)-C(422)	108.2(8)
N(42)-C(421)-C(423)	112.3(9)	C(422)-C(421)-C(423)	110.0(10)
N(42)-C(421)-C(424)	108.9(9)	C(422)-C(421)-C(424)	110.1(9)
C(423)-C(421)-C(424)	107.3(9)	C(421)-C(422)-H(42A)	109.5
C(421)-C(422)-H(42B)	109.5	H(42A)-C(422)-H(42B)	109.5
C(421)-C(422)-H(42C)	109.5	H(42A)-C(422)-H(42C)	109.5
H(42B)-C(422)-H(42C)	109.5	C(421)-C(424)-H(42D)	109.5
C(421)-C(424)-H(42E)	109.5	H(42D)-C(424)-H(42E)	109.5
C(421)-C(424)-H(42F)	109.5	H(42D)-C(424)-H(42F)	109.5
H(42E)-C(424)-H(42F)	109.5	C(421)-C(423)-H(42G)	109.5
C(421)-C(423)-H(42H)	109.5	H(42G)-C(423)-H(42H)	109.5
C(421)-C(423)-H(42I)	109.5	H(42G)-C(423)-H(42I)	109.5
H(42H)-C(423)-H(42I)	109.5		

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1.

The anisotropic displacement factor exponent takes the form:

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

	U11	U22	U33	U23	U13	U12
Ga(11)	38(1)	30(1)	41(1)	-1(1)	4(1)	3(1)
Ga(12)	25(1)	30(1)	30(1)	0(1)	5(1)	1(1)
Cl(11)	51(1)	53(1)	77(1)	3(1)	-2(1)	24(1)
Cl(12)	73(1)	39(1)	74(1)	0(1)	20(1)	-15(1)
N(11)	31(3)	32(3)	27(3)	1(2)	4(2)	2(2)
N(12)	25(3)	40(3)	36(3)	3(3)	4(2)	5(2)
N(13)	37(3)	31(3)	32(3)	-1(2)	6(2)	1(2)
N(14)	33(3)	39(3)	46(3)	0(3)	14(3)	-3(2)
C(11)	37(4)	37(4)	34(4)	5(3)	10(3)	-5(3)
C(12)	27(3)	46(4)	42(4)	-5(3)	5(3)	-1(3)
C(13)	37(4)	46(4)	48(5)	-3(4)	15(3)	9(3)
C(14)	24(4)	55(5)	57(5)	2(4)	11(3)	-3(3)
C(111)	36(4)	44(4)	29(4)	-1(3)	-1(3)	0(3)
C(112)	34(4)	61(5)	51(5)	-6(4)	-5(3)	-2(3)
C(113)	52(4)	51(4)	39(4)	-10(4)	0(3)	-2(4)
C(114)	57(5)	56(5)	43(4)	10(4)	-5(4)	4(4)
C(121)	36(4)	45(4)	55(5)	7(4)	10(3)	14(3)
C(122)	70(6)	49(5)	84(6)	-5(5)	25(5)	16(4)
C(123)	58(5)	70(6)	63(6)	24(5)	5(4)	22(4)
C(124)	35(4)	86(7)	85(6)	8(5)	-1(4)	11(4)
C(131)	49(4)	41(4)	41(4)	-14(3)	2(3)	7(3)
C(132)	44(4)	56(5)	47(4)	-13(4)	-6(3)	-6(4)
C(133)	68(5)	74(6)	38(5)	1(4)	6(4)	5(4)
C(134)	87(6)	52(5)	64(6)	-26(4)	4(5)	6(5)
C(141)	45(4)	40(4)	57(5)	4(4)	16(4)	-10(3)
C(142)	73(6)	83(6)	68(6)	31(5)	23(5)	1(5)
C(143)	45(5)	61(5)	115(8)	5(5)	7(5)	-23(4)
C(144)	55(5)	35(4)	72(5)	-9(4)	8(4)	-19(3)
Ga(21)	74(1)	29(1)	46(1)	2(1)	11(1)	12(1)
Ga(22)	33(1)	28(1)	36(1)	-3(1)	2(1)	3(1)
Cl(21)	116(2)	41(1)	65(1)	-15(1)	6(1)	-5(1)
Cl(22)	127(2)	52(1)	88(2)	22(1)	15(2)	41(1)
N(21)	102(6)	31(3)	62(4)	7(3)	42(4)	4(3)
N(22)	78(5)	27(3)	94(6)	8(3)	-51(4)	-3(3)
N(23)	38(3)	41(3)	72(5)	-19(3)	12(3)	3(3)
N(24)	48(3)	39(3)	48(4)	-5(3)	-6(3)	-9(3)
C(21)	70(6)	61(5)	59(6)	-1(4)	-23(4)	25(5)
C(22)	68(6)	68(6)	87(7)	3(5)	-4(5)	15(5)
C(23)	102(8)	65(6)	73(7)	-9(5)	2(6)	24(6)
C(24)	63(6)	83(7)	87(7)	1(6)	2(5)	0(5)
C(211)	67(6)	46(5)	114(8)	-9(5)	47(6)	-15(4)
C(212)	97(8)	117(9)	66(6)	-29(6)	-33(6)	42(7)
C(213)	75(6)	55(5)	62(5)	0(4)	15(4)	-26(4)
C(214)	45(4)	68(5)	77(6)	-6(5)	22(4)	-8(4)
C(221)	48(4)	39(4)	96(7)	23(4)	13(4)	11(4)
C(222)	78(6)	72(6)	93(7)	-3(6)	20(6)	1(5)
C(223)	115(9)	54(6)	168(12)	-2(7)	89(9)	3(6)
C(224)	258(17)	139(11)	44(6)	5(7)	-22(8)	120(12)

C(231)	133(10)	51(6)	144(11)	-5(6)	95(9)	9(6)
C(232)	88(7)	58(6)	87(7)	12(5)	40(5)	-9(5)
C(233)	98(8)	56(6)	107(8)	3(6)	-15(7)	1(5)
C(241)	51(5)	66(5)	66(6)	-29(5)	11(4)	-13(4)
C(242)	72(6)	73(6)	94(7)	-16(6)	29(5)	10(5)
C(243)	138(11)	74(8)	350(20)	-93(11)	159(14)	-57(8)
C(244)	125(10)	123(10)	72(7)	-33(7)	-20(7)	16(8)
Ga(31)	35(1)	31(1)	52(1)	-1(1)	11(1)	-2(1)
Ga(32)	28(1)	32(1)	46(1)	-2(1)	8(1)	-1(1)
Cl(31)	68(1)	41(1)	67(1)	-9(1)	25(1)	-1(1)
Cl(32)	58(1)	40(1)	74(1)	3(1)	21(1)	-12(1)
N(31)	31(3)	35(3)	48(3)	-3(3)	4(3)	-3(2)
N(32)	34(3)	39(3)	49(3)	-8(3)	9(3)	4(3)
N(33)	28(3)	35(3)	46(3)	1(3)	8(2)	-2(2)
N(34)	46(3)	35(3)	64(4)	4(3)	19(3)	-8(3)
C(31)	31(4)	46(4)	57(5)	-5(4)	12(3)	-4(3)
C(32)	32(4)	49(5)	59(5)	5(4)	17(4)	5(3)
C(33)	38(4)	41(4)	61(5)	-5(4)	20(4)	2(3)
C(34)	40(4)	43(4)	64(5)	0(4)	23(4)	-5(3)
C(311)	34(4)	49(4)	57(5)	-5(4)	-6(3)	-4(3)
C(312)	70(5)	61(5)	40(4)	0(4)	2(4)	-4(4)
C(313)	52(5)	55(5)	65(5)	-2(4)	-16(4)	16(4)
C(314)	64(5)	55(5)	77(6)	-21(5)	-9(5)	-7(4)
C(321)	47(4)	41(4)	46(4)	-6(3)	5(3)	11(3)
C(322)	55(5)	59(5)	65(5)	-23(4)	2(4)	3(4)
C(323)	98(7)	64(6)	59(5)	-13(5)	26(5)	11(5)
C(324)	54(5)	60(5)	75(6)	-3(5)	0(4)	26(4)
C(331)	34(4)	44(4)	53(4)	5(4)	5(3)	8(3)
C(332)	49(4)	62(5)	52(5)	9(4)	10(4)	6(4)
C(333)	34(4)	71(6)	69(6)	-1(5)	3(4)	-4(4)
C(334)	51(5)	63(5)	80(6)	9(5)	14(4)	23(4)
C(341)	61(5)	35(4)	76(6)	3(4)	19(4)	-8(4)
C(342)	58(5)	36(4)	77(6)	15(4)	8(4)	6(4)
C(343)	55(5)	43(5)	136(9)	-2(5)	9(5)	-13(4)
C(344)	101(7)	52(5)	95(7)	18(5)	45(6)	3(5)
Ga(41)	45(1)	33(1)	88(1)	0	8(1)	0
Ga(42)	39(1)	36(1)	52(1)	0	-3(1)	0
Cl(4)	88(2)	76(2)	188(3)	77(2)	-2(2)	-2(2)
N(41)	36(3)	39(3)	68(4)	0(3)	9(3)	0(3)
N(42)	80(5)	54(4)	60(5)	-13(4)	-20(4)	17(4)
C(41)	58(5)	54(5)	68(6)	-5(4)	-1(4)	8(4)
C(42)	83(7)	66(6)	72(6)	-3(5)	-14(5)	-1(5)
C(411)	52(5)	80(7)	134(10)	-3(7)	41(6)	-4(5)
C(412)	101(8)	141(11)	70(7)	-1(7)	29(6)	-12(8)
C(413)	55(6)	105(9)	161(11)	-16(8)	28(7)	34(6)
C(414)	56(6)	120(10)	152(11)	7(8)	24(7)	-33(6)
C(421)	86(7)	64(6)	95(8)	-33(6)	-26(6)	24(5)
C(422)	86(8)	81(8)	187(13)	-40(8)	-38(8)	23(6)
C(424)	99(9)	61(7)	183(13)	-22(8)	-47(9)	11(6)
C(423)	158(12)	134(11)	93(9)	-62(8)	2(8)	34(10)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H(11A)	2501	8859	1790	76
H(11B)	2562	7401	1927	76
H(11C)	2597	8484	2320	76
H(11D)	2025	9076	2319	73
H(11E)	2174	9886	2033	73
H(11F)	2272	9497	2560	73
H(11G)	2117	6804	2519	81
H(11H)	2363	7221	2765	81
H(11I)	2327	6142	2370	81
H(12A)	1587	10800	1433	100
H(12B)	1536	11776	1005	100
H(12C)	1787	11497	1259	100
H(12D)	1735	9776	193	97
H(12E)	1875	10884	495	97
H(12F)	1623	11139	244	97
H(12G)	1361	9147	941	106
H(12H)	1422	8738	457	106
H(12I)	1315	10114	510	106
H(13A)	1771	5760	623	76
H(13B)	1682	6049	83	76
H(13C)	1728	7206	447	76
H(13D)	2182	7423	-142	91
H(13E)	1979	8220	-18	91
H(13F)	1932	7064	-383	91
H(13G)	2254	5192	142	103
H(13H)	2006	4778	-92	103
H(13I)	2097	4541	451	103
H(14A)	2462	10717	222	110
H(14B)	2429	12131	408	110
H(14C)	2221	11188	278	110
H(14D)	2760	10360	925	112
H(14E)	2707	10525	1433	112
H(14F)	2720	11758	1117	112
H(14G)	2330	11169	1524	82
H(14H)	2141	11479	1078	82
H(14I)	2351	12408	1215	82
H(11)	1853(8)	6990(50)	1893(18)	16(14)
H(12)	1593(10)	8250(50)	1393(19)	30(16)
H(13)	2463(9)	6530(60)	578(19)	24(15)
H(14)	2601(13)	8610(80)	750(30)	70(30)
H(21)	1991	3013	3540	82
H(22)	2000	924	3861	93
H(23)	966	3040	2971	98
H(24)	966	1664	2367	96
H(21A)	1452	2368	2225	150
H(21B)	1571	3456	1979	150
H(21C)	1432	3838	2365	150
H(21D)	1770	4948	2822	96
H(21E)	1907	4553	2433	96

H(21F)	2004	4229	2968	96
H(21G)	1807	1187	2490	93
H(21H)	2027	1879	2761	93
H(21I)	1931	2214	2227	93
H(22A)	1773	-1701	3071	121
H(22B)	1896	-2583	3490	121
H(22C)	2007	-1261	3377	121
H(22D)	1438	-1633	3358	156
H(22E)	1435	-1264	3885	156
H(22F)	1547	-2578	3770	156
H(22G)	1796	-577	4404	231
H(22H)	2020	-616	4204	231
H(22I)	1900	-1923	4297	231
H(23A)	882	1177	3513	112
H(23B)	966	778	4045	112
H(23C)	1085	201	3652	112
H(23D)	1463	1052	4097	138
H(23E)	1349	1672	4490	138
H(23F)	1491	2549	4211	138
H(23G)	919	3412	3670	147
H(23H)	1145	4045	3942	147
H(23I)	999	3169	4215	147
H(24A)	1521	-599	2203	117
H(24B)	1377	-1873	2073	117
H(24C)	1472	-1522	2606	117
H(24D)	908	-777	2473	260
H(24E)	1106	-1594	2775	260
H(24F)	1008	-1979	2247	260
H(24G)	1227	654	1714	168
H(24H)	978	589	1799	168
H(24I)	1083	-620	1587	168
H(31A)	839	4119	1278	87
H(31B)	840	5609	1406	87
H(31C)	1016	4663	1710	87
H(31D)	1348	4109	854	92
H(31E)	1150	3197	939	92
H(31F)	1326	3736	1372	92
H(31G)	1343	6418	1047	103
H(31H)	1323	6079	1568	103
H(31I)	1145	7011	1261	103
H(32A)	701	1602	-277	91
H(32B)	735	1196	-784	91
H(32C)	598	2465	-718	91
H(32D)	1103	3694	-933	108
H(32E)	840	3717	-1112	108
H(32F)	978	2457	-1180	108
H(32G)	1270	2327	-254	97
H(32H)	1141	1113	-509	97
H(32I)	1111	1495	2	97
H(33A)	644	6852	-571	81
H(33B)	458	6323	-990	81
H(33C)	632	5355	-691	81
H(33D)	131	4687	-300	89
H(33E)	321	4036	-525	89
H(33F)	147	5001	-826	89
H(33G)	355	7859	-217	97
H(33H)	154	7023	-104	97
H(33I)	166	7343	-632	97
H(34A)	888	1718	962	87

H(34B)	808	1307	430	87
H(34C)	768	366	836	87
H(34D)	223	1546	386	119
H(34E)	365	258	495	119
H(34F)	403	1178	83	119
H(34G)	353	2196	1225	119
H(34H)	613	2260	1441	119
H(34I)	495	904	1315	119
H(31)	1216(13)	6070(80)	290(30)	70(30)
H(32)	1184(10)	4700(60)	-320(20)	34(17)
H(33)	288(13)	5760(80)	570(30)	70(30)
H(34)	322(11)	3900(60)	880(20)	40(20)
H(41)	422	5227	3252	74
H(42)	321	6967	3622	93
H(41A)	204	4998	1712	154
H(41B)	426	5633	1611	154
H(41C)	233	6521	1730	154
H(41D)	440	3620	2354	159
H(41E)	605	4299	2774	159
H(41F)	663	4276	2267	159
H(41G)	503	7522	2389	163
H(41H)	699	6634	2285	163
H(41I)	642	6652	2793	163
H(42A)	-263	9070	3067	190
H(42B)	-113	9815	2765	190
H(42C)	-155	10424	3240	190
H(42D)	408	9367	3538	187
H(42E)	256	10618	3518	187
H(42F)	298	9983	3047	187
H(42G)	180	8277	4011	197
H(42H)	-84	8159	3841	197
H(42I)	26	9522	3993	197

Figure 1. Asymmetric Unit of 1

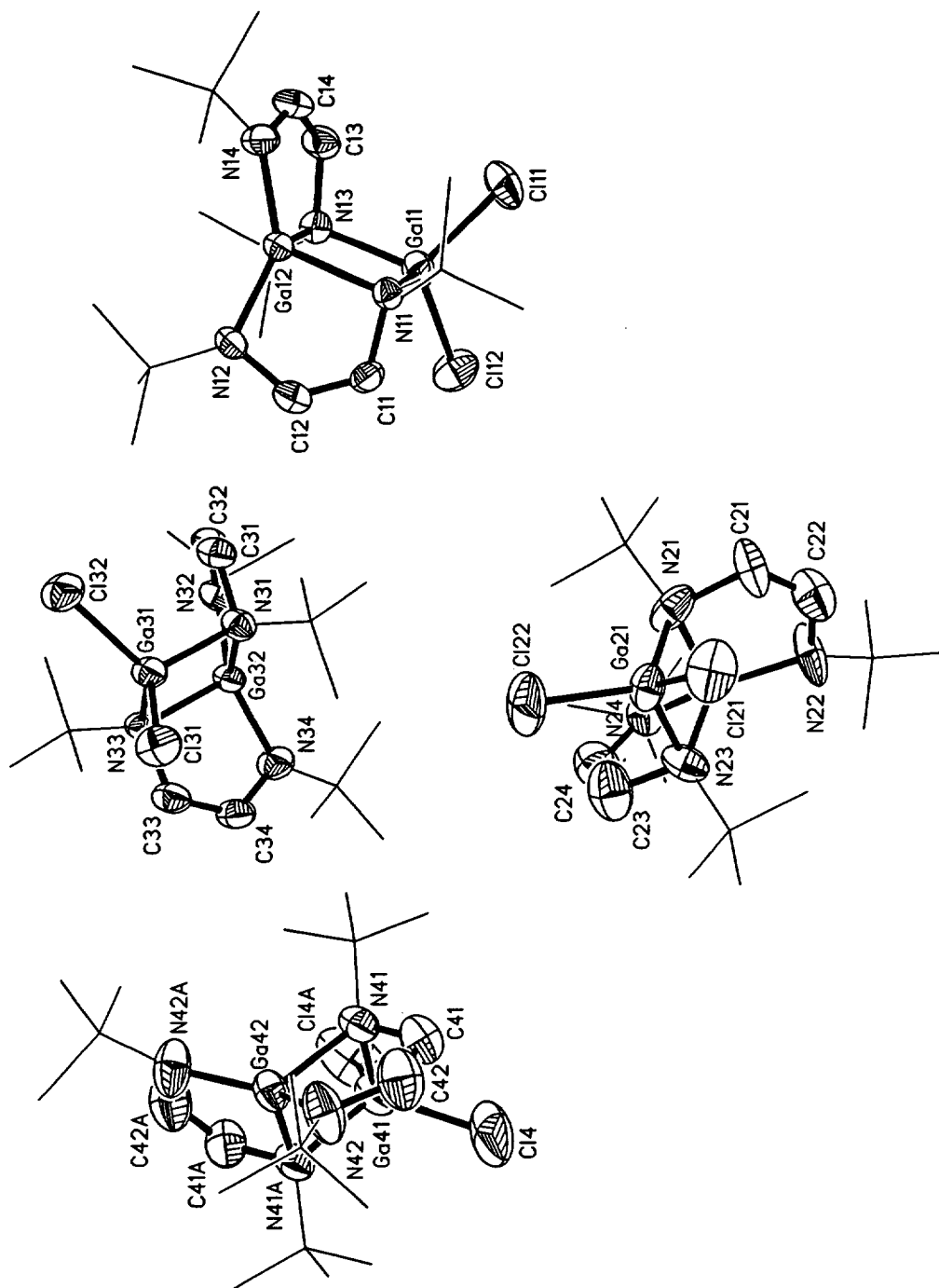


Table 6. Crystal Data, Data Collection and Structure Refinement for **3**.

<i>Crystal data</i>	
empirical formula	C ₃₀ H ₆₀ GaKN ₂ O ₈
formula weight	685.62
crystal system	triclinic
space group	$P\bar{1}$ (no. 2)
<i>a</i> , Å	9.718(2)
<i>b</i> , Å	10.116(2)
<i>c</i> , Å	10.318(2)
α , deg	77.67(2)
β , deg	69.64(2)
γ , deg	88.51(2)
<i>V</i> , Å ³	927.7(3)
ρ_{calcd} , g cm ⁻³	1.227
<i>Z</i>	1
F(000)	368
μ (Mo <i>K</i> α), cm ⁻¹	8.98
crystal dimensions, mm	0.3 × 0.3 × 0.4
<i>Data collection</i>	
temperature, K	143
scan mode	ω/θ
<i>hkl</i> range	-12→12; -13→13; -14→13
$\sin(\theta/\lambda)_{\text{max}}$, Å ⁻¹	0.64
measured reflns	8192
unique reflns	4122 (<i>R</i> _{int} = 0.0347)
reflns used for refinement	4122
<i>Refinement</i>	
least-squares parameters	315
restraints	72
final <i>R</i> values [<i>I</i> > 2σ(<i>I</i>)]:	
<i>R</i> 1 ^a	0.0336
<i>wR</i> 2 ^b	0.0751
goodness-of-fit on <i>F</i> ²	1.017
ρ_{fin} (max/min), e Å ⁻³	0.272/-0.421

^a $R1 = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|$; ^b $wR2 = \{[\Sigma w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (ap)^2 + bp]$; $p = (F_o^2 + 2F_c^2)/3$; $a = 0.0445$; $b = 0.0719$.

Restraints applied in the molecular structure of 3

Two models have been used to describe the disorder of the anion. Application of “soft” restraints led to a slightly asymmetric structure for the galla-heterocycle with distances Ga-N1 1.942(12), Ga-N2A 1.934(11) Å and N1-C1 1.428(14), N2A-C2A 1.434(13) Å. Because a molecular symmetry close to point group C_{2v} is chemically more reasonable, the following “hard” restraints have been applied:

1. Geometrical restraints: The distances of the following atoms are restrained to be equal (standard deviation 0 Å):

$$\begin{array}{llll}
 d(\text{Ga-N1}) & = & d(\text{Ga-N2A}) & \\
 d(\text{C1-N1}) & = & d(\text{C2-N2}) & \\
 d(\text{C31-C4}) & = & d(\text{C32A-C7A}) & \\
 d(\text{C31-C5}) & = & d(\text{C31-C6}) & = d(\text{C32A-C8A}) = d(\text{C32A-C9A}) \\
 d(\text{N1-C31}) & = & d(\text{N2-C32}) &
 \end{array}$$

2. Restraints on anisotropic displacement parameters: The components of the anisotropic displacement parameters of two bonded atoms along the line joining them are restrained to be equal with an effective standard deviation of 0.0001 Å (rigid-bond restraints).

Table 7. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 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	4696(1)	670(1)	1157(1)	28(1)
N(1)	4203(10)	632(9)	-548(9)	24(1)
N(2)	4004(10)	778(9)	-497(9)	25(1)
C(1)	4974(8)	-278(6)	-1294(6)	27(1)
C(2)	4103(4)	1043(4)	712(3)	25(1)
C(31)	3228(4)	1464(5)	-1151(7)	31(1)
C(4)	2485(5)	2425(4)	-172(4)	57(1)
C(5)	4073(4)	2344(4)	-2602(4)	43(1)
C(6)	2031(4)	616(4)	-1284(5)	53(1)
C(32)	2993(4)	1546(5)	-1102(7)	32(1)
C(7)	2983(6)	998(5)	-2377(5)	54(1)
C(8)	1430(4)	1414(5)	-35(4)	48(1)
C(9)	3499(5)	3039(3)	-1631(5)	48(1)
K	0	5000	5000	27(1)
O(1)	2261(1)	6437(1)	2634(1)	34(1)
O(2)	2211(1)	3597(1)	3319(1)	35(1)
O(3)	255(1)	2280(1)	6039(1)	35(1)
O(4)	-1637(2)	4330(2)	3532(2)	61(1)
C(11)	1903(2)	7722(2)	1974(2)	46(1)
C(12)	3050(2)	5668(2)	1640(2)	40(1)
C(13)	3494(2)	4412(2)	2414(2)	38(1)
C(14)	2544(2)	2421(2)	4168(2)	40(1)
C(15)	1158(2)	1584(2)	5017(2)	42(1)
C(16)	-1098(2)	1543(2)	6899(3)	45(1)
C(41)	-3044(3)	3643(3)	4196(3)	58(1)
C(42)	-3004(3)	2482(3)	3494(3)	67(1)
C(43)	-2061(6)	3212(6)	1963(5)	67(1)
C(43')	-1646(9)	2551(8)	2327(9)	62(2)
C(44)	-955(3)	4019(3)	2180(3)	65(1)

Table 8. Bond lengths [Å] and angles [°] for 3.

Ga-N(2)#1	1.984(6)	Ga-N(1)	1.985(6)
N(1)-C(1)	1.367(8)	N(1)-C(31)	1.463(3)
N(2)-C(2)	1.367(8)	N(2)-C(32)	1.462(3)
N(2)-Ga#1	1.984(6)	C(1)-C(2)#1	1.380(6)
C(1)-H(1)	1.01(3)	C(2)-C(1)#1	1.380(6)
C(2)-H(2)	0.86(3)	C(31)-C(6)	1.523(5)
C(31)-C(5)	1.524(5)	C(31)-C(4)	1.536(9)
C(4)-H(4A)	0.9800	C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800	C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800	C(5)-H(5C)	0.9800
C(6)-H(6A)	0.9800	C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800	C(32)-C(8)	1.523(5)
C(32)-C(9)	1.523(4)	C(32)-C(7)	1.536(9)
C(7)-H(7A)	0.9800	C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800	C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800	C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800	C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800	K-O(4)#2	2.7304(16)
K-O(4)	2.7304(16)	K-O(3)#2	2.7702(13)
K-O(3)	2.7702(13)	K-O(1)#2	2.7965(15)
K-O(1)	2.7965(15)	K-O(2)#2	2.8180(14)
K-O(2)	2.8180(14)	O(1)-C(12)	1.417(2)
O(1)-C(11)	1.427(2)	O(2)-C(14)	1.421(2)
O(2)-C(13)	1.422(2)	O(3)-C(15)	1.421(2)
O(3)-C(16)	1.424(2)	O(4)-C(44)	1.420(3)
O(4)-C(41)	1.420(3)	C(11)-C(16)#2	1.491(3)
C(11)-H(111)	0.97(2)	C(11)-H(112)	0.94(2)
C(12)-C(13)	1.489(3)	C(12)-H(121)	0.96(2)
C(12)-H(122)	0.97(2)	C(13)-H(131)	0.98(2)
C(13)-H(132)	1.02(2)	C(14)-C(15)	1.490(3)
C(14)-H(141)	0.98(2)	C(14)-H(142)	0.94(2)
C(15)-H(151)	0.97(2)	C(15)-H(152)	1.00(2)
C(16)-C(11)#2	1.491(3)	C(16)-H(161)	0.98(2)
C(16)-H(162)	0.98(2)	C(41)-C(42)	1.499(3)
C(41)-H(41A)	0.9900	C(41)-H(41B)	0.9900
C(42)-C(43')	1.435(8)	C(42)-C(43)	1.553(6)
C(42)-H(42A)	0.9900	C(42)-H(42B)	0.9900
C(43)-C(44)	1.471(5)	C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900	C(43')-C(44)	1.602(8)
C(43')-H(43C)	0.9900	C(43')-H(43D)	0.9900
C(44)-H(44A)	0.9900	C(44)-H(44B)	0.9900
N(2)#1-Ga-N(1)	81.8(3)	C(1)-N(1)-C(31)	116.4(6)
C(1)-N(1)-Ga	113.1(3)	C(31)-N(1)-Ga	130.4(5)
C(2)-N(2)-C(32)	118.2(5)	C(2)-N(2)-Ga#1	112.1(2)
C(32)-N(2)-Ga#1	129.7(5)	N(1)-C(1)-C(2)#1	115.5(5)
N(1)-C(1)-H(1)	123(2)	C(2)#1-C(1)-H(1)	121.9(19)
N(2)-C(2)-C(1)#1	117.5(3)	N(2)-C(2)-H(2)	122(2)
C(1)#1-C(2)-H(2)	121(2)	N(1)-C(31)-C(6)	112.3(5)
N(1)-C(31)-C(5)	111.8(5)	C(6)-C(31)-C(5)	108.7(5)
N(1)-C(31)-C(4)	108.4(5)	C(6)-C(31)-C(4)	108.3(4)
C(5)-C(31)-C(4)	107.1(4)	C(31)-C(4)-H(4A)	109.5
C(31)-C(4)-H(4B)	109.5	H(4A)-C(4)-H(4B)	109.5
C(31)-C(4)-H(4C)	109.5	H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5	C(31)-C(5)-H(5A)	109.5

C(31)-C(5)-H(5B)	109.5	H(5A)-C(5)-H(5B)	109.5
C(31)-C(5)-H(5C)	109.5	H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5	C(31)-C(6)-H(6A)	109.5
C(31)-C(6)-H(6B)	109.5	H(6A)-C(6)-H(6B)	109.5
C(31)-C(6)-H(6C)	109.5	H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5	N(2)-C(32)-C(8)	111.8(5)
N(2)-C(32)-C(9)	110.8(6)	C(8)-C(32)-C(9)	109.2(5)
N(2)-C(32)-C(7)	108.7(5)	C(8)-C(32)-C(7)	108.4(4)
C(9)-C(32)-C(7)	107.8(4)	C(32)-C(7)-H(7A)	109.5
C(32)-C(7)-H(7B)	109.5	H(7A)-C(7)-H(7B)	109.5
C(32)-C(7)-H(7C)	109.5	H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5	C(32)-C(8)-H(8A)	109.5
C(32)-C(8)-H(8B)	109.5	H(8A)-C(8)-H(8B)	109.5
C(32)-C(8)-H(8C)	109.5	H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5	C(32)-C(9)-H(9A)	109.5
C(32)-C(9)-H(9B)	109.5	H(9A)-C(9)-H(9B)	109.5
C(32)-C(9)-H(9C)	109.5	H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5	O(4)#2-K-O(4)	180.0
O(4)#2-K-O(3)#2	90.24(5)	O(4)-K-O(3)#2	89.76(5)
O(4)#2-K-O(3)	89.76(5)	O(4)-K-O(3)	90.24(5)
O(3)#2-K-O(3)	180.0	O(4)#2-K-O(1)#2	96.06(5)
O(4)-K-O(1)#2	83.94(5)	O(3)#2-K-O(1)#2	119.77(4)
O(3)-K-O(1)#2	60.23(4)	O(4)#2-K-O(1)	83.94(5)
O(4)-K-O(1)	96.06(5)	O(3)#2-K-O(1)	60.23(4)
O(3)-K-O(1)	119.77(4)	O(1)#2-K-O(1)	180.00(5)
O(4)#2-K-O(2)#2	84.55(5)	O(4)-K-O(2)#2	95.45(5)
O(3)#2-K-O(2)#2	61.19(4)	O(3)-K-O(2)#2	118.81(4)
O(1)#2-K-O(2)#2	59.98(4)	O(1)-K-O(2)#2	120.02(4)
O(4)#2-K-O(2)	95.45(5)	O(4)-K-O(2)	84.55(5)
O(3)#2-K-O(2)	118.81(4)	O(3)-K-O(2)	61.19(4)
O(1)#2-K-O(2)	120.02(4)	O(1)-K-O(2)	59.98(4)
O(2)#2-K-O(2)	180.0	C(12)-O(1)-C(11)	112.58(15)
C(12)-O(1)-K	115.31(10)	C(11)-O(1)-K	115.73(11)
C(14)-O(2)-C(13)	112.11(15)	C(14)-O(2)-K	110.77(11)
C(13)-O(2)-K	114.39(10)	C(15)-O(3)-C(16)	112.39(15)
C(15)-O(3)-K	114.79(11)	C(16)-O(3)-K	114.88(11)
C(44)-O(4)-C(41)	109.15(17)	C(44)-O(4)-K	121.05(14)
C(41)-O(4)-K	123.29(14)	O(1)-C(11)-C(16)#2	108.45(17)
O(1)-C(11)-H(111)	111.9(13)	C(16)#2-C(11)-H(111)	108.3(13)
O(1)-C(11)-H(112)	108.3(13)	C(16)#2-C(11)-H(112)	111.0(14)
H(111)-C(11)-H(112)	108.9(18)	O(1)-C(12)-C(13)	108.56(16)
O(1)-C(12)-H(121)	110.7(13)	C(13)-C(12)-H(121)	110.1(13)
O(1)-C(12)-H(122)	110.7(12)	C(13)-C(12)-H(122)	109.5(12)
H(121)-C(12)-H(122)	107.2(17)	O(2)-C(13)-C(12)	108.96(15)
O(2)-C(13)-H(131)	109.0(12)	C(12)-C(13)-H(131)	109.7(11)
O(2)-C(13)-H(132)	111.4(12)	C(12)-C(13)-H(132)	111.8(12)
H(131)-C(13)-H(132)	105.9(16)	O(2)-C(14)-C(15)	108.73(17)
O(2)-C(14)-H(141)	108.9(12)	C(15)-C(14)-H(141)	111.1(12)
O(2)-C(14)-H(142)	110.0(13)	C(15)-C(14)-H(142)	111.4(14)
H(141)-C(14)-H(142)	106.7(17)	O(3)-C(15)-C(14)	108.88(16)
O(3)-C(15)-H(151)	109.6(13)	C(14)-C(15)-H(151)	109.5(13)
O(3)-C(15)-H(152)	109.9(12)	C(14)-C(15)-H(152)	110.5(12)
H(151)-C(15)-H(152)	108.5(17)	O(3)-C(16)-C(11)#2	108.60(17)
O(3)-C(16)-H(161)	108.7(12)	C(11)#2-C(16)-H(161)	109.7(13)
O(3)-C(16)-H(162)	111.8(13)	C(11)#2-C(16)-H(162)	108.0(13)
H(161)-C(16)-H(162)	110.0(18)	O(4)-C(41)-C(42)	106.29(19)
O(4)-C(41)-H(41A)	110.5	C(42)-C(41)-H(41A)	110.5
O(4)-C(41)-H(41B)	110.5	C(42)-C(41)-H(41B)	110.5
H(41A)-C(41)-H(41B)	108.7	C(43')-C(42)-C(41)	110.2(4)

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C(43')-C(42)-C(43)	33.1(3)	C(41)-C(42)-C(43)	97.8(3)
C(43')-C(42)-H(42A)	128.2	C(41)-C(42)-H(42A)	112.2
C(43)-C(42)-H(42A)	112.2	C(43')-C(42)-H(42B)	79.2
C(41)-C(42)-H(42B)	112.2	C(43)-C(42)-H(42B)	112.2
H(42A)-C(42)-H(42B)	109.8	C(44)-C(43)-C(42)	103.0(3)
C(44)-C(43)-H(43A)	111.2	C(42)-C(43)-H(43A)	111.2
C(44)-C(43)-H(43B)	111.2	C(42)-C(43)-H(43B)	111.2
H(43A)-C(43)-H(43B)	109.1	C(42)-C(43')-C(44)	102.3(5)
C(42)-C(43')-H(43C)	111.3	C(44)-C(43')-H(43C)	111.3
C(42)-C(43')-H(43D)	111.3	C(44)-C(43')-H(43D)	111.3
H(43C)-C(43')-H(43D)	109.2	O(4)-C(44)-C(43)	106.1(3)
O(4)-C(44)-C(43')	104.9(3)	C(43)-C(44)-C(43')	32.1(3)
O(4)-C(44)-H(44A)	110.5	C(43)-C(44)-H(44A)	110.5
C(43')-C(44)-H(44A)	81.7	O(4)-C(44)-H(44B)	110.5
C(43)-C(44)-H(44B)	110.5	C(43')-C(44)-H(44B)	135.8
H(44A)-C(44)-H(44B)	108.7		

Symmetry transformations used to generate equivalent atoms:

. #1 -x+1,-y,-z #2 -x,-y+1,-z+1

Table 9. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 3.

The anisotropic displacement factor exponent takes the form:

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

	U11	U22	U33	U23	U13	U12
Ga	33(1)	26(1)	23(1)	-8(1)	-6(1)	0(1)
N(1)	24(2)	21(2)	25(1)	-3(1)	-7(1)	-1(1)
N(2)	25(2)	21(2)	26(1)	-3(1)	-7(1)	0(1)
C(1)	40(3)	16(3)	27(2)	-5(2)	-14(2)	0(1)
C(2)	26(2)	18(2)	30(1)	-8(1)	-6(1)	0(1)
C(31)	26(2)	27(2)	37(1)	1(1)	-11(1)	-1(1)
C(4)	57(3)	54(2)	60(2)	-17(2)	-21(2)	32(2)
C(5)	47(2)	35(2)	41(1)	10(1)	-20(1)	-7(1)
C(6)	36(2)	41(2)	84(3)	9(2)	-35(2)	-8(1)
C(32)	33(2)	22(2)	36(2)	2(1)	-13(1)	0(1)
C(7)	78(3)	49(2)	52(2)	-11(2)	-45(2)	14(3)
C(8)	25(1)	60(3)	52(2)	10(2)	-17(1)	1(2)
C(9)	53(2)	25(1)	61(3)	12(2)	-26(2)	-5(2)
K	28(1)	18(1)	30(1)	-4(1)	-6(1)	-4(1)
O(1)	31(1)	30(1)	33(1)	2(1)	-6(1)	-3(1)
O(2)	30(1)	33(1)	39(1)	-4(1)	-10(1)	0(1)
O(3)	34(1)	19(1)	46(1)	-2(1)	-10(1)	-4(1)
O(4)	56(1)	71(1)	70(1)	-31(1)	-29(1)	-8(1)
C(11)	38(1)	35(1)	49(1)	17(1)	-9(1)	-8(1)
C(12)	31(1)	49(1)	31(1)	-3(1)	-4(1)	-8(1)
C(13)	27(1)	44(1)	39(1)	-15(1)	-5(1)	0(1)
C(14)	42(1)	37(1)	42(1)	-12(1)	-16(1)	14(1)
C(15)	51(1)	24(1)	53(1)	-10(1)	-21(1)	5(1)
C(16)	37(1)	22(1)	67(2)	9(1)	-16(1)	-9(1)
C(41)	47(1)	66(2)	72(2)	-30(1)	-26(1)	9(1)
C(42)	55(2)	66(2)	91(2)	-36(2)	-28(1)	1(1)
C(43)	75(3)	79(4)	61(3)	-33(3)	-33(2)	8(3)
C(43')	67(5)	54(5)	70(5)	-27(4)	-21(4)	-4(4)
C(44)	67(2)	70(2)	56(2)	-16(1)	-18(1)	-6(1)

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

	x	y	z	U(eq)
H(1)	4840(40)	-420(30)	-2180(40)	24(9)
H(2)	3560(40)	1620(30)	1140(40)	21(8)
H(4A)	1883	3037	-597	85
H(4B)	3239	2957	-46	85
H(4C)	1859	1893	750	85
H(5A)	3389	2900	-2963	64
H(5B)	4566	1764	-3257	64
H(5C)	4808	2935	-2519	64
H(6A)	1439	1209	-1738	79
H(6B)	1400	134	-339	79
H(6C)	2484	-42	-1859	79
H(7A)	3982	1072	-3073	81
H(7B)	2335	1527	-2812	81
H(7C)	2625	46	-2059	81
H(8A)	1417	1759	788	72
H(8B)	1083	458	272	72
H(8C)	786	1939	-477	72
H(9A)	3520	3414	-837	71
H(9B)	2816	3532	-2045	71
H(9C)	4486	3132	-2351	71
H(111)	1280(20)	7630(20)	1440(20)	48(6)
H(112)	2780(30)	8200(20)	1350(20)	51(6)
H(121)	3900(20)	6180(20)	940(20)	47(6)
H(122)	2450(20)	5430(20)	1140(20)	36(5)
H(131)	4030(20)	4650(20)	2990(20)	38(5)
H(132)	4200(20)	3890(20)	1740(20)	47(6)
H(141)	3000(20)	2700(20)	4780(20)	40(5)
H(142)	3240(20)	1930(20)	3590(20)	47(6)
H(151)	650(20)	1440(20)	4400(20)	48(6)
H(152)	1380(20)	680(20)	5500(20)	48(6)
H(161)	-890(20)	640(20)	7330(20)	49(6)
H(162)	-1720(30)	1470(20)	6350(20)	50(6)
H(41A)	-3819	4259	4071	69
H(41B)	-3249	3307	5223	69
H(42A)	-3996	2187	3566	80
H(42B)	-2515	1700	3871	80
H(43A)	-1592	2551	1381	80
H(43B)	-2663	3800	1499	80
H(43C)	-1820	2480	1454	74
H(43D)	-1001	1827	2541	74
H(44A)	-75	3495	2155	78
H(44B)	-652	4860	1433	78

Figure 2. Molecular structure of the cation $[\text{K}(\text{18-crown-6})(\text{thf})_2]^+$ of **3** (ORTEP drawing with 50% probability ellipsoids).

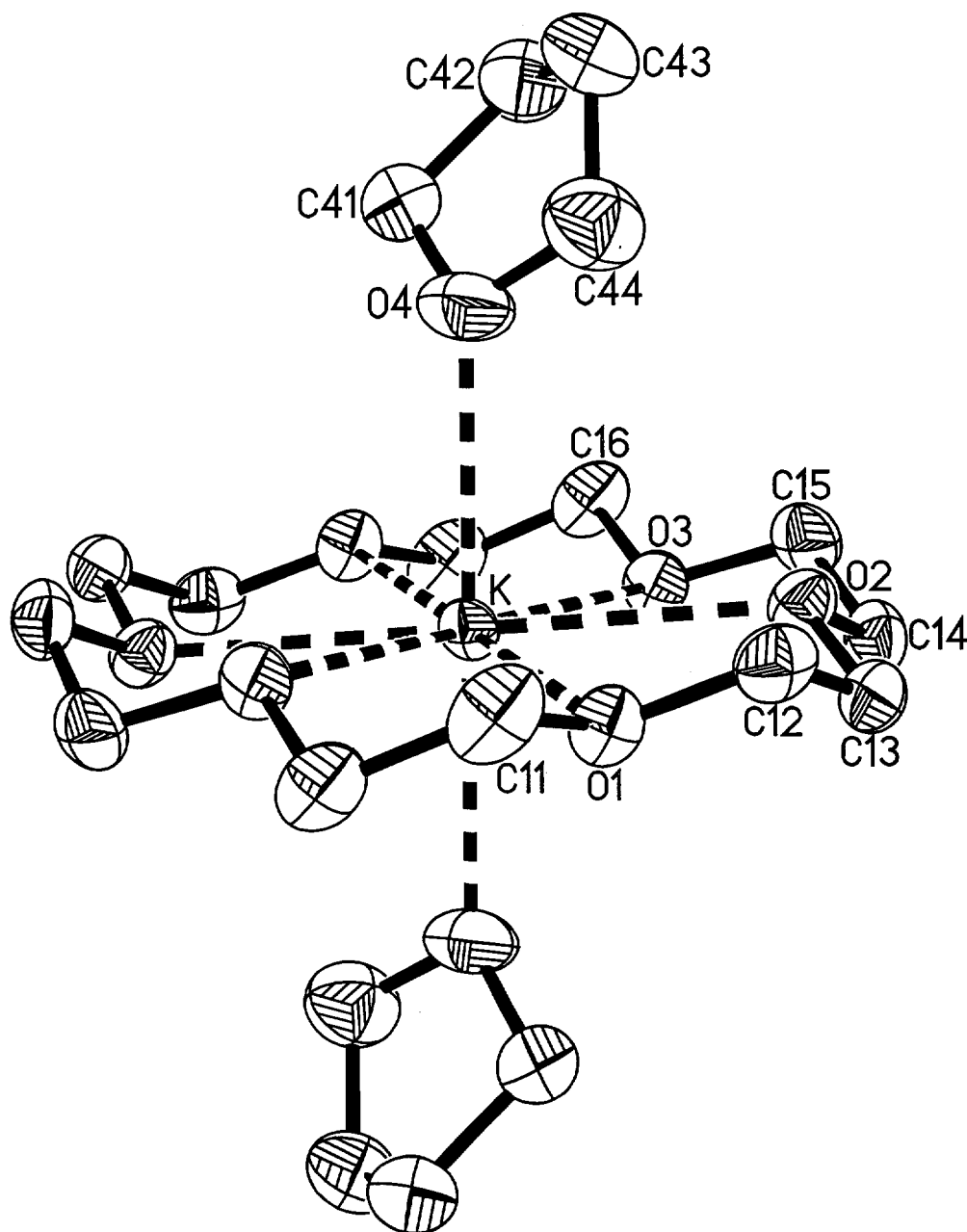
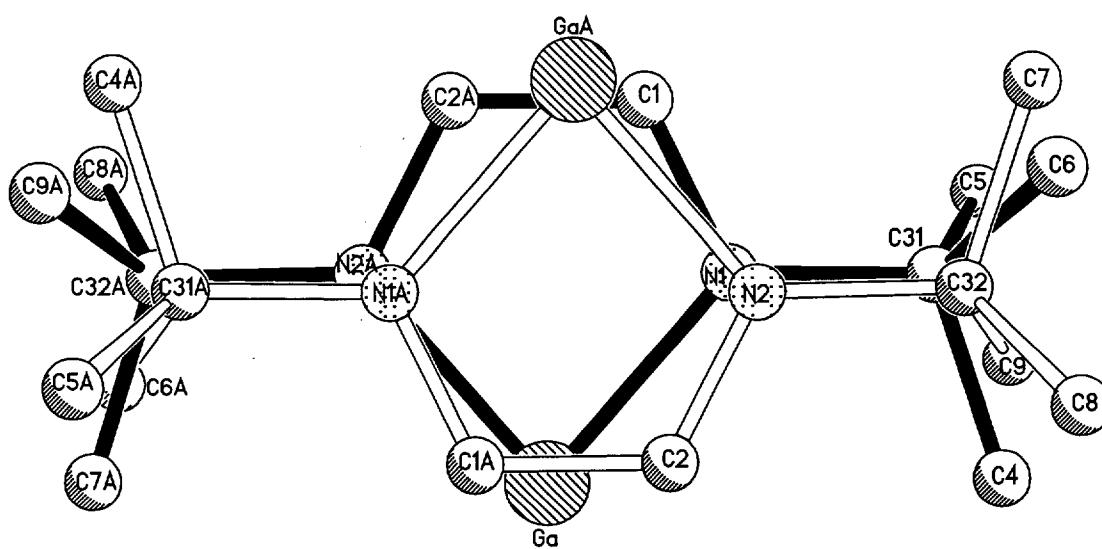
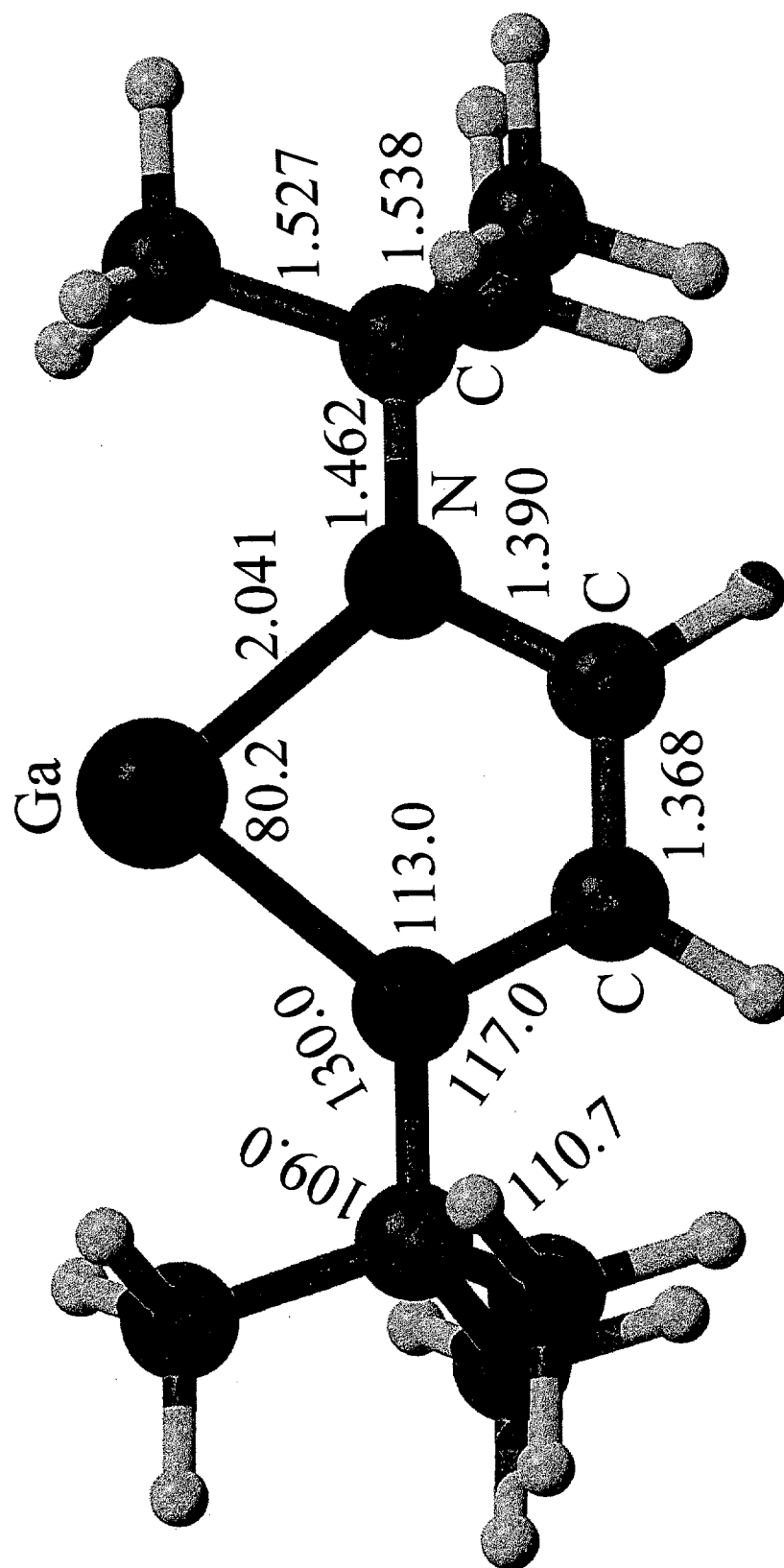


Figure 3. Split positions of the anion of **3**.



Å/°