

ORGANOMETALLICS

Organometallics, 1998, 17(2), 156-160, DOI:[10.1021/om970740p](https://doi.org/10.1021/om970740p)

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1998 American Chemical Society

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

	x	y	z	U(eq)
Al(1)	1440(1)	2400(1)	1954(1)	30(1)
Al(2)	887(1)	784(1)	2235(1)	38(1)
Al(3)	1911(1)	2357(1)	655(1)	49(1)
C(1)	1780(1)	3754(2)	2216(2)	43(1)
C(2)	865(1)	917(2)	3208(2)	50(1)
C(3)	546(2)	-506(3)	1645(2)	67(1)
C(4)	1767(2)	1404(3)	-215(3)	100(2)
C(5)	2724(2)	2279(4)	1631(3)	97(2)
C(6)	1647(2)	3749(3)	204(2)	64(1)
N(1)	1698(1)	1098(2)	2525(1)	33(1)
N(2)	1377(1)	1853(2)	1006(1)	37(1)
N(3)	617(1)	2047(2)	1541(1)	34(1)
O(1)	2095(1)	2837(2)	3997(1)	45(1)
O(2)	949(1)	3524(2)	3157(1)	50(1)
C(7)	2621(1)	2675(2)	4064(2)	39(1)
C(8)	3088(1)	3357(2)	4420(2)	49(1)
C(9)	3598(1)	3119(3)	4447(2)	55(1)
C(10)	3644(1)	2223(3)	4131(2)	55(1)
C(11)	3182(1)	1528(2)	3799(2)	47(1)
C(12)	2662(1)	1734(2)	3753(2)	36(1)
C(13)	2157(1)	978(2)	3410(2)	39(1)
C(14)	1882(1)	509(2)	2043(2)	43(1)
C(15)	1465(1)	721(2)	1151(2)	44(1)
C(16)	753(1)	2103(3)	374(2)	47(1)
C(17)	333(1)	1847(3)	649(2)	45(1)
C(18)	214(1)	2688(2)	1684(2)	40(1)
C(19)	333(1)	3825(2)	1771(2)	41(1)
C(20)	71(2)	4484(3)	1122(2)	62(1)
C(21)	189(2)	5528(3)	1227(3)	82(1)
C(22)	559(2)	5914(3)	1985(3)	78(1)
C(23)	824(2)	5284(2)	2653(2)	60(1)
C(24)	710(1)	4236(2)	2544(2)	45(1)
C(25)	1356(1)	3807(2)	3978(2)	48(1)
C(26)	1980(1)	3835(2)	4188(2)	45(1)

Table 2. Bond lengths [Å] and angles [°] for 1.

Al(1)-N(2)	1.928(3)	Al(1)-C(1)	1.932(3)
Al(1)-N(1)	1.953(2)	Al(1)-N(3)	1.968(2)
Al(2)-C(2)	1.967(4)	Al(2)-C(3)	1.972(3)
Al(2)-N(1)	1.990(2)	Al(2)-N(3)	2.016(2)
Al(3)-C(6)	1.982(4)	Al(3)-C(4)	1.987(4)
Al(3)-C(5)	1.993(4)	Al(3)-N(2)	2.023(2)
N(1)-C(14)	1.505(4)	N(1)-C(13)	1.508(4)
N(2)-C(16)	1.494(4)	N(2)-C(15)	1.503(4)
N(3)-C(17)	1.518(4)	N(3)-C(18)	1.520(3)
O(1)-C(7)	1.373(3)	O(1)-C(26)	1.440(3)
O(2)-C(24)	1.380(4)	O(2)-C(25)	1.433(4)
C(7)-C(8)	1.387(4)	C(7)-C(12)	1.408(4)
C(8)-C(9)	1.388(4)	C(9)-C(10)	1.367(5)
C(10)-C(11)	1.390(4)	C(11)-C(12)	1.387(4)
C(12)-C(13)	1.516(4)	C(14)-C(15)	1.519(4)
C(16)-C(17)	1.541(4)	C(18)-C(19)	1.512(4)
C(19)-C(20)	1.381(4)	C(19)-C(24)	1.407(4)
C(20)-C(21)	1.392(5)	C(21)-C(22)	1.371(6)
C(22)-C(23)	1.383(5)	C(23)-C(24)	1.396(4)
C(25)-C(26)	1.504(4)		
N(2)-Al(1)-C(1)	112.31(12)	N(2)-Al(1)-N(1)	93.10(11)
C(1)-Al(1)-N(1)	132.53(12)	N(2)-Al(1)-N(3)	91.55(10)
C(1)-Al(1)-N(3)	126.38(11)	N(1)-Al(1)-N(3)	90.25(10)
C(2)-Al(2)-C(3)	113.7(2)	C(2)-Al(2)-N(1)	108.4(2)
C(3)-Al(2)-N(1)	115.9(3)	C(2)-Al(2)-N(3)	113.8(2)
C(3)-Al(2)-N(3)	114.7(2)	N(1)-Al(2)-N(3)	87.82(9)
C(6)-Al(3)-C(4)	109.5(2)	C(6)-Al(3)-C(5)	114.9(2)
C(4)-Al(3)-C(5)	113.7(2)	C(6)-Al(3)-N(2)	107.72(13)
C(4)-Al(3)-N(2)	104.6(2)	C(5)-Al(3)-N(2)	105.6(2)
C(14)-N(1)-C(13)	109.6(2)	C(14)-N(1)-Al(1)	102.6(2)
C(13)-N(1)-Al(1)	125.0(2)	C(14)-N(1)-Al(2)	113.9(2)
C(13)-N(1)-Al(2)	113.4(2)	Al(1)-N(1)-Al(2)	91.20(9)
C(16)-N(2)-C(15)	111.4(2)	C(16)-N(2)-Al(1)	101.3(2)
C(15)-N(2)-Al(1)	105.0(2)	C(16)-N(2)-Al(3)	109.6(2)
C(15)-N(2)-Al(3)	108.6(2)	Al(1)-N(2)-Al(3)	120.75(12)
C(17)-N(3)-C(18)	110.6(2)	C(17)-N(3)-Al(1)	105.6(2)
C(18)-N(3)-Al(1)	124.0(2)	C(17)-N(3)-Al(2)	114.7(2)
C(18)-N(3)-Al(2)	110.8(2)	Al(1)-N(3)-Al(2)	90.00(10)
C(7)-O(1)-C(26)	118.4(2)	C(24)-O(2)-C(25)	121.8(2)
O(1)-C(7)-C(8)	124.2(3)	O(1)-C(7)-C(12)	114.6(2)
C(8)-C(7)-C(12)	121.2(3)	C(7)-C(8)-C(9)	119.2(3)
C(10)-C(9)-C(8)	120.8(3)	C(9)-C(10)-C(11)	119.6(3)
C(12)-C(11)-C(10)	121.7(3)	C(11)-C(12)-C(7)	117.3(3)
C(11)-C(12)-C(13)	122.5(3)	C(7)-C(12)-C(13)	120.1(2)
N(1)-C(13)-C(12)	115.3(2)	N(1)-C(14)-C(15)	110.5(2)
N(2)-C(15)-C(14)	110.1(2)	N(2)-C(16)-C(17)	112.0(2)
N(3)-C(17)-C(16)	111.6(2)	C(19)-C(18)-N(3)	115.8(2)
C(20)-C(19)-C(18)	118.4(3)	C(20)-C(19)-C(21)	122.6(3)
C(24)-C(19)-C(18)	119.0(3)	C(19)-C(20)-C(21)	120.9(4)
C(22)-C(21)-C(20)	119.8(4)	C(21)-C(22)-C(23)	121.2(4)
C(22)-C(23)-C(24)	118.8(3)	O(2)-C(24)-C(23)	124.7(3)
O(2)-C(24)-C(19)	114.5(3)	C(23)-C(24)-C(19)	120.8(3)
O(2)-C(25)-C(26)	112.2(2)	O(1)-C(26)-C(25)	106.0(2)

Symmetry transformations used to generate equivalent atoms:

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
Al(1)	27(1)	28(1)	35(1)	0(1)	16(1)	-1(1)
Al(2)	35(1)	34(1)	45(1)	-1(1)	22(1)	-6(1)
Al(3)	57(1)	49(1)	56(1)	5(1)	40(1)	1(1)
C(1)	48(2)	35(2)	48(2)	-1(1)	28(2)	-6(1)
C(2)	48(2)	52(2)	53(2)	11(2)	30(2)	1(2)
C(3)	70(2)	50(2)	87(3)	-16(2)	46(2)	-25(2)
C(4)	179(5)	69(3)	120(4)	-14(3)	124(4)	-8(3)
C(5)	55(2)	143(4)	97(3)	53(3)	44(2)	14(3)
C(6)	75(2)	55(2)	63(2)	8(2)	39(2)	-6(2)
N(1)	31(1)	28(1)	38(1)	1(1)	17(1)	2(1)
N(2)	38(1)	34(1)	39(1)	-1(1)	22(1)	0(1)
N(3)	27(1)	37(1)	35(1)	-2(1)	16(1)	0(1)
O(1)	41(1)	37(1)	60(1)	-2(1)	29(1)	-1(1)
O(2)	51(1)	41(1)	45(1)	1(1)	18(1)	6(1)
C(7)	28(1)	41(2)	37(2)	8(1)	11(1)	1(1)
C(8)	44(2)	40(2)	53(2)	1(2)	20(2)	-3(1)
C(9)	35(2)	51(2)	63(2)	8(2)	16(2)	-9(2)
C(10)	33(2)	62(2)	66(2)	9(2)	24(2)	5(2)
C(11)	39(2)	45(2)	51(2)	6(2)	21(2)	7(1)
C(12)	30(1)	36(2)	33(2)	6(1)	12(1)	1(1)
C(13)	35(2)	33(2)	43(2)	7(1)	16(1)	2(1)
C(14)	46(2)	29(1)	61(2)	2(1)	34(2)	5(1)
C(15)	54(2)	34(2)	55(2)	-9(1)	36(2)	-5(1)
C(16)	42(2)	58(2)	35(2)	-1(1)	17(1)	0(1)
C(17)	34(2)	57(2)	36(2)	-5(1)	14(1)	-6(1)
C(18)	27(1)	47(2)	46(2)	1(1)	20(1)	1(1)
C(19)	34(2)	42(2)	49(2)	5(1)	24(1)	10(1)
C(20)	63(2)	55(2)	58(2)	9(2)	27(2)	12(2)
C(21)	99(3)	60(3)	81(3)	32(2)	43(3)	23(2)
C(22)	99(3)	38(2)	103(3)	11(2)	59(3)	6(2)
C(23)	65(2)	40(2)	69(2)	-4(2)	33(2)	5(2)
C(24)	38(2)	40(2)	58(2)	5(2)	28(2)	10(1)
C(25)	54(2)	46(2)	44(2)	-5(1)	27(2)	2(2)
C(26)	51(2)	41(2)	41(2)	-3(1)	24(2)	0(1)

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

	x	y	z	U(eq)
H(1A)	1802(1)	3996(2)	2690(2)	64
H(1B)	1538(1)	4209(2)	1776(2)	64
H(1C)	2167(1)	3731(2)	2312(2)	64
H(2A)	1036(1)	1558(2)	3465(2)	74
H(2B)	1083(1)	367(2)	3571(2)	74
H(2C)	464(1)	889(2)	3062(2)	74
H(3A)	571(2)	-522(3)	1179(2)	101
H(3B)	142(2)	-551(3)	1481(2)	101
H(3C)	761(2)	-1073(3)	1989(2)	101
H(4A)	1894(2)	729(3)	3(3)	150
H(4B)	1982(2)	1629(3)	-444(3)	150
H(4C)	1354(2)	1391(3)	-625(3)	150
H(5A)	2815(2)	1582(4)	1808(3)	145
H(5B)	2749(2)	2691(4)	2050(3)	145
H(5C)	2998(2)	2527(4)	1504(3)	145
H(6A)	1717(2)	4209(3)	625(2)	96
H(6B)	1235(2)	3736(3)	-205(2)	96
H(6C)	1863(2)	3975(3)	-25(2)	96
H(8A)	3059(1)	3967(2)	4638(2)	58
H(9A)	3911(1)	3575(3)	4683(2)	66
H(10A)	3983(1)	2078(3)	4138(2)	66
H(11A)	3222(1)	909(2)	3603(2)	56
H(13A)	2318(1)	292(2)	3502(2)	47
H(13B)	1966(1)	1044(2)	3704(2)	47
H(14A)	1882(1)	-217(2)	2144(2)	52
H(14B)	2279(1)	704(2)	2211(2)	52
H(15A)	1627(1)	439(2)	857(2)	53
H(15B)	1090(1)	393(2)	958(2)	53
H(16A)	636(1)	1720(3)	-110(2)	56
H(16B)	722(1)	2825(3)	246(2)	56
H(17A)	-21(1)	2258(3)	346(2)	54
H(17B)	219(1)	1133(3)	536(2)	54
H(18A)	-188(1)	2577(2)	1240(2)	48
H(18B)	246(1)	2442(2)	2169(2)	48
H(20A)	-186(2)	4227(3)	608(2)	74
H(21A)	17(2)	5961(3)	784(3)	99
H(22A)	632(2)	6613(3)	2052(3)	93
H(23A)	1074(2)	5553(2)	3165(2)	71
H(25A)	1328(1)	3322(2)	4327(2)	57
H(25B)	1251(1)	4476(2)	4074(2)	57
H(26A)	2025(1)	4356(2)	3877(2)	54
H(26B)	2249(1)	3983(2)	4755(2)	54

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

	x	y	z	U(eq)
Al(1)	1931(2)	6364(1)	7102(1)	53(1)
Al(2)	278(2)	4748(1)	6488(1)	44(1)
C(1)	3589(6)	5830(4)	7567(4)	74(3)
C(2)	435(6)	6334(4)	7895(4)	69(2)
C(3)	2469(6)	7506(3)	6738(3)	75(3)
C(4)	1231(6)	4126(3)	7348(3)	66(2)
C(5)	-1681(5)	4836(4)	6674(3)	54(2)
N(1)	1299(4)	5700(3)	6094(3)	40(2)
N(2)	455(5)	4055(3)	5470(3)	39(1)
O(1)	-1560(4)	5479(2)	4676(2)	49(1)
O(2)	-1718(4)	3804(2)	4350(2)	50(1)
C(6)	-1908(7)	6138(3)	5189(3)	42(2)
C(7)	-3265(6)	6385(4)	5300(4)	56(2)
C(8)	-3528(7)	7030(4)	5830(4)	64(2)
C(9)	-2502(7)	7433(4)	6230(4)	69(3)
C(10)	-1155(7)	7167(4)	6101(4)	59(2)
C(11)	-840(6)	6512(4)	5604(4)	42(2)
C(12)	616(6)	6260(4)	5467(3)	44(2)
C(13)	2630(6)	5404(4)	5706(4)	62(2)
C(14)	2497(6)	4814(4)	4966(3)	56(2)
C(15)	1912(6)	3990(4)	5174(4)	53(2)
C(16)	-136(6)	3203(3)	5589(3)	50(2)
C(17)	-287(6)	2739(4)	4781(4)	44(2)
C(18)	411(7)	1990(4)	4644(4)	70(2)
C(19)	278(7)	1612(4)	3879(4)	69(2)
C(20)	-453(6)	1971(4)	3247(4)	64(2)
C(21)	-1151(6)	2711(4)	3389(4)	53(2)
C(22)	-1060(6)	3081(4)	4165(4)	41(2)
C(23)	-2033(7)	4399(3)	3725(3)	55(2)
C(24)	-2612(6)	5149(4)	4172(3)	55(2)

Table 2. Bond lengths [Å] and angles [°] for 2.

Al(1)-C(2)	1.962(6)	Al(1)-C(1)	1.995(6)
Al(1)-C(3)	2.007(5)	Al(1)-N(1)	2.060(5)
Al(2)-N(1)	1.945(5)	Al(2)-C(5)	1.958(6)
Al(2)-C(4)	1.965(6)	Al(2)-N(2)	2.011(5)
N(1)-C(12)	1.521(7)	N(1)-C(13)	1.533(7)
N(2)-C(16)	1.504(6)	N(2)-C(15)	1.517(7)
O(1)-C(6)	1.396(6)	O(1)-C(24)	1.426(6)
O(2)-C(22)	1.368(6)	O(2)-C(23)	1.435(6)
C(6)-C(11)	1.389(8)	C(6)-C(7)	1.406(8)
C(7)-C(8)	1.379(8)	C(8)-C(9)	1.367(9)
C(9)-C(10)	1.410(8)	C(10)-C(11)	1.368(8)
C(11)-C(12)	1.507(8)	C(13)-C(14)	1.543(7)
C(14)-C(15)	1.487(8)	C(16)-C(17)	1.524(8)
C(17)-C(22)	1.377(8)	C(17)-C(18)	1.408(8)
C(18)-C(19)	1.396(9)	C(19)-C(20)	1.386(9)
C(20)-C(21)	1.397(8)	C(21)-C(22)	1.404(8)
C(23)-C(24)	1.522(7)		
C(2)-Al(1)-C(1)	110.7(3)	C(2)-Al(1)-C(3)	114.6(3)
C(1)-Al(1)-C(3)	107.0(3)	C(2)-Al(1)-N(1)	106.7(2)
C(1)-Al(1)-N(1)	109.1(2)	C(3)-Al(1)-N(1)	108.6(2)
N(1)-Al(2)-C(5)	120.2(2)	N(1)-Al(2)-C(4)	113.1(2)
C(5)-Al(2)-C(4)	113.4(3)	N(1)-Al(2)-N(2)	96.9(2)
C(5)-Al(2)-N(2)	104.8(2)	C(4)-Al(2)-N(2)	105.4(2)
C(12)-N(1)-C(13)	106.5(4)	C(12)-N(1)-Al(2)	117.6(3)
C(13)-N(1)-Al(2)	109.4(4)	C(12)-N(1)-Al(1)	111.3(3)
C(13)-N(1)-Al(1)	103.5(3)	Al(2)-N(1)-Al(1)	107.6(2)
C(16)-N(2)-C(15)	110.1(4)	C(16)-N(2)-Al(2)	111.5(3)
C(15)-N(2)-Al(2)	112.6(3)	C(6)-O(1)-C(24)	116.9(4)
C(22)-O(2)-C(23)	121.1(4)	C(11)-C(6)-O(1)	115.9(5)
C(11)-C(6)-C(7)	122.3(6)	O(1)-C(6)-C(7)	121.8(6)
C(8)-C(7)-C(6)	118.3(6)	C(9)-C(8)-C(7)	121.3(6)
C(8)-C(9)-C(10)	118.6(6)	C(11)-C(10)-C(9)	122.5(7)
C(10)-C(11)-C(6)	116.9(6)	C(10)-C(11)-C(12)	120.8(6)
C(6)-C(11)-C(12)	122.1(5)	C(11)-C(12)-N(1)	118.7(5)
N(1)-C(13)-C(14)	116.3(4)	C(15)-C(14)-C(13)	113.8(5)
C(14)-C(15)-N(2)	112.2(5)	N(2)-C(16)-C(17)	112.0(5)
C(22)-C(17)-C(18)	119.8(6)	C(22)-C(17)-C(16)	119.3(5)
C(18)-C(17)-C(16)	120.8(6)	C(19)-C(18)-C(17)	118.1(6)
C(20)-C(19)-C(18)	122.2(6)	C(19)-C(20)-C(21)	119.3(6)
C(20)-C(21)-C(22)	118.8(6)	O(2)-C(22)-C(17)	116.3(5)
O(2)-C(22)-C(21)	122.0(6)	C(17)-C(22)-C(21)	121.7(6)
O(2)-C(23)-C(24)	105.7(4)	O(1)-C(24)-C(23)	107.5(5)

Symmetry transformations used to generate equivalent atoms:

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

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
Al(1)	53(1)	56(1)	49(1)	-4(1)	-8(1)	-4(1)
Al(2)	44(1)	45(1)	43(1)	5(1)	-3(1)	-4(1)
C(1)	62(5)	83(5)	77(5)	-5(5)	-28(4)	-10(5)
C(2)	85(5)	70(5)	53(4)	-12(4)	12(5)	-13(5)
C(3)	86(5)	69(5)	71(5)	0(4)	-16(5)	-40(5)
C(4)	81(5)	71(5)	47(4)	12(4)	-2(4)	-6(5)
C(5)	67(5)	48(4)	47(4)	4(4)	9(4)	-19(4)
N(1)	32(3)	46(3)	41(3)	9(3)	-2(3)	-7(3)
N(2)	47(3)	26(3)	45(3)	-5(2)	10(3)	-8(3)
O(1)	47(3)	51(3)	50(3)	-5(2)	-8(2)	2(2)
O(2)	66(3)	39(2)	44(3)	0(2)	1(3)	7(3)
C(6)	61(4)	35(4)	30(4)	3(3)	-1(4)	15(4)
C(7)	49(4)	62(5)	56(4)	-6(4)	-8(4)	10(4)
C(8)	64(5)	74(5)	55(5)	3(4)	3(4)	38(5)
C(9)	99(6)	52(5)	58(5)	-9(4)	-11(5)	32(5)
C(10)	79(5)	38(4)	60(5)	17(4)	-21(5)	-4(4)
C(11)	52(4)	36(4)	38(4)	11(3)	-7(4)	5(4)
C(12)	52(4)	47(4)	34(4)	-1(4)	0(4)	-7(4)
C(13)	27(4)	89(6)	68(5)	5(5)	4(4)	0(4)
C(14)	45(4)	73(5)	48(4)	-14(4)	13(4)	-5(4)
C(15)	49(4)	65(5)	46(4)	1(4)	-10(4)	-3(4)
C(16)	51(4)	51(4)	47(4)	-2(4)	-10(4)	-3(4)
C(17)	42(4)	42(4)	49(4)	3(4)	-12(4)	-6(4)
C(18)	69(5)	53(4)	87(6)	8(5)	-3(5)	14(5)
C(19)	57(5)	58(5)	93(6)	-31(5)	19(5)	2(4)
C(20)	53(5)	74(5)	64(5)	-17(4)	11(5)	-19(5)
C(21)	43(4)	66(5)	50(4)	-11(4)	4(4)	-1(4)
C(22)	43(4)	31(4)	48(4)	5(4)	6(4)	-3(4)
C(23)	73(5)	44(4)	47(4)	5(4)	-20(4)	3(4)
C(24)	51(4)	62(5)	53(4)	4(4)	-19(4)	7(4)

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

	x	y	z	U(eq)
H(1A)	4309 (6)	5850 (4)	7171 (4)	111
H(1B)	3393 (6)	5263 (4)	7700 (4)	111
H(1C)	3861 (6)	6120 (4)	8053 (4)	111
H(2A)	-353 (6)	6593 (4)	7661 (4)	104
H(2B)	696 (6)	6626 (4)	8382 (4)	104
H(2C)	228 (6)	5769 (4)	8029 (4)	104
H(3A)	3203 (6)	7468 (3)	6353 (3)	113
H(3B)	2755 (6)	7825 (3)	7204 (3)	113
H(3C)	1707 (6)	7773 (3)	6483 (3)	113
H(4A)	2183 (6)	4104 (3)	7223 (3)	100
H(4B)	874 (6)	3572 (3)	7376 (3)	100
H(4C)	1101 (6)	4397 (3)	7866 (3)	100
H(5A)	-2089 (5)	5145 (4)	6236 (3)	81
H(5B)	-1844 (5)	5115 (4)	7184 (3)	81
H(5C)	-2072 (5)	4291 (4)	6694 (3)	81
H(7A)	-3966 (6)	6120 (4)	5023 (4)	67
H(8A)	-4422 (7)	7195 (4)	5917 (4)	77
H(9A)	-2689 (7)	7873 (4)	6580 (4)	83
H(10A)	-454 (7)	7448 (4)	6363 (4)	71
H(12A)	1152 (6)	6763 (4)	5424 (3)	53
H(12B)	666 (6)	5984 (4)	4940 (3)	53
H(13A)	3160 (6)	5125 (4)	6125 (4)	74
H(13B)	3141 (6)	5888 (4)	5534 (4)	74
H(14A)	1927 (6)	5076 (4)	4556 (3)	67
H(14B)	3388 (6)	4733 (4)	4726 (3)	67
H(15A)	2461 (6)	3734 (4)	5598 (4)	64
H(15B)	1944 (6)	3636 (4)	4695 (4)	64
H(16A)	-1019 (6)	3252 (3)	5847 (3)	60
H(16B)	447 (6)	2887 (3)	5952 (3)	60
H(18A)	946 (7)	1753 (4)	5051 (4)	84
H(19A)	694 (7)	1102 (4)	3790 (4)	83
H(20A)	-478 (6)	1722 (4)	2733 (4)	77
H(21A)	-1667 (6)	2955 (4)	2977 (4)	63
H(23A)	-2694 (7)	4175 (3)	3344 (3)	66
H(23B)	-1222 (7)	4551 (3)	3423 (3)	66
H(24A)	-2914 (6)	5563 (4)	3781 (3)	66
H(24B)	-3382 (6)	4984 (4)	4505 (3)	66

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

	x	y	z	U(eq)
Ga(1)	3031(1)	2049(1)	5446(1)	58(1)
Ga(2)	4772(1)	711(1)	3435(1)	53(1)
O(1)	3582(4)	398(4)	6131(3)	58(1)
O(2)	4197(4)	1890(3)	4210(3)	57(1)
C(1)	1143(7)	2487(7)	5343(6)	90(2)
C(2)	3567(8)	3005(7)	6010(6)	95(3)
C(3)	3455(7)	-109(7)	3857(5)	75(2)
C(4)	5240(7)	1478(6)	2053(4)	68(2)
O(3)	8074(4)	2008(4)	758(3)	66(1)
O(4)	6117(4)	4398(4)	953(3)	63(1)
C(5)	9452(6)	1509(6)	516(5)	56(2)
C(6)	10209(7)	2012(6)	-292(5)	66(2)
C(7)	11588(7)	1441(7)	-472(5)	73(2)
C(8)	12220(7)	373(7)	144(6)	78(2)
C(9)	11424(7)	-114(6)	956(5)	67(2)
C(10)	10049(6)	434(6)	1152(5)	55(2)
C(11)	9195(7)	-126(6)	2018(5)	64(2)
C(12)	9635(7)	573(6)	3256(5)	68(2)
C(13)	8988(7)	1346(7)	3978(6)	76(2)
C(14)	7087(9)	3173(7)	4238(6)	86(2)
C(15)	6001(8)	4185(6)	3746(5)	73(2)
C(16)	4378(7)	4699(6)	2703(5)	66(2)
C(17)	4796(7)	5720(6)	1995(5)	59(2)
C(18)	4345(8)	6849(7)	2201(6)	78(2)
C(19)	4755(9)	7783(7)	1554(7)	84(2)
C(20)	5622(8)	7580(7)	693(7)	80(2)
C(21)	6085(7)	6469(6)	472(5)	69(2)
C(22)	5693(6)	5531(6)	1119(5)	57(2)
C(23)	7027(6)	4150(6)	54(5)	65(2)
C(24)	7309(6)	2862(6)	44(5)	61(2)
N(1)	8622(5)	490(5)	2836(4)	59(1)
N(2)	8123(6)	2530(5)	3547(4)	74(2)
N(3)	5398(5)	3732(5)	3231(4)	59(1)
C(25)	10570(15)	4656(12)	2756(7)	135(4)
C(26)	11422(10)	3595(12)	2524(10)	124(4)
C(27)	11239(13)	3188(10)	1842(10)	129(4)
C(28)	10189(19)	3876(15)	1359(9)	165(7)
C(29)	9335(13)	4950(14)	1574(12)	167(8)
C(30)	9537(13)	5339(9)	2272(10)	141(5)

Table 2. Bond lengths [Å] and angles [°] for 3.

Ga(1)-O(1)	1.910(4)	Ga(1)-O(2)	1.917(4)
Ga(1)-C(2)	1.956(7)	Ga(1)-C(1)	1.967(7)
Ga(2)-O(2)	1.914(4)	Ga(2)-O(1)#1	1.921(4)
Ga(2)-C(3)	1.957(6)	Ga(2)-C(4)	1.973(6)
O(1)-Ga(2)#1	1.921(4)	O(3)-C(5)	1.379(7)
O(3)-C(24)	1.420(7)	O(4)-C(22)	1.364(7)
O(4)-C(23)	1.446(7)	C(5)-C(6)	1.380(9)
C(5)-C(10)	1.398(8)	C(6)-C(7)	1.384(9)
C(7)-C(8)	1.389(9)	C(8)-C(9)	1.399(9)
C(9)-C(10)	1.378(9)	C(10)-C(11)	1.517(9)
C(11)-N(1)	1.466(8)	C(12)-N(1)	1.460(7)
C(12)-C(13)	1.475(9)	C(13)-N(2)	1.452(8)
C(14)-N(2)	1.441(9)	C(14)-C(15)	1.500(9)
C(15)-N(3)	1.464(8)	C(16)-N(3)	1.460(8)
C(16)-C(17)	1.514(9)	C(17)-C(18)	1.379(9)
C(17)-C(22)	1.402(9)	C(18)-C(19)	1.398(9)
C(19)-C(20)	1.375(9)	C(20)-C(21)	1.366(9)
C(21)-C(22)	1.393(8)	C(23)-C(24)	1.499(9)
C(25)-C(30)	1.349(8)	C(25)-C(26)	1.352(8)
C(26)-C(27)	1.332(8)	C(27)-C(28)	1.362(9)
C(28)-C(29)	1.356(9)	C(29)-C(30)	1.348(9)
O(1)-Ga(1)-O(2)	99.6(2)	O(1)-Ga(1)-C(2)	110.1(3)
O(2)-Ga(1)-C(2)	106.7(3)	O(1)-Ga(1)-C(1)	106.0(3)
O(2)-Ga(1)-C(1)	111.5(3)	C(2)-Ga(1)-C(1)	120.9(3)
O(2)-Ga(2)-O(1)#1	102.1(2)	O(2)-Ga(2)-C(3)	106.8(2)
O(1)#1-Ga(2)-C(3)	108.4(3)	O(2)-Ga(2)-C(4)	108.7(2)
O(1)#1-Ga(2)-C(4)	107.4(2)	C(3)-Ga(2)-C(4)	121.8(3)
Ga(1)-O(1)-Ga(2)#1	133.5(2)	Ga(2)-O(2)-Ga(1)	132.6(2)
C(5)-O(3)-C(24)	120.3(5)	C(22)-O(4)-C(23)	118.4(5)
O(3)-C(5)-C(6)	123.6(6)	O(3)-C(5)-C(10)	115.1(5)
C(6)-C(5)-C(10)	121.4(6)	C(5)-C(6)-C(7)	119.2(7)
C(6)-C(7)-C(8)	121.2(7)	C(7)-C(8)-C(9)	118.2(6)
C(10)-C(9)-C(8)	121.8(6)	C(9)-C(10)-C(5)	118.2(6)
C(9)-C(10)-C(11)	121.2(6)	C(5)-C(10)-C(11)	120.6(5)
N(1)-C(11)-C(10)	116.0(5)	N(1)-C(12)-C(13)	110.4(6)
N(2)-C(13)-C(12)	111.1(6)	N(2)-C(14)-C(15)	111.5(6)
N(3)-C(15)-C(14)	110.9(6)	N(3)-C(16)-C(17)	116.8(5)
C(18)-C(17)-C(22)	118.0(6)	C(18)-C(17)-C(16)	121.5(7)
C(22)-C(17)-C(16)	120.6(6)	C(17)-C(18)-C(19)	121.2(8)
C(20)-C(19)-C(18)	119.8(7)	C(21)-C(20)-C(19)	120.2(8)
C(20)-C(21)-C(22)	120.4(8)	O(4)-C(22)-C(21)	123.8(6)
O(4)-C(22)-C(17)	115.7(5)	C(21)-C(22)-C(17)	120.5(6)
O(4)-C(23)-C(24)	107.6(5)	O(3)-C(24)-C(23)	113.7(5)
C(12)-N(1)-C(11)	113.4(5)	C(14)-N(2)-C(13)	114.8(6)
C(16)-N(3)-C(15)	112.5(5)	C(30)-C(25)-C(26)	120.0(9)
C(27)-C(26)-C(25)	121.1(9)	C(26)-C(27)-C(28)	118.8(9)
C(29)-C(28)-C(27)	120.9(9)	C(30)-C(29)-C(28)	119.3(9)
C(29)-C(30)-C(25)	120.0(9)		

Symmetry transformations used to generate equivalent atoms:

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

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

The anisotropic displacement factor exponent takes the form:

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

	U11	U22	U33	U23	U13	U12
Ga(1)	57(1)	55(1)	58(1)	-11(1)	-2(1)	-23(1)
Ga(2)	51(1)	61(1)	49(1)	-7(1)	-5(1)	-29(1)
O(1)	53(2)	64(3)	57(3)	-2(2)	-7(2)	-30(2)
O(2)	67(3)	55(3)	47(2)	-4(2)	-6(2)	-29(2)
C(1)	64(5)	94(6)	89(6)	-6(5)	-9(4)	-16(4)
C(2)	101(6)	85(6)	104(6)	-46(5)	12(5)	-39(5)
C(3)	62(4)	92(5)	89(5)	-28(4)	-3(4)	-44(4)
C(4)	64(4)	88(5)	46(4)	-5(3)	-1(3)	-33(4)
O(3)	46(3)	73(3)	58(3)	5(2)	-7(2)	-14(2)
O(4)	62(3)	55(3)	62(3)	-3(2)	-2(2)	-22(2)
C(5)	46(4)	60(4)	62(4)	-16(3)	-4(3)	-19(3)
C(6)	61(4)	73(5)	64(4)	-10(4)	-7(3)	-30(4)
C(7)	60(5)	96(6)	67(5)	-22(4)	7(4)	-39(4)
C(8)	50(4)	79(5)	97(6)	-28(5)	-2(4)	-16(4)
C(9)	62(5)	55(4)	78(5)	-6(4)	-15(4)	-19(4)
C(10)	48(4)	53(4)	66(4)	-15(3)	-11(3)	-16(3)
C(11)	59(4)	57(4)	77(5)	-3(4)	-17(4)	-25(3)
C(12)	63(4)	84(5)	62(4)	5(4)	-21(4)	-37(4)
C(13)	75(5)	88(6)	76(5)	-7(4)	-24(4)	-38(4)
C(14)	122(7)	80(5)	69(5)	-6(4)	-25(5)	-51(5)
C(15)	97(6)	68(5)	63(5)	-16(4)	-18(4)	-34(4)
C(16)	58(4)	71(5)	72(5)	-15(4)	-3(4)	-29(4)
C(17)	61(4)	51(4)	66(4)	-4(3)	-21(4)	-20(3)
C(18)	84(5)	64(5)	87(5)	-16(4)	-27(4)	-20(4)
C(19)	96(6)	52(5)	114(7)	-9(5)	-51(6)	-19(4)
C(20)	75(5)	64(5)	108(7)	6(5)	-45(5)	-29(4)
C(21)	58(4)	63(5)	85(5)	7(4)	-27(4)	-27(4)
C(22)	50(4)	58(4)	66(4)	0(3)	-26(3)	-23(3)
C(23)	50(4)	74(5)	58(4)	-1(3)	-8(3)	-20(3)
C(24)	53(4)	73(5)	54(4)	-9(3)	-9(3)	-23(3)
N(1)	59(3)	58(3)	62(3)	-3(3)	-14(3)	-29(3)
N(2)	82(4)	76(4)	73(4)	-4(3)	-11(3)	-47(4)
N(3)	70(4)	58(3)	57(3)	-13(3)	-7(3)	-31(3)
C(25)	196(14)	122(9)	98(8)	-17(8)	-38(9)	-65(9)
C(26)	92(8)	125(9)	137(9)	9(8)	-45(7)	-31(7)
C(27)	124(9)	128(9)	119(9)	-40(9)	54(7)	-67(9)
C(28)	238(21)	232(19)	103(9)	-6(13)	-41(13)	-176(16)
C(29)	126(12)	221(19)	155(15)	83(13)	-95(12)	-103(12)
C(30)	112(10)	100(8)	124(10)	27(8)	19(7)	-10(7)

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

	x	y	z	U(eq)
H(1D)	2971(4)	90(4)	6274(3)	69
H(2D)	4521(4)	2454(3)	3957(3)	68
H(1C)	813(7)	3314(7)	5002(6)	135
H(1B)	615(7)	2387(7)	5986(6)	135
H(1A)	1080(7)	1974(7)	4990(6)	135
H(2C)	3286(8)	3832(7)	5661(6)	142
H(2B)	4526(8)	2696(7)	5959(6)	142
H(2A)	3152(8)	2956(7)	6685(6)	142
H(3C)	3707(7)	-711(7)	3485(5)	113
H(3B)	2584(7)	469(7)	3755(5)	113
H(3A)	3426(7)	-488(7)	4539(5)	113
H(4A)	5531(7)	895(6)	1656(4)	102
H(4B)	5951(7)	1774(6)	1983(4)	102
H(4C)	4466(7)	2138(6)	1847(4)	102
H(6A)	9797(7)	2726(6)	-710(5)	79
H(7A)	12101(7)	1779(7)	-1015(5)	88
H(8A)	13147(7)	-8(7)	20(6)	93
H(9A)	11834(7)	-828(6)	1374(5)	80
H(11A)	8463(7)	-154(6)	1788(5)	77
H(11B)	9741(7)	-953(6)	2261(5)	77
H(12A)	10240(7)	908(6)	2740(5)	82
H(12B)	10158(7)	-228(6)	3571(5)	82
H(13A)	8461(7)	964(7)	4528(6)	92
H(13B)	9674(7)	1435(7)	4218(6)	92
H(14A)	7481(9)	3498(7)	4564(6)	103
H(14B)	6699(9)	2617(7)	4731(6)	103
H(15A)	5313(8)	4589(6)	4231(5)	88
H(15B)	6376(8)	4771(6)	3284(5)	88
H(16A)	3617(7)	5042(6)	3180(5)	80
H(16B)	4070(7)	4343(6)	2342(5)	80
H(18A)	3758(8)	6992(7)	2782(6)	94
H(19A)	4442(9)	8538(7)	1705(7)	101
H(20A)	5894(8)	8200(7)	260(7)	97
H(21A)	6665(7)	6339(6)	-114(5)	83
H(23A)	7855(6)	4271(6)	23(5)	78
H(23B)	6622(6)	4688(6)	-505(5)	78
H(24A)	6461(6)	2737(6)	154(5)	73
H(24B)	7789(6)	2719(6)	-598(5)	73
H(1A)	8095(5)	1248(5)	2609(4)	70
H(2A)	8636(6)	2981(5)	3206(4)	88
H(3A)	6055(5)	3358(5)	2788(4)	71
H(25A)	10695(15)	4915(12)	3249(7)	162
H(26A)	12148(10)	3142(12)	2847(10)	149
H(27A)	11817(13)	2448(10)	1697(10)	155
H(28A)	10057(19)	3605(15)	876(9)	197
H(29A)	8618(13)	5412(14)	1244(12)	201
H(30A)	8965(13)	6079(9)	2419(10)	170

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

	x	y	z	$U(\text{eq})$
Ga(1)	541(1)	5439(1)	3718(1)	50(1)
Ga(2)	-2916(1)	4428(1)	3675(1)	57(1)
Ga(3)	-2161(1)	5926(1)	2636(1)	51(1)
O(1)	-839(4)	4563(2)	3917(2)	70(1)
O(2)	-2699(4)	4830(2)	2872(1)	54(1)
O(3)	-871(4)	6123(2)	3321(1)	50(1)
C(1)	1919(7)	5006(4)	3108(3)	79(2)
C(2)	1160(8)	5957(4)	4482(3)	82(2)
C(3)	-3276(8)	3229(4)	3674(3)	83(2)
C(4)	-4093(7)	5220(4)	4127(3)	90(2)
C(5)	-929(7)	5833(4)	1901(2)	73(2)
C(6)	-3834(7)	6692(4)	2727(3)	86(2)
O(4)	173(4)	8597(2)	4858(1)	55(1)
O(5)	2881(4)	9301(2)	4438(2)	54(1)
N(1)	-805(5)	7821(3)	3654(2)	49(1)
N(2)	2653(5)	8719(2)	3114(2)	46(1)
C(7)	-793(6)	8002(3)	5067(2)	51(1)
C(8)	-700(7)	7643(4)	5636(3)	68(2)
C(9)	-1749(9)	7067(4)	5806(3)	90(2)
C(10)	-2859(9)	6850(5)	5423(4)	98(3)
C(11)	-2971(7)	7208(4)	4857(3)	78(2)
C(12)	-1931(6)	7789(3)	4667(2)	52(1)
C(13)	-1984(6)	8164(3)	4048(2)	60(2)
C(14)	-666(6)	8293(3)	3095(2)	62(2)
C(15)	539(7)	7936(4)	2685(2)	67(2)
C(16)	2085(6)	7896(3)	2961(2)	59(2)
C(17)	4151(6)	8697(3)	3409(2)	54(1)
C(18)	4552(5)	9535(3)	3646(2)	47(1)
C(19)	5554(6)	10048(4)	3349(3)	65(2)
C(20)	5826(7)	10835(4)	3546(3)	76(2)
C(21)	5091(7)	11137(4)	4042(3)	75(2)
C(22)	4086(6)	10644(3)	4356(3)	58(2)
C(23)	3834(5)	9846(3)	4160(2)	50(1)
C(24)	2138(6)	9579(3)	4968(2)	55(1)
C(25)	1362(6)	8865(4)	5244(2)	60(2)

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

Ga(1)-O(3)	1.892(3)	Ga(1)-O(1)	1.927(4)
Ga(1)-C(1)	1.957(5)	Ga(1)-C(2)	1.962(6)
Ga(2)-O(2)	1.899(3)	Ga(2)-C(4)	1.935(6)
Ga(2)-O(1)	1.945(4)	Ga(2)-C(3)	1.960(6)
Ga(3)-O(2)	1.905(3)	Ga(3)-O(3)	1.928(3)
Ga(3)-C(6)	1.952(6)	Ga(3)-C(5)	1.969(5)
O(4)-C(7)	1.372(6)	O(4)-C(25)	1.429(6)
O(5)-C(23)	1.370(6)	O(5)-C(24)	1.422(6)
N(1)-C(14)	1.457(6)	N(1)-C(13)	1.477(6)
N(2)-C(16)	1.461(6)	N(2)-C(17)	1.490(6)
C(7)-C(8)	1.386(7)	C(7)-C(12)	1.390(7)
C(8)-C(9)	1.373(8)	C(9)-C(10)	1.350(10)
C(10)-C(11)	1.381(9)	C(11)-C(12)	1.386(8)
C(12)-C(13)	1.496(7)	C(14)-C(15)	1.523(7)
C(15)-C(16)	1.512(8)	C(17)-C(18)	1.492(7)
C(18)-C(19)	1.386(7)	C(18)-C(23)	1.400(7)
C(19)-C(20)	1.364(9)	C(20)-C(21)	1.371(9)
C(21)-C(22)	1.388(8)	C(22)-C(23)	1.375(7)
C(24)-C(25)	1.477(7)		
O(3)-Ga(1)-O(1)	96.1(2)	O(3)-Ga(1)-C(1)	108.0(2)
O(1)-Ga(1)-C(1)	107.5(2)	O(3)-Ga(1)-C(2)	109.7(2)
O(1)-Ga(1)-C(2)	107.2(2)	C(1)-Ga(1)-C(2)	124.5(3)
O(2)-Ga(2)-C(4)	108.3(2)	O(2)-Ga(2)-O(1)	96.9(2)
C(4)-Ga(2)-O(1)	107.7(2)	O(2)-Ga(2)-C(3)	110.6(2)
C(4)-Ga(2)-C(3)	124.2(3)	O(1)-Ga(2)-C(3)	105.5(2)
O(2)-Ga(3)-O(3)	95.13(14)	O(2)-Ga(3)-C(6)	111.4(2)
O(3)-Ga(3)-C(6)	105.8(2)	O(2)-Ga(3)-C(5)	107.3(2)
O(3)-Ga(3)-C(5)	108.9(2)	C(6)-Ga(3)-C(5)	124.3(3)
Ga(1)-O(1)-Ga(2)	129.1(2)	Ga(2)-O(2)-Ga(3)	126.8(2)
Ga(1)-O(3)-Ga(3)	131.7(2)	C(7)-O(4)-C(25)	118.6(4)
C(23)-O(5)-C(24)	117.3(4)	C(14)-N(1)-C(13)	111.5(4)
C(16)-N(2)-C(17)	113.0(4)	O(4)-C(7)-C(8)	124.1(5)
O(4)-C(7)-C(12)	114.7(5)	C(8)-C(7)-C(12)	121.1(5)
C(9)-C(8)-C(7)	119.4(6)	C(10)-C(9)-C(8)	120.4(7)
C(9)-C(10)-C(11)	120.8(7)	C(10)-C(11)-C(12)	120.7(6)
C(11)-C(12)-C(7)	117.7(6)	C(11)-C(12)-C(13)	122.0(5)
C(7)-C(12)-C(13)	120.3(5)	N(1)-C(13)-C(12)	111.5(4)
N(1)-C(14)-C(15)	111.7(5)	C(16)-C(15)-C(14)	115.0(4)
N(2)-C(16)-C(15)	111.8(5)	N(2)-C(17)-C(18)	110.4(4)
C(19)-C(18)-C(23)	118.0(5)	C(19)-C(18)-C(17)	121.9(5)
C(23)-C(18)-C(17)	120.0(5)	C(20)-C(19)-C(18)	121.3(6)
C(19)-C(20)-C(21)	120.1(6)	C(20)-C(21)-C(22)	120.6(6)
C(23)-C(22)-C(21)	119.0(6)	O(5)-C(23)-C(22)	124.1(5)
O(5)-C(23)-C(18)	114.8(4)	C(22)-C(23)-C(18)	121.1(5)
O(5)-C(24)-C(25)	108.4(4)	O(4)-C(25)-C(24)	109.8(4)

Symmetry transformations used to generate equivalent atoms:

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

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(1)	51(1)	55(1)	43(1)	2(1)	-1(1)	2(1)
Ga(2)	64(1)	54(1)	52(1)	0(1)	16(1)	-12(1)
Ga(3)	67(1)	38(1)	48(1)	0(1)	-13(1)	-3(1)
O(1)	66(2)	69(3)	76(3)	27(2)	-8(2)	-9(2)
O(2)	74(2)	40(2)	47(2)	-6(2)	5(2)	-9(2)
O(3)	60(2)	43(2)	48(2)	-3(2)	-10(2)	1(2)
C(1)	66(4)	96(5)	74(4)	-10(4)	16(3)	8(4)
C(2)	98(5)	92(5)	56(4)	-6(3)	-22(4)	9(4)
C(3)	104(5)	61(4)	82(4)	10(3)	22(4)	-19(4)
C(4)	86(5)	95(5)	91(5)	-19(4)	32(4)	2(4)
C(5)	104(5)	68(4)	48(3)	1(3)	3(3)	-28(4)
C(6)	85(5)	59(4)	114(5)	-21(4)	-41(4)	15(4)
O(4)	46(2)	69(2)	51(2)	-4(2)	-5(2)	-11(2)
O(5)	50(2)	50(2)	63(2)	-15(2)	9(2)	-7(2)
N(1)	46(3)	48(3)	53(3)	-4(2)	-12(2)	2(2)
N(2)	54(3)	35(2)	49(3)	0(2)	5(2)	2(2)
C(7)	48(3)	53(3)	52(3)	-8(3)	12(3)	0(3)
C(8)	81(4)	65(4)	59(4)	-10(3)	16(3)	0(4)
C(9)	120(6)	78(5)	71(5)	-4(4)	40(5)	-12(5)
C(10)	106(6)	82(5)	105(6)	-14(5)	56(5)	-37(5)
C(11)	66(4)	74(4)	94(5)	-23(4)	17(4)	-20(4)
C(12)	43(3)	50(3)	64(4)	-20(3)	9(3)	0(3)
C(13)	45(3)	58(4)	79(4)	-18(3)	-16(3)	4(3)
C(14)	64(4)	52(3)	70(4)	10(3)	-21(3)	-11(3)
C(15)	91(4)	60(4)	49(3)	2(3)	-9(3)	-37(3)
C(16)	81(4)	48(3)	48(3)	-1(3)	14(3)	-6(3)
C(17)	46(3)	60(4)	54(3)	1(3)	4(3)	15(3)
C(18)	41(3)	44(3)	57(3)	6(3)	-7(3)	1(3)
C(19)	53(3)	81(4)	61(4)	16(3)	-4(3)	-12(3)
C(20)	67(4)	85(5)	76(4)	25(4)	-19(4)	-31(4)
C(21)	70(4)	57(4)	98(5)	11(4)	-39(4)	-12(4)
C(22)	48(3)	47(3)	79(4)	-11(3)	-17(3)	-2(3)
C(23)	35(3)	50(3)	66(4)	6(3)	-14(3)	0(3)
C(24)	47(3)	61(4)	57(3)	-16(3)	0(3)	-2(3)
C(25)	48(3)	80(4)	50(3)	-11(3)	-4(3)	-11(3)

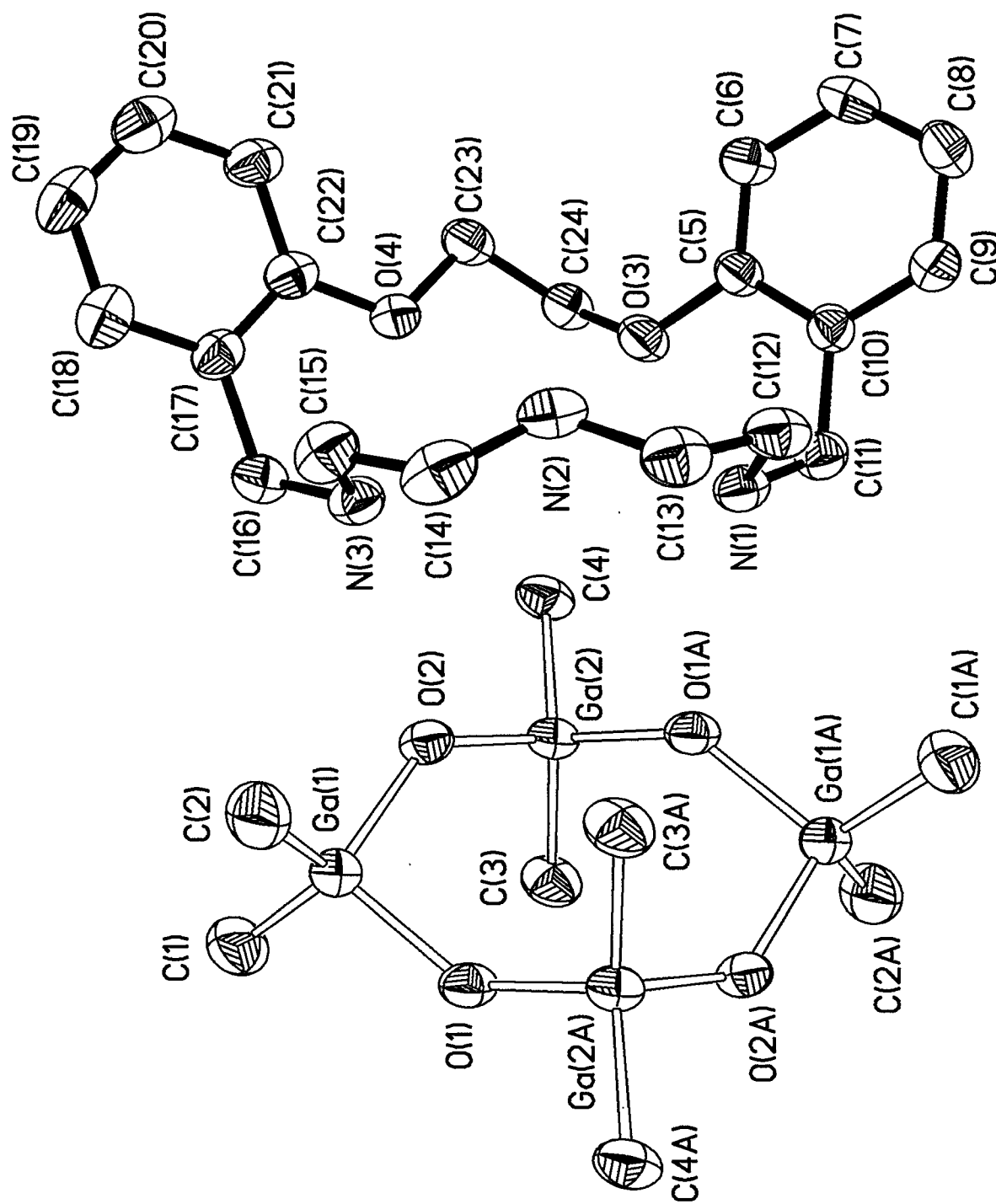
Table 4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4.

	x	y	z	U(eq)
H(10)	-490(4)	4183(2)	4143(2)	84
H(20)	-2861(4)	4485(2)	2588(1)	64
H(30)	-949(4)	6606(2)	3471(1)	60
H(1A)	2647(7)	4656(4)	3300(3)	118
H(1B)	2416(7)	5459(4)	2912(3)	118
H(1C)	1370(7)	4691(4)	2814(3)	118
H(2A)	1876(8)	5608(4)	4682(3)	123
H(2B)	304(8)	6030(4)	4737(3)	123
H(2C)	1605(8)	6487(4)	4400(3)	123
H(3A)	-2556(8)	2962(4)	3418(3)	124
H(3B)	-4265(8)	3119(4)	3524(3)	124
H(3C)	-3183(8)	3019(4)	4079(3)	124
H(4A)	-4214(7)	5026(4)	4535(3)	136
H(4B)	-5057(7)	5279(4)	3940(3)	136
H(4C)	-3592(7)	5746(4)	4131(3)	136
H(5A)	-637(7)	6377(4)	1770(2)	110
H(5B)	-1496(7)	5566(4)	1588(2)	110
H(5C)	-53(7)	5511(4)	1989(2)	110
H(6A)	-3530(7)	7238(4)	2605(3)	129
H(6B)	-4142(7)	6704(4)	3143(3)	129
H(6C)	-4653(7)	6512(4)	2478(3)	129
H(8A)	65(7)	7791(4)	5900(3)	82
H(9A)	-1694(9)	6825(4)	6187(3)	107
H(10A)	-3556(9)	6454(5)	5541(4)	117
H(11A)	-3751(7)	7058(4)	4601(3)	94
H(13A)	-2955(6)	8058(3)	3868(2)	73
H(13B)	-1859(6)	8760(3)	4080(2)	73
H(14A)	-421(6)	8865(3)	3191(2)	74
H(14B)	-1616(6)	8290(3)	2883(2)	74
H(15A)	243(7)	7381(4)	2566(2)	80
H(15B)	587(7)	8270(4)	2320(2)	80
H(16A)	2053(6)	7558(3)	3324(2)	71
H(16B)	2762(6)	7632(3)	2678(2)	71
H(17A)	4896(6)	8519(3)	3118(2)	64
H(17B)	4141(6)	8301(3)	3739(2)	64
H(19A)	6050(6)	9851(4)	3008(3)	78
H(20A)	6512(7)	11167(4)	3343(3)	91
H(21A)	5268(7)	11678(4)	4170(3)	90
H(22A)	3590(6)	10849(3)	4694(3)	70
H(24A)	1421(6)	10008(3)	4865(2)	66
H(24B)	2856(6)	9809(3)	5251(2)	66
H(25A)	2064(6)	8414(4)	5305(2)	71
H(25B)	964(6)	9023(4)	5635(2)	71
H(2D)	2095(43)	8950(25)	3385(17)	20(11)
H(1D)	15(53)	7820(29)	3838(20)	44(15)

Supporting Information

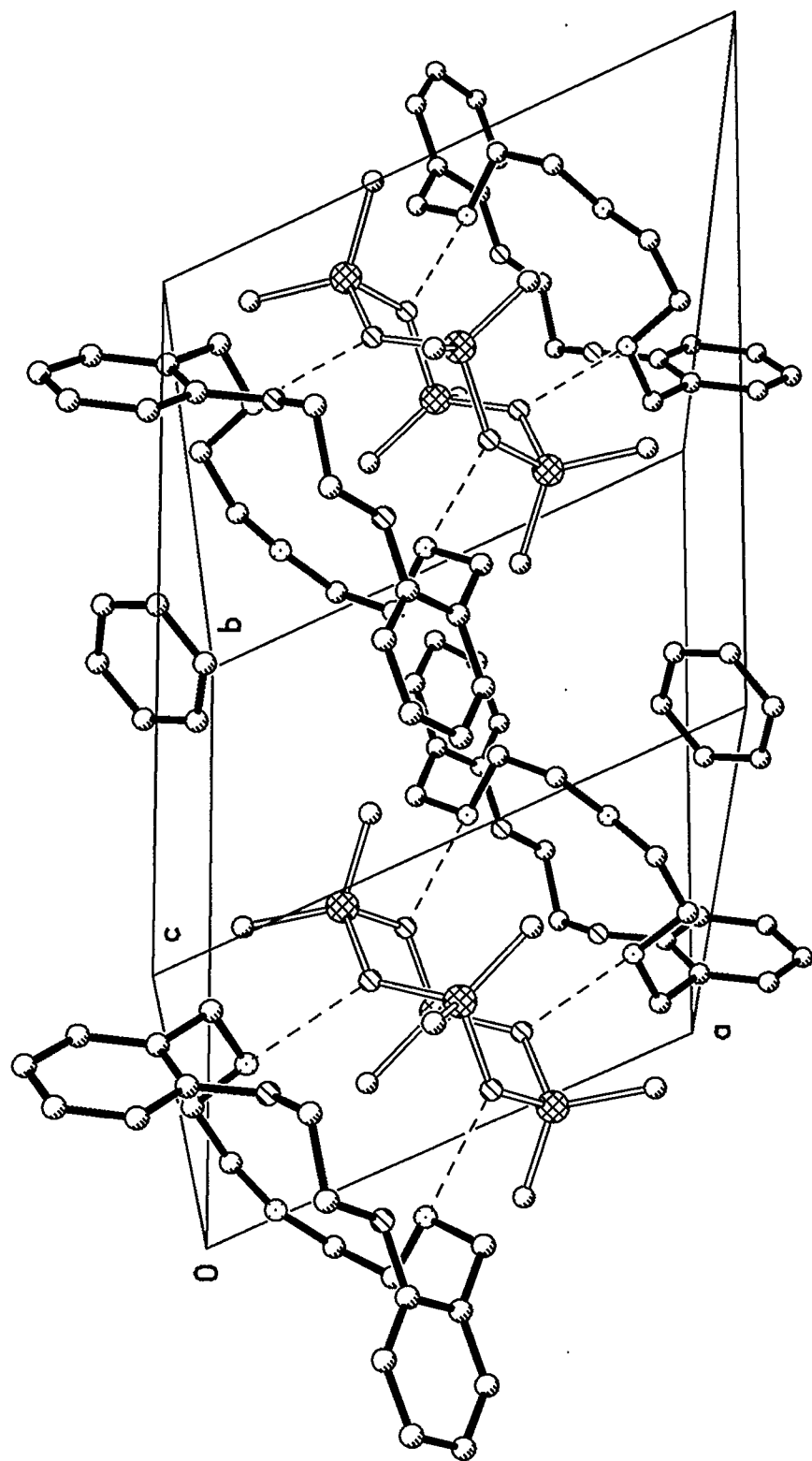
Mass spectra data for complexes 1-4.

Compound	MS (EI mode), m/e
(AlMe)(AlMe ₂)(OenNdienH ₄) (AlMe ₃) (1)	422.1 (M ⁺ -AlMe ₃ -Me) 378.1 (M ⁺ -AlMe ₃ -AlMe ₂) 338.1 (OenNdienH ⁺) 57.0 (AlMe ₂ ⁺)
(AlMe ₂)(OenNtnH ₄)(AlMe ₃) (2)	423.1 (M ⁺ -Me) 365.1 (M ⁺ -AlMe ₃) 351.1 (M ⁺ -AlMe ₃ -Me) 310.2 (OenNtnH ₂ ⁺) 57.1 (AlMe ₂ ⁺)
(OenNdienH ₄) ₂ (GaMe ₂ OH) ₄ (3)	86 (GaMe ⁺) 101 (GaMe ₂ ⁺) 341 (OenNdienH ₄ ⁺)
(OenNtnH ₄)(GaMe ₂ OH) ₃ (4)	86 (GaMe ⁺) 101 (GaMe ₂ ⁺) 312 (OenNtnH ₄ ⁺)

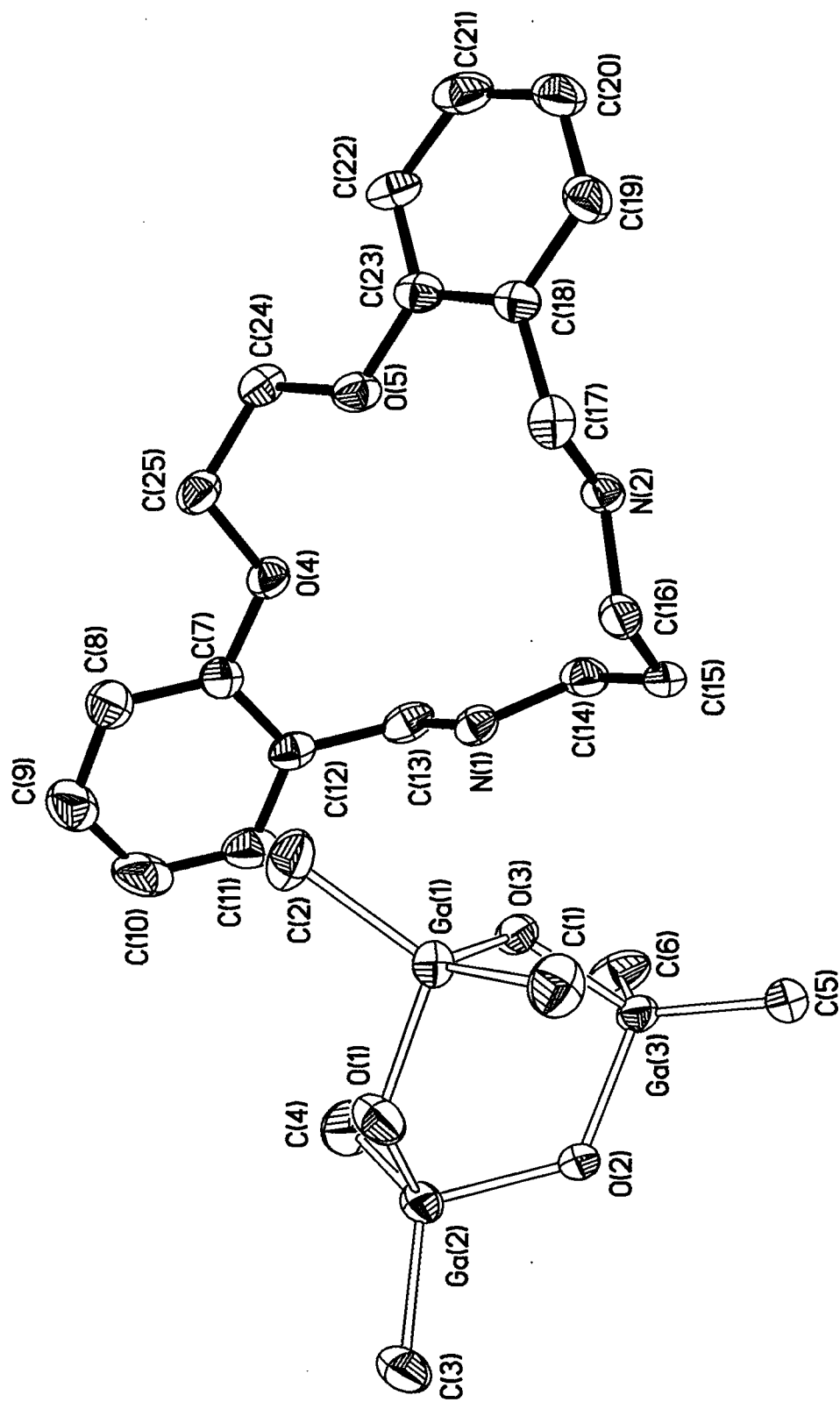


Supporting Information

Figure Molecular diagram (30% probability ellipsoids) showing the solid-state structure and atom-numbering scheme of $(\text{OenNdienHL})_2(\text{GaMe}_2\text{OH})_4$ (3). Hydrogen atoms are omitted for clarity.

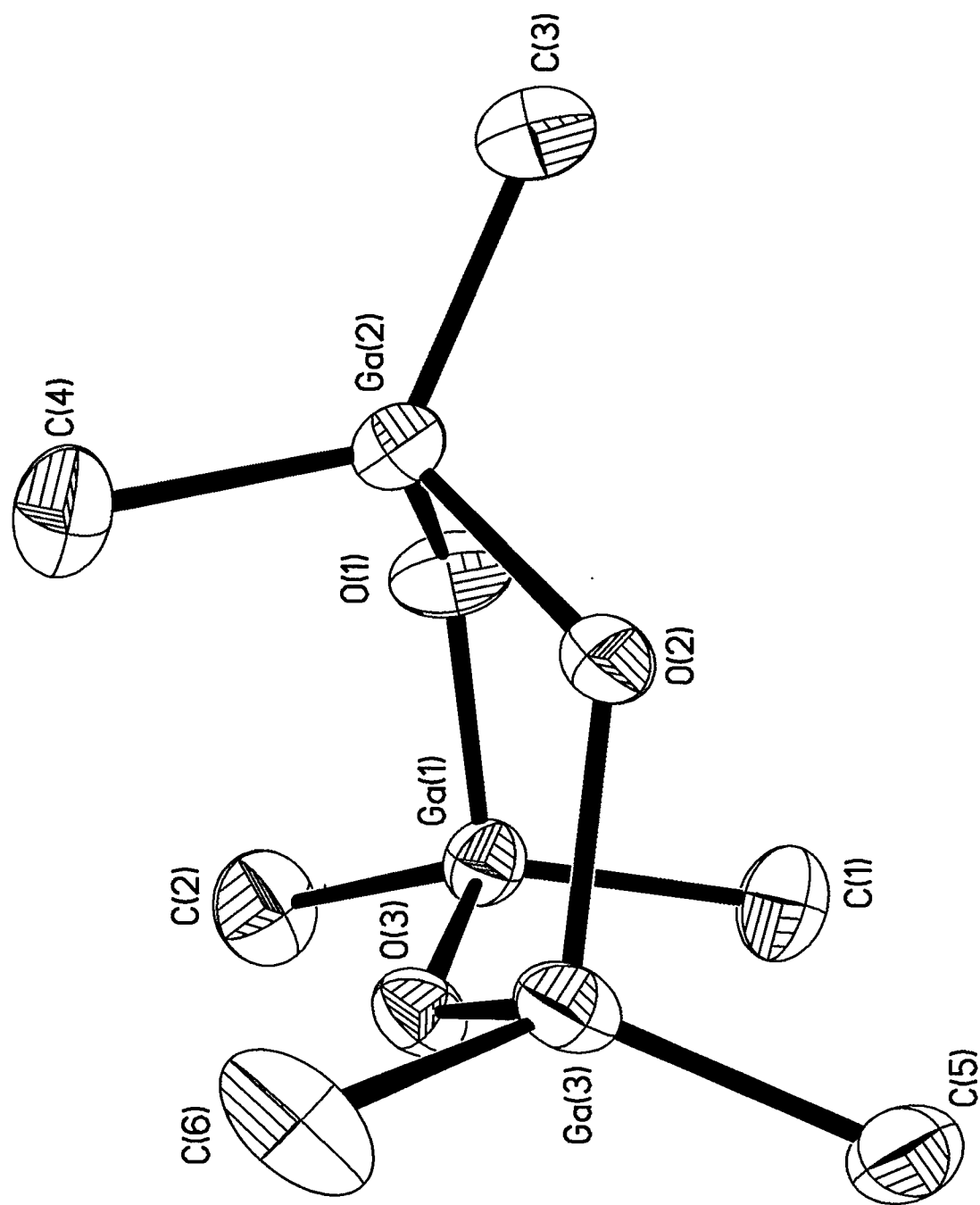


Supporting Information
Figure unit cell diagram showing the hydrogen bonding pattern in $(\text{OenNdienH}_4)_2(\text{GaMe}_2\text{OH})_4$ (3).

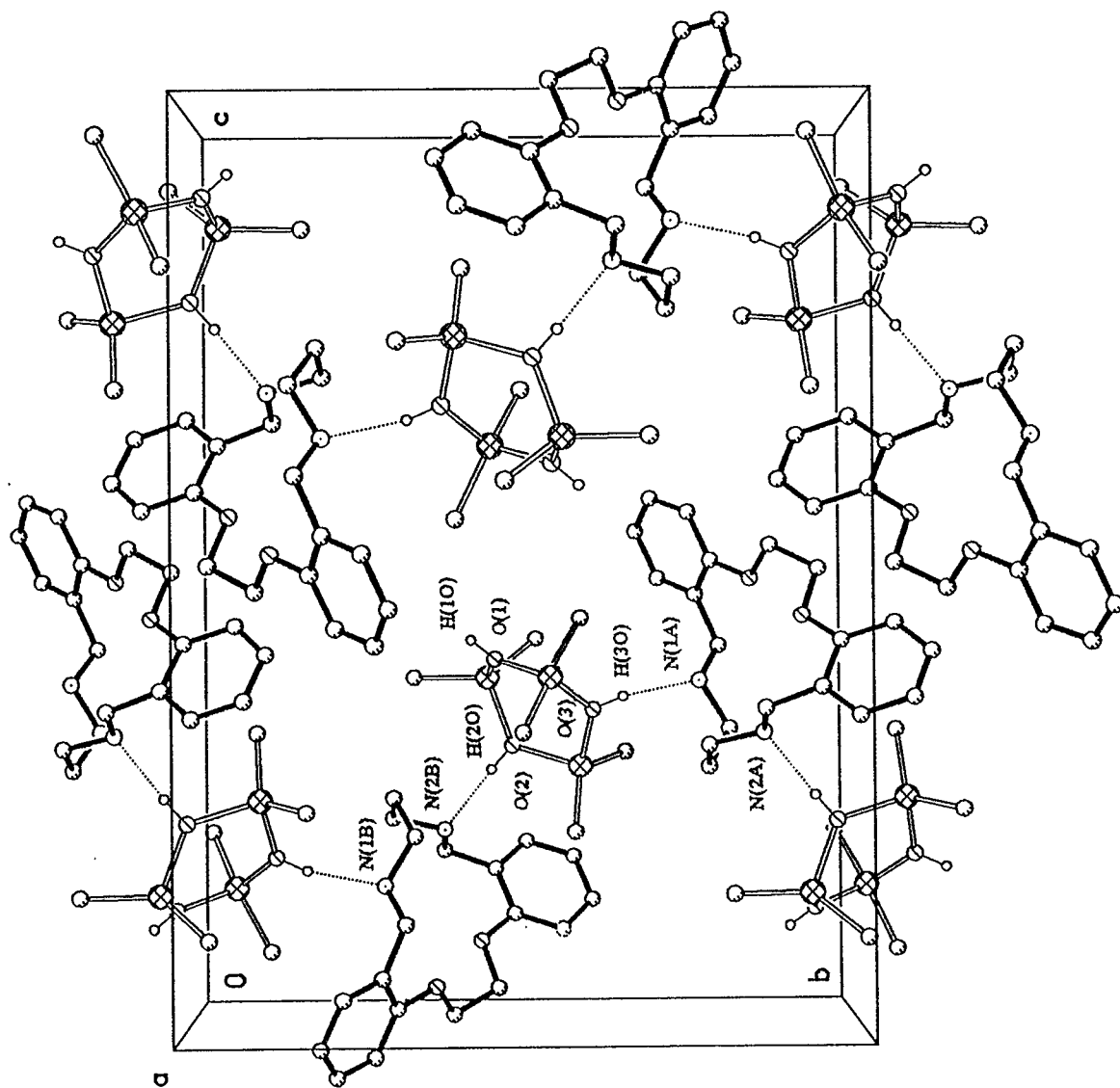


Supporting Information

Figure Molecular diagram (30% probability ellipsoids) showing the solid-state structure and atom-numbering scheme of $(\text{OenNtmHL}_4)(\text{GaMe}_2\text{OH})_3$ (4). Hydrogen atoms are omitted for clarity.



Supporting Information
Figure Skewed-boat conformation of $(\text{GaMe}_2\text{OH})_3$ in 4.



Supporting Information

Figure unit cell diagram showing the hydrogen bonding pattern in $(\text{OenNtmH}_4)(\text{GaMe}_2\text{OH})_3$ (4).