Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information File

Te-Te and Te-C bond activation reactions using a monovalent Gallanediyl

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Content

[RGa-μ-Te]$_2$ (1)

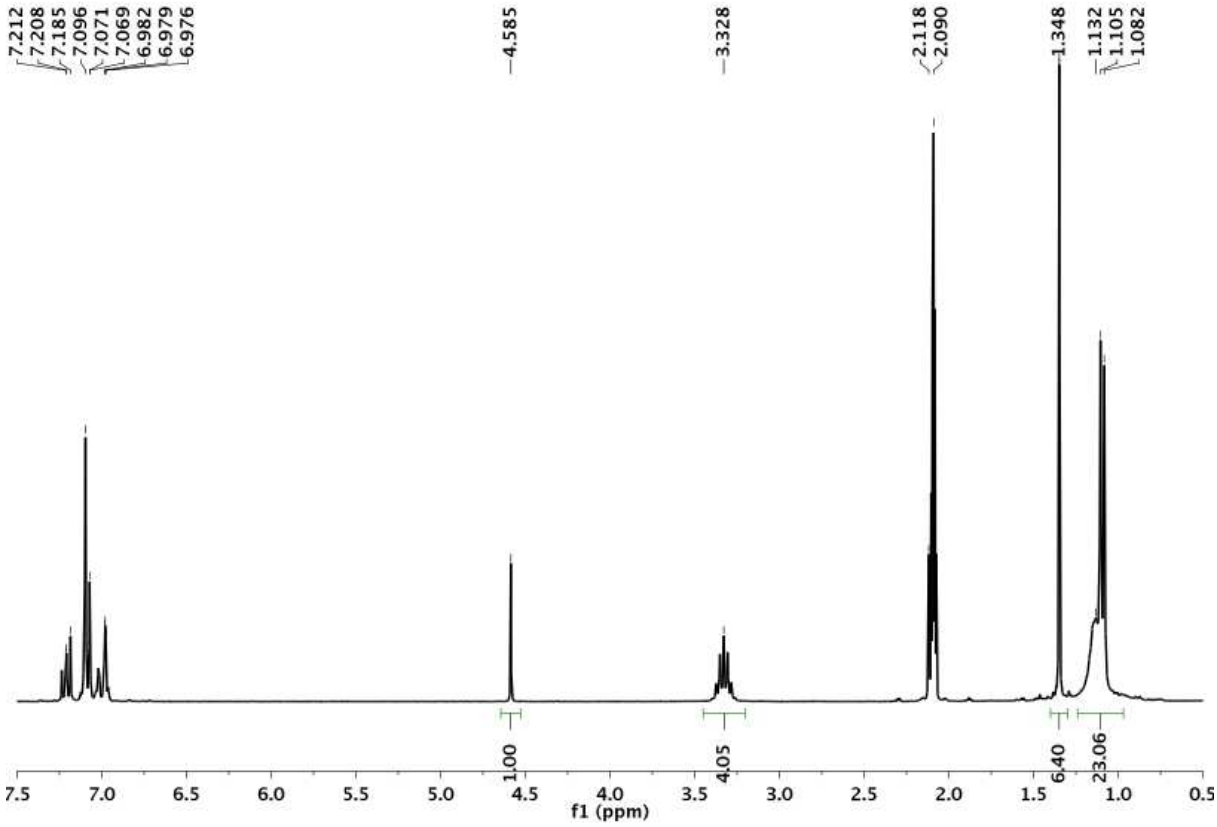

Figure S1. ^{1}H NMR spectrum of [LGa-μ-Te]$_2$ (**1**) in toluene-d_8.

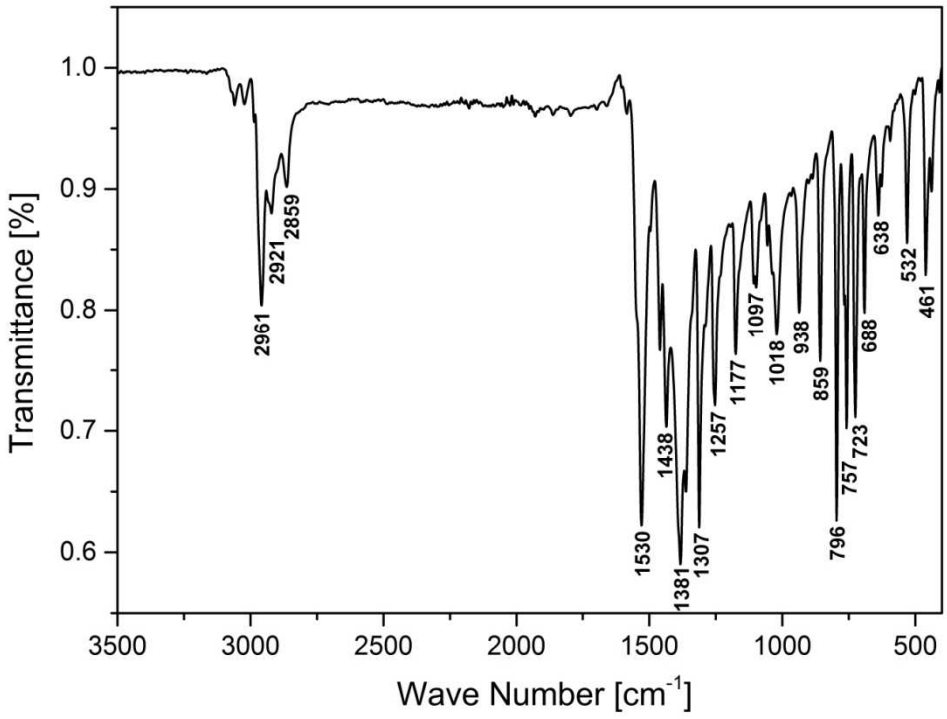

Figure S2. ATR-IR spectrum of [LGa-μ-Te]$_2$ (**1**).

[RGa(TePh)$_2$] (2)

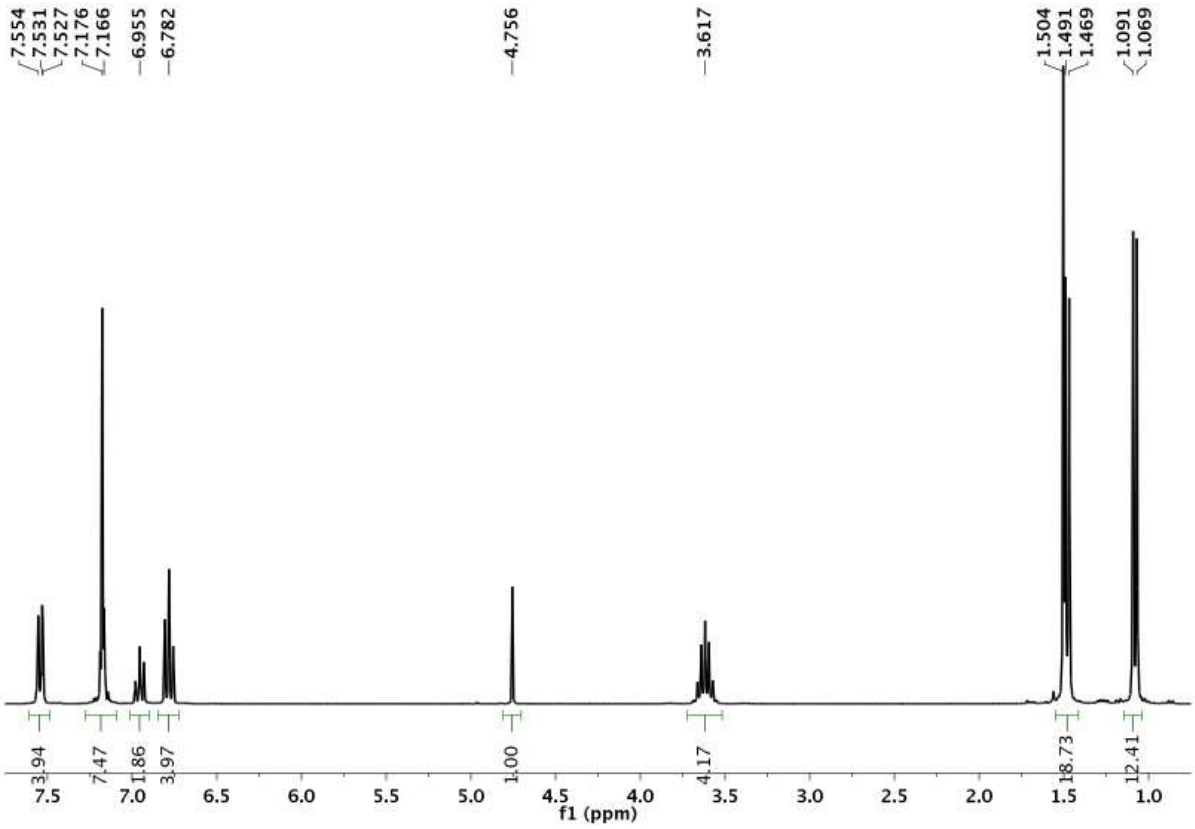

Figure S3. ^{1}H NMR spectrum of [LGa(TePh)$_2$] (**2**) in C_6D_6.

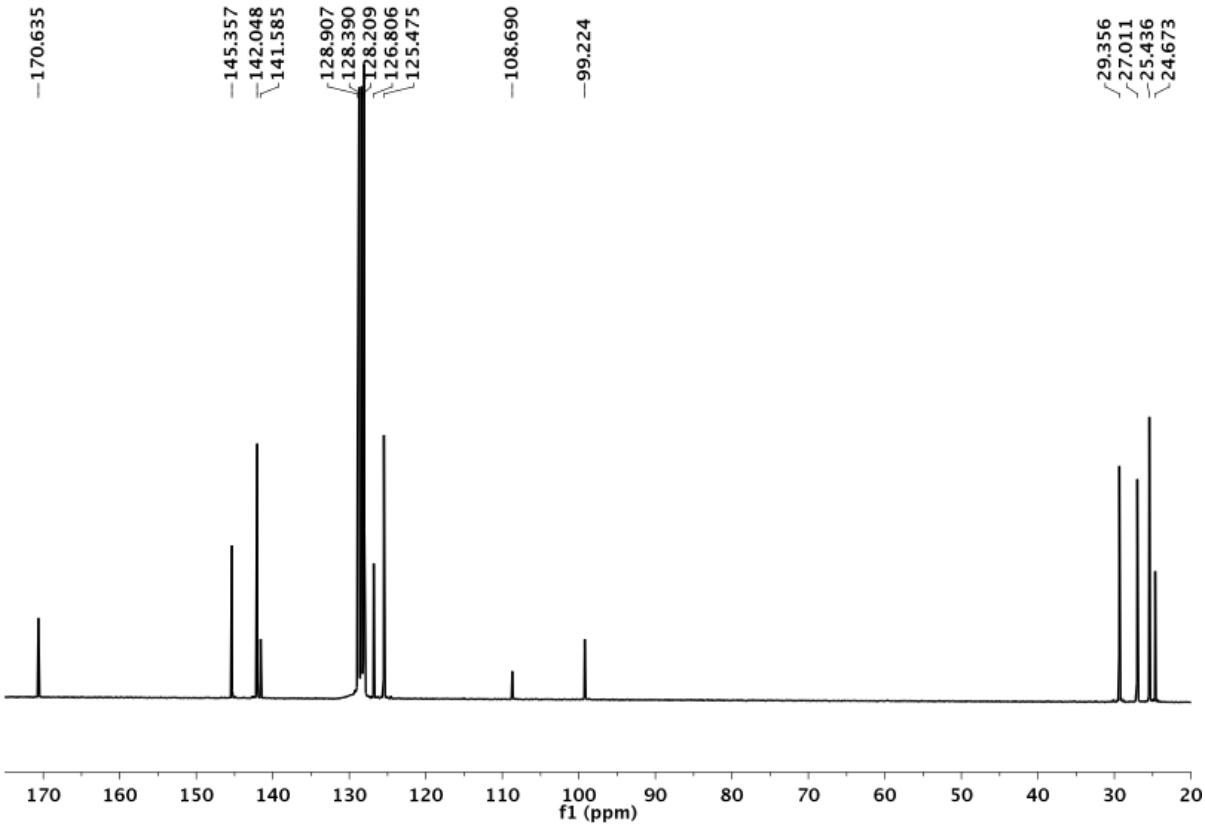

Figure S4. ^{13}C NMR spectrum of [LGa(TePh)$_2$] (**2**) in C_6D_6.

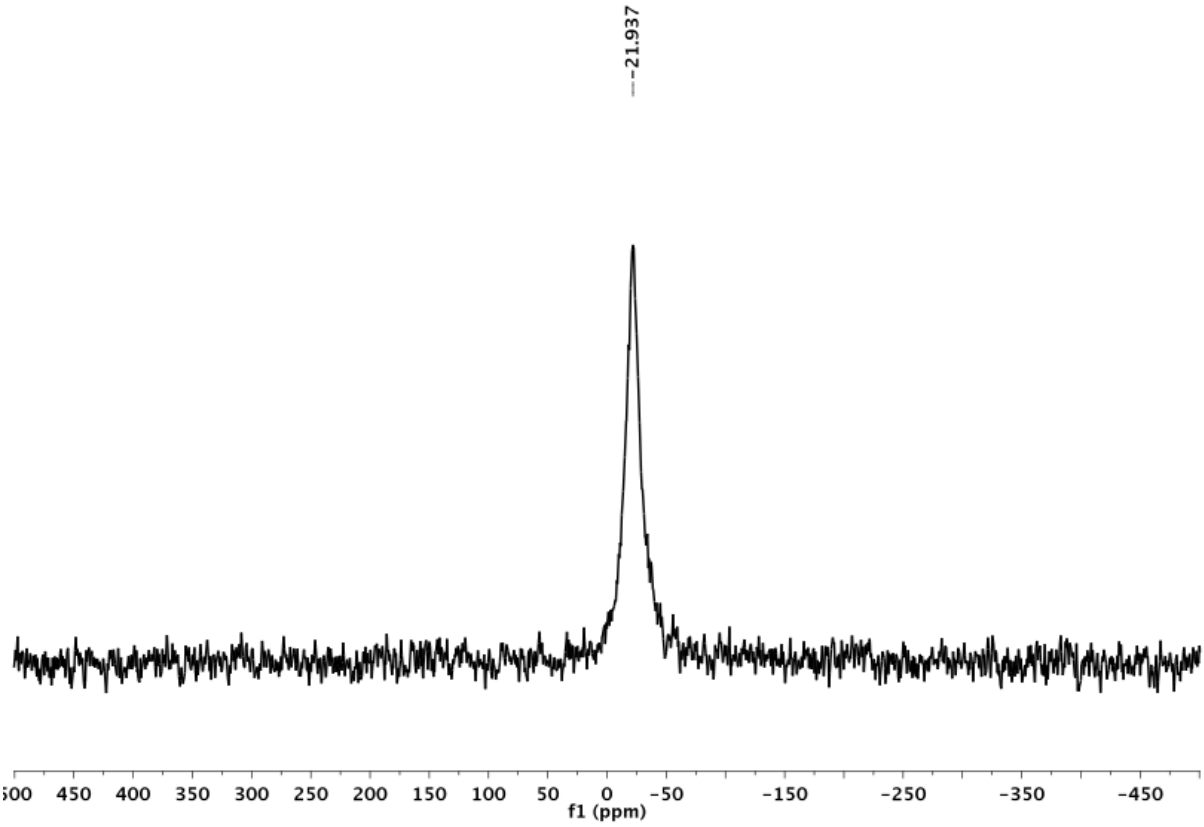

Figure S5. ^{125}Te NMR spectrum of [LGa(TePh)$_2$] (**2**) in C_6D_6.

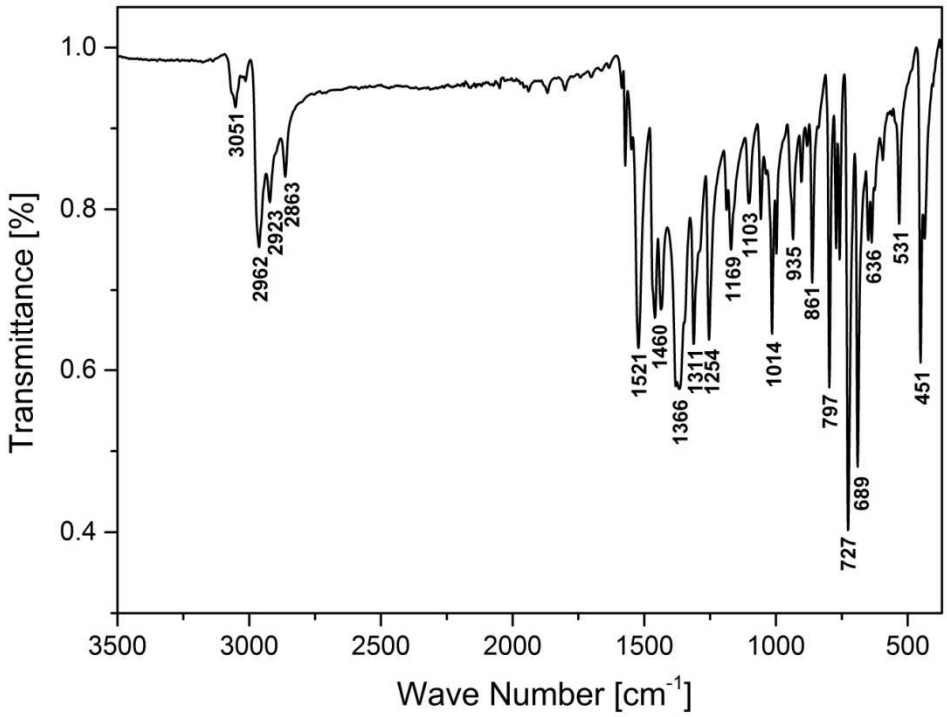

Figure S6. ATR-IR spectrum of [LGa(TePh)$_2$] (**2**).

[RGa(*i*-Pr)Te-*i*-Pr] (3)

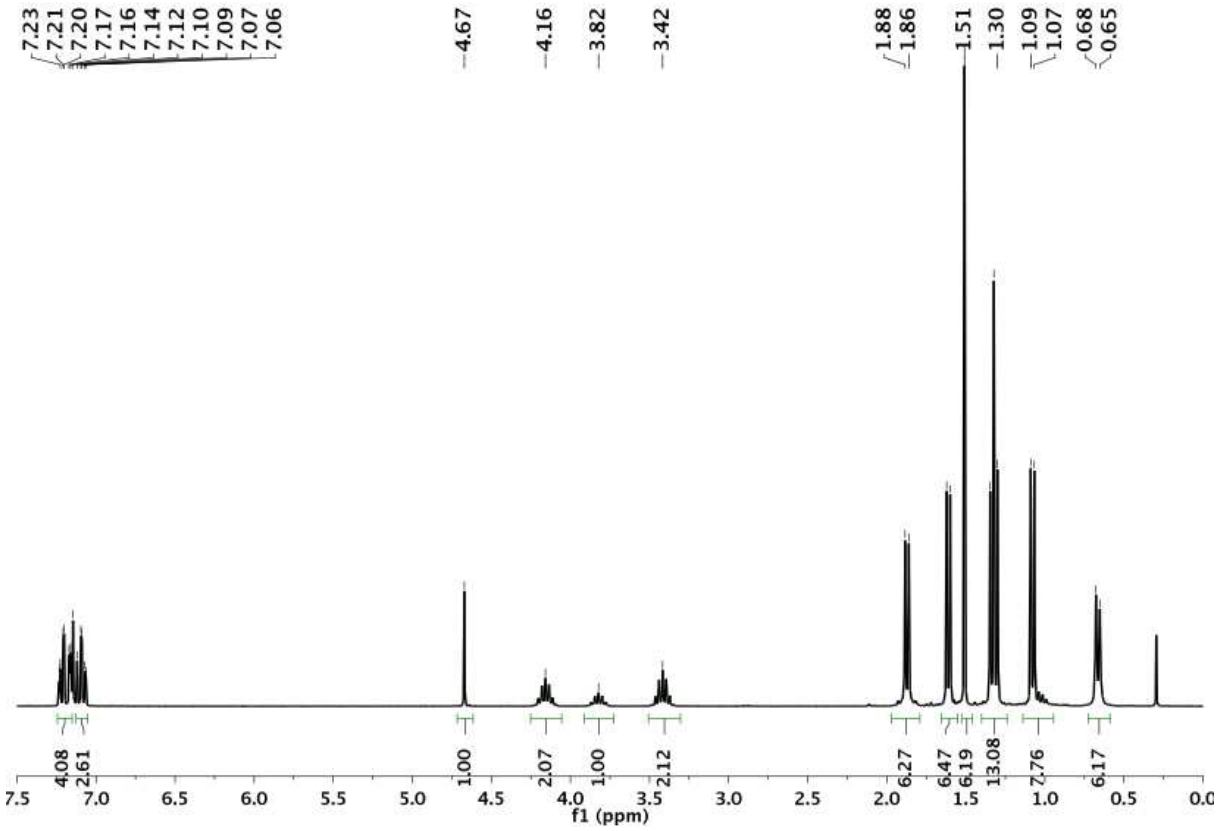

Figure S7. ^{1}H NMR spectrum of [LGa(*i*-Pr)Te-*i*-Pr] (**3**) in C_6D_6.

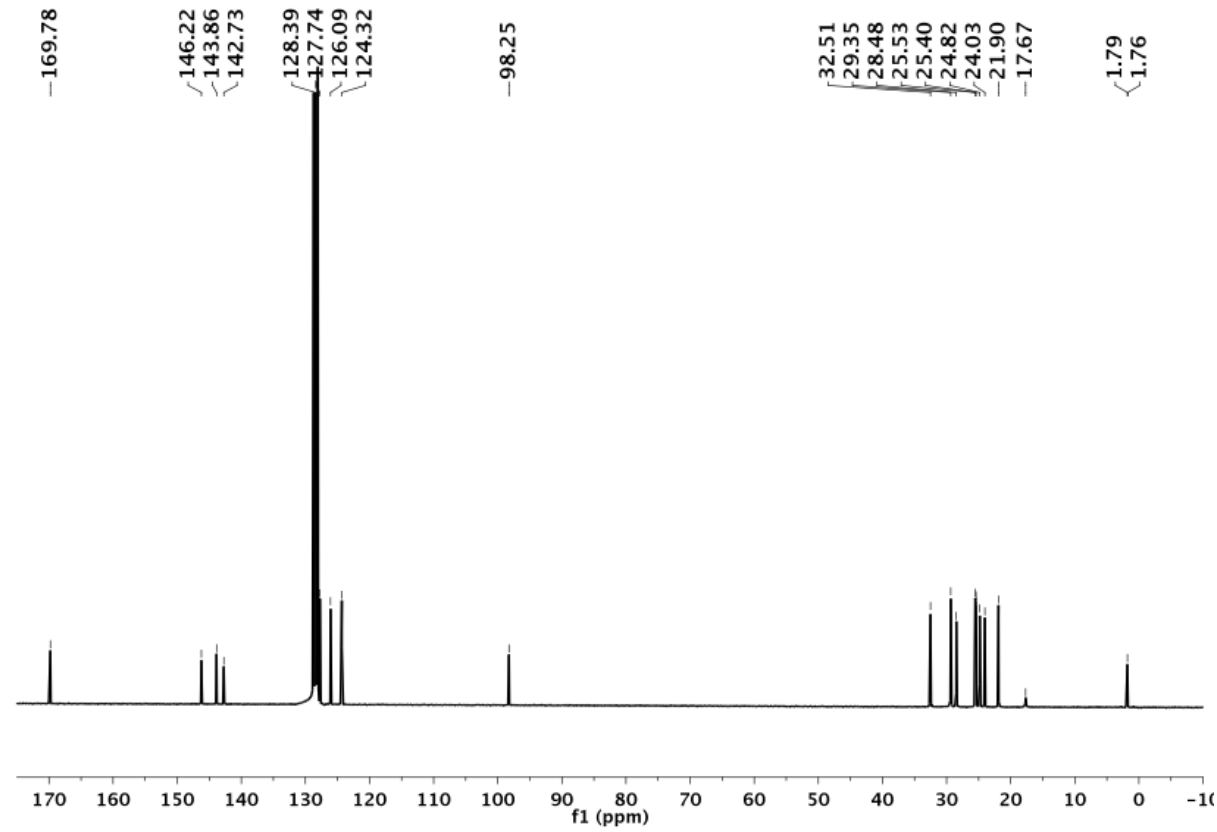

Figure S8. ^{13}C NMR spectrum of [LGa(*i*-Pr)Te-*i*-Pr] (**3**) in C_6D_6.

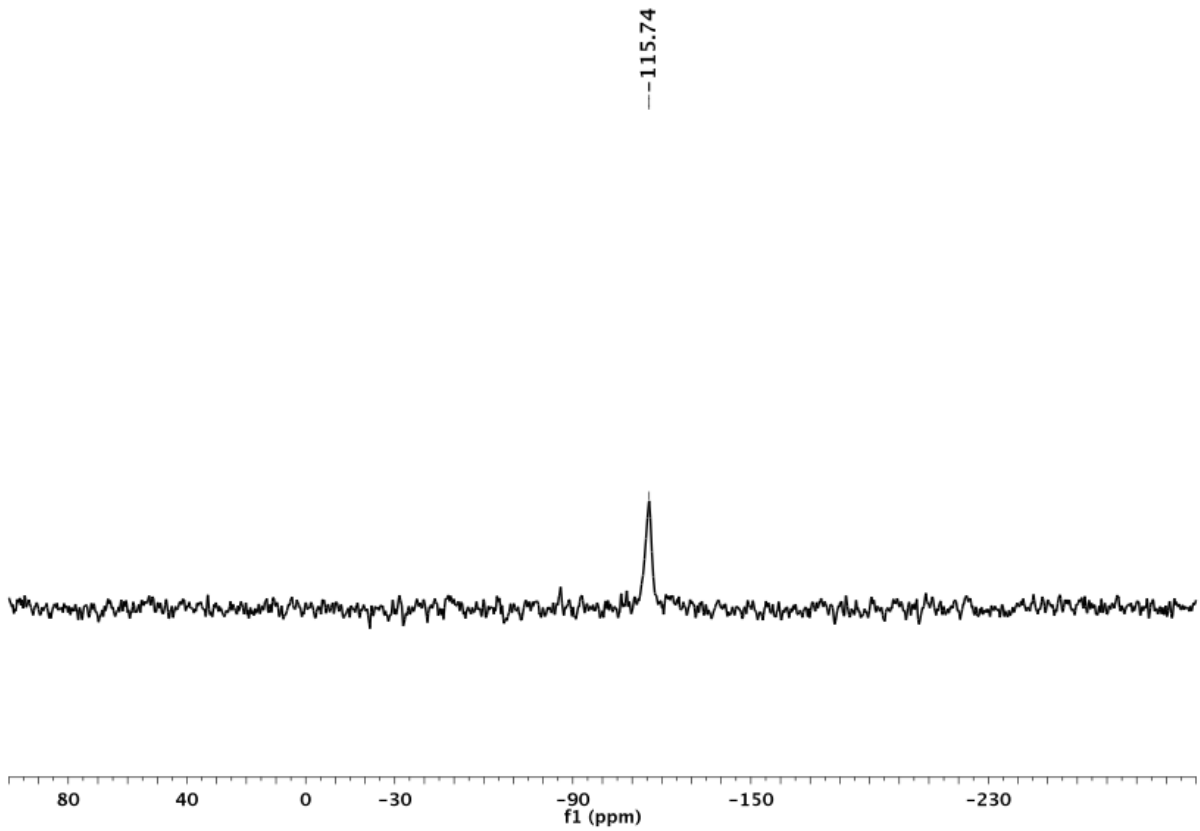

Figure S9. ^{125}Te NMR spectrum of [LGa(*i*-Pr)Te-*i*-Pr] (**3**) in C_6D_6.

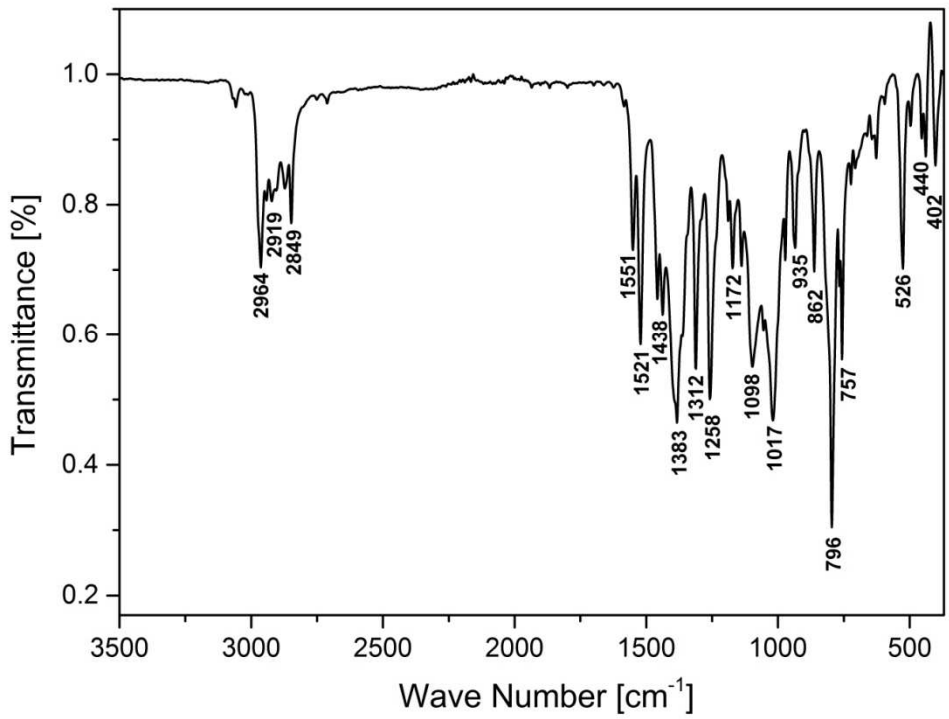

Figure S10. ATR-IR spectrum of [LGa(*i*-Pr)Te-*i*-Pr] (**3**).

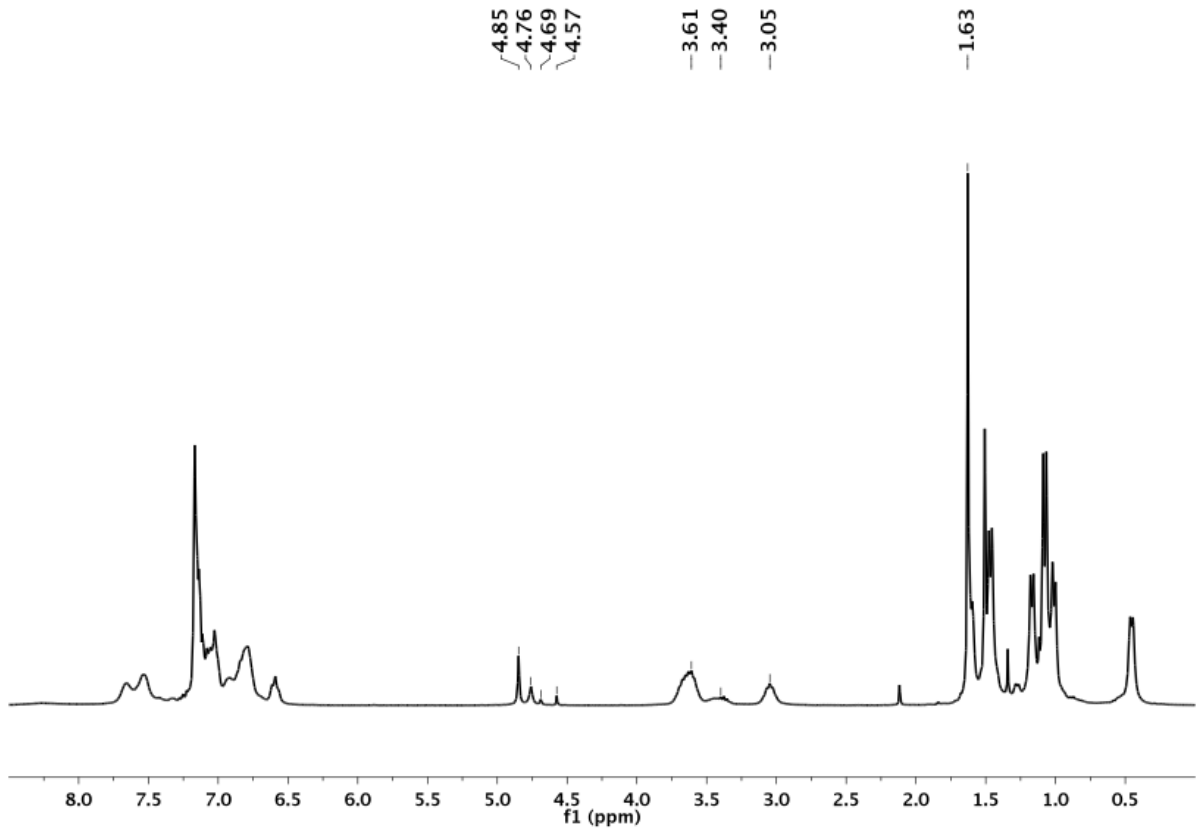

Figure S11. ^{1}H NMR spectrum of the 1:1 reaction mixture of Ph_2Te_2 and LGa→B(C_6F_5)$_3$ in C_6D_6 after 3 days.

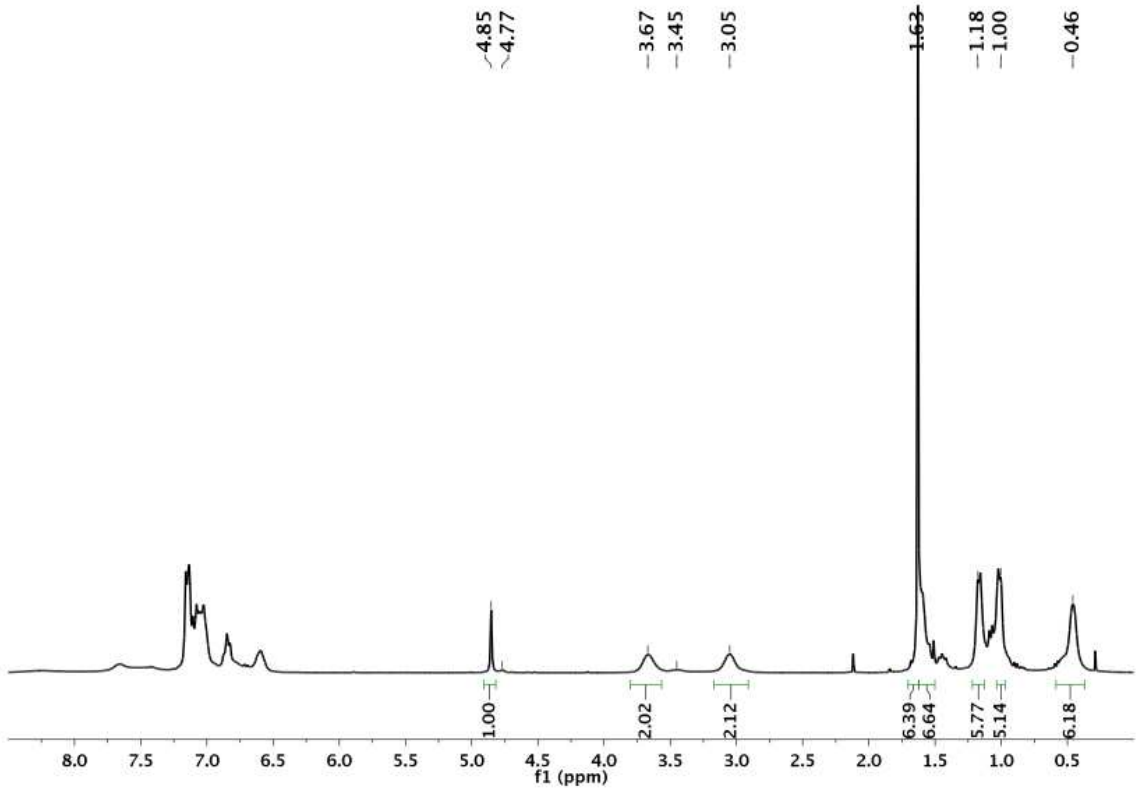

Figure S12. ^{1}H NMR spectrum of the 1:1 reaction mixture of Ph_2Te_2 and LGa→B(C_6F_5)$_3$ in C_6D_6 after 10 days; after isolated the pale yellow crystals of **1**.

Crystallographic data of 1-3

*Compound **1a***

Table 1: Crystal structure data

Identification code	cg_004m
Empirical formula	$C_{58}\ H_{82}\ Ga_2\ N_4\ Te_2$
Formula weight	1229.91
Density (calculated)	1.434 $g \cdot cm^{-1}$
F(000)	1248
Temperature	130(1) K
Crystal size	0.280 × 0.220 × 0.180 mm
Crystal colour	colourless
Crystal description	block
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	$P\ 2_1/n$
Unit cell dimensions	
a [Å]	14.0688(10)
b [Å]	13.8376(10)
c [Å]	15.2807(11)
α [°]	90
β [°]	106.759(2)
γ [°]	90
Volume	2848.5(4) $Å^3$
Z	2
Cell measurement reflections used	24228
Cell measurement ϑ min/max	2.76°/32.50°
Diffractometer control software	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Diffractometer measurement device	Bruker D8 KAPPA series II with APEX II area detector system
Diffractometer measurement method	Data collection strategy APEX 2/COSMO
ϑ range for data collection	2.110°- 32.618°
Completeness to ϑ = 25.242°	99.6%
Completeness to ϑ_{max} = 32.618°	98.6%
Index ranges	$-20 \le h \le 21$
	$-20 \le k \le 20$
	$-21 \le l \le 22$
Computing data reduction	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Absorption coefficient	1.988 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Computation absorption correction	BRUKER AXS SMART APEX 2 Vers. 3.0-2009
Max./min. Transmission	0.75/0.50
R_{merg} before/after correction	0.0935 / 0.0492
Computing structure solution	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Computing structure refinement	BRUKER AXS Inc. 2013 Vers. 2013/4
Refinement method	Full-matrix least-squares on F^2
Reflections collected	43835
Independent reflections	10256
R_{int}	0.0375
Reflections with $I > 2\sigma(I)$	8525
Restraints	0
Parameter	298
GooF	1.081
Weighting details	$w = 1/[\sigma^2(F_{obs}^2) + (0.0679P)^2 + 6.9476P]$

	where P = (F_{obs}^2 + 2F_{calc}^2)/3
R_1 [$I > 2\sigma(I)$]	0.0440
wR_2 [$I > 2\sigma(I)$]	0.1175
R_1 [all data]	0.0573
wR_2 [all data]	0.1300
Absolute structure parameter	
Largest diff. peak and hole	3.763/-1.417

Table 2: Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for cg_004m. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	U_{eq}
Te(1)	4218(1)	6119(1)	4406(1)	17(1)
Ga(1)	4427(1)	4301(1)	4104(1)	13(1)
N(1)	4755(2)	4007(2)	2955(2)	18(1)
N(2)	3181(2)	3544(2)	3781(2)	16(1)
C(1)	4050(2)	3754(2)	2195(2)	21(1)
C(2)	3074(2)	3534(2)	2174(2)	23(1)
H(2)	2610	3500	1584	27
C(3)	2693(2)	3357(2)	2908(2)	20(1)
C(4)	4282(3)	3644(3)	1291(2)	32(1)
H(4A)	4014	4199	898	48
H(4B)	3979	3048	990	48
H(4C)	5003	3615	1400	48
C(5)	1673(2)	2904(3)	2653(2)	31(1)
H(5A)	1564	2591	3191	47
H(5B)	1623	2421	2172	47
H(5C)	1170	3405	2429	47
C(6)	5759(2)	4087(2)	2901(2)	20(1)
C(7)	6071(2)	4923(3)	2542(2)	24(1)
C(8)	7036(3)	4933(3)	2450(2)	32(1)
H(8)	7262	5490	2206	39
C(9)	7662(3)	4149(4)	2705(3)	36(1)
H(9)	8307	4166	2626	44
C(10)	7348(3)	3338(3)	3077(2)	33(1)
H(10)	7788	2807	3261	39
C(11)	6398(2)	3285(2)	3189(2)	25(1)
C(12)	5424(3)	5814(3)	2250(2)	28(1)
H(12)	4765	5682	2351	34
C(13)	5890(3)	6683(3)	2839(3)	34(1)
H(13A)	5987	6530	3485	50
H(13B)	5448	7243	2668	50
H(13C)	6532	6833	2741	50
C(14)	5250(4)	6068(4)	1234(3)	43(1)
H(14A)	5891	6177	1116	65
H(14B)	4847	6656	1087	65
H(14C)	4903	5534	852	65
C(15)	6063(3)	2379(2)	3573(2)	28(1)
H(15)	5531	2575	3852	34
C(16)	6887(3)	1899(3)	4326(3)	38(1)
H(16A)	7397	1647	4065	56
H(16B)	6607	1366	4596	56
H(16C)	7185	2375	4801	56
C(17)	5603(3)	1643(3)	2817(3)	43(1)

H(17A)	6100	1448	2516	65
H(17B)	5035	1938	2367	65
H(17C)	5380	1074	3086	65
C(18)	2740(2)	3187(2)	4467(2)	19(1)
C(19)	3031(2)	2268(2)	4849(2)	26(1)
C(20)	2555(3)	1900(3)	5465(3)	34(1)
H(20)	2736	1279	5725	41
C(21)	1834(3)	2414(3)	5703(3)	37(1)
H(21)	1525	2150	6127	45
C(22)	1555(3)	3318(3)	5325(2)	32(1)
H(22)	1060	3672	5500	39
C(23)	1991(2)	3722(2)	4689(2)	22(1)
C(24)	1599(2)	4676(2)	4248(2)	24(1)
H(24)	1962	4841	3793	29
C(25)	480(3)	4617(3)	3742(3)	37(1)
H(25A)	109	4501	4185	55
H(25B)	360	4086	3300	55
H(25C)	261	5226	3421	55
C(26)	1773(3)	5485(3)	4955(3)	38(1)
H(26A)	1391	5353	5386	56
H(26B)	1559	6101	4646	56
H(26C)	2481	5518	5287	56
C(27)	3810(3)	1663(2)	4583(3)	33(1)
H(27A)	4176	2097	4269	40
C(28)	4562(4)	1220(3)	5406(4)	46(1)
H(28A)	4835	1725	5858	70
H(28B)	5100	922	5212	70
H(28C)	4236	727	5679	70
C(29)	3303(5)	871(4)	3904(4)	60(2)
H(29A)	2891	469	4177	90
H(29B)	3810	468	3758	90
H(29C)	2886	1170	3343	90

Table 3: Anisotropic displacement parameters ($Å^2 \times 10^3$) for cg_004m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Te(1)	19(1)	13(1)	16(1)	0(1)	1(1)	2(1)
Ga(1)	12(1)	13(1)	13(1)	-2(1)	3(1)	0(1)
N(1)	13(1)	23(1)	17(1)	-2(1)	3(1)	0(1)
N(2)	15(1)	16(1)	16(1)	-1(1)	4(1)	0(1)
C(1)	18(1)	28(1)	14(1)	-4(1)	2(1)	0(1)
C(2)	17(1)	32(2)	17(1)	-4(1)	2(1)	-1(1)
C(3)	16(1)	20(1)	21(1)	-5(1)	3(1)	-1(1)
C(4)	25(2)	54(2)	18(1)	-11(1)	7(1)	-7(2)
C(5)	21(1)	44(2)	26(2)	-10(1)	4(1)	-10(1)
C(6)	16(1)	30(1)	17(1)	-6(1)	6(1)	0(1)
C(7)	16(1)	38(2)	18(1)	-4(1)	7(1)	-4(1)
C(8)	21(2)	53(2)	26(2)	-5(1)	11(1)	-8(1)
C(9)	17(1)	63(3)	32(2)	-13(2)	12(1)	-1(2)
C(10)	20(1)	49(2)	30(2)	-13(2)	8(1)	8(1)
C(11)	20(1)	32(2)	22(1)	-10(1)	4(1)	4(1)
C(12)	21(1)	36(2)	27(2)	4(1)	7(1)	-4(1)
C(13)	31(2)	34(2)	40(2)	4(1)	16(2)	-7(1)

C(14)	40(2)	57(3)	28(2)	13(2)	2(2)	-5(2)
C(15)	24(2)	27(1)	33(2)	-8(1)	6(1)	7(1)
C(16)	38(2)	36(2)	36(2)	-3(2)	6(2)	15(2)
C(17)	45(2)	32(2)	44(2)	-15(2)	0(2)	5(2)
C(18)	16(1)	20(1)	18(1)	0(1)	3(1)	-4(1)
C(19)	24(1)	22(1)	28(2)	4(1)	2(1)	-3(1)
C(20)	31(2)	34(2)	34(2)	14(1)	2(1)	-8(1)
C(21)	28(2)	53(2)	30(2)	13(2)	7(1)	-13(2)
C(22)	22(2)	51(2)	25(2)	4(1)	9(1)	-5(1)
C(23)	15(1)	29(1)	20(1)	-1(1)	5(1)	-3(1)
C(24)	18(1)	28(1)	27(1)	-3(1)	9(1)	2(1)
C(25)	24(2)	44(2)	39(2)	1(2)	2(1)	9(2)
C(26)	31(2)	40(2)	48(2)	-16(2)	22(2)	-4(2)
C(27)	36(2)	20(1)	40(2)	3(1)	6(2)	2(1)
C(28)	42(2)	21(2)	64(3)	2(2)	-4(2)	6(1)
C(29)	68(4)	43(2)	61(3)	-15(2)	4(3)	14(2)

Table 4: Bond lengths [Å] for cg_004m.

Te(1)-Ga(1)#1	2.5777(4)	C(9)-C(10)	1.387(6)
Te(1)-Ga(1)	2.5898(4)	C(10)-C(11)	1.398(5)
Te(1)-Te(1)#1	3.9260(4)	C(11)-C(15)	1.516(5)
Ga(1)-N(2)	1.979(2)	C(12)-C(13)	1.532(5)
Ga(1)-N(1)	1.982(2)	C(12)-C(14)	1.542(5)
Ga(1)-Te(1)#1	2.5777(4)	C(15)-C(16)	1.530(5)
N(1)-C(1)	1.339(4)	C(15)-C(17)	1.537(5)
N(1)-C(6)	1.443(4)	C(18)-C(23)	1.407(4)
N(2)-C(3)	1.337(4)	C(18)-C(19)	1.409(4)
N(2)-C(18)	1.450(4)	C(19)-C(20)	1.400(5)
C(1)-C(2)	1.397(4)	C(19)-C(27)	1.525(5)
C(1)-C(4)	1.516(4)	C(20)-C(21)	1.371(6)
C(2)-C(3)	1.397(4)	C(21)-C(22)	1.387(6)
C(3)-C(5)	1.511(4)	C(22)-C(23)	1.407(5)
C(6)-C(7)	1.403(5)	C(23)-C(24)	1.513(5)
C(6)-C(11)	1.416(4)	C(24)-C(26)	1.525(5)
C(7)-C(8)	1.404(4)	C(24)-C(25)	1.543(5)
C(7)-C(12)	1.521(5)	C(27)-C(28)	1.520(6)
C(8)-C(9)	1.380(6)	C(27)-C(29)	1.536(6)

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

Table 5: Bond angles [°] for cg_004m.

Ga(1)#1-Te(1)-Ga(1)	81.117(11)	C(8)-C(9)-C(10)	120.0(3)
Ga(1)#1-Te(1)-Te(1)#1	40.673(7)	C(9)-C(10)-C(11)	121.4(3)
Ga(1)-Te(1)-Te(1)#1	40.444(8)	C(10)-C(11)-C(6)	117.7(3)
N(2)-Ga(1)-N(1)	94.92(10)	C(10)-C(11)-C(15)	120.4(3)
N(2)-Ga(1)-Te(1)#1	118.56(7)	C(6)-C(11)-C(15)	121.9(3)
N(1)-Ga(1)-Te(1)#1	115.72(7)	C(7)-C(12)-C(13)	110.2(3)
N(2)-Ga(1)-Te(1)	114.87(7)	C(7)-C(12)-C(14)	112.9(3)
N(1)-Ga(1)-Te(1)	115.13(7)	C(13)-C(12)-C(14)	109.2(3)
Te(1)#1-Ga(1)-Te(1)	98.883(11)	C(11)-C(15)-C(16)	113.4(3)
C(1)-N(1)-C(6)	117.5(2)	C(11)-C(15)-C(17)	111.5(3)
C(1)-N(1)-Ga(1)	121.3(2)	C(16)-C(15)-C(17)	109.9(3)

C(6)-N(1)-Ga(1)	121.15(18)	C(23)-C(18)-C(19)	121.5(3)
C(3)-N(2)-C(18)	116.8(2)	C(23)-C(18)-N(2)	120.0(3)
C(3)-N(2)-Ga(1)	121.0(2)	C(19)-C(18)-N(2)	118.3(3)
C(18)-N(2)-Ga(1)	122.16(18)	C(20)-C(19)-C(18)	118.0(3)
N(1)-C(1)-C(2)	123.6(3)	C(20)-C(19)-C(27)	120.0(3)
N(1)-C(1)-C(4)	121.1(3)	C(18)-C(19)-C(27)	122.0(3)
C(2)-C(1)-C(4)	115.2(3)	C(21)-C(20)-C(19)	121.6(3)
C(3)-C(2)-C(1)	128.4(3)	C(20)-C(21)-C(22)	120.0(3)
N(2)-C(3)-C(2)	124.1(3)	C(21)-C(22)-C(23)	121.2(4)
N(2)-C(3)-C(5)	120.9(3)	C(22)-C(23)-C(18)	117.7(3)
C(2)-C(3)-C(5)	114.9(3)	C(22)-C(23)-C(24)	118.6(3)
C(7)-C(6)-C(11)	121.7(3)	C(18)-C(23)-C(24)	123.7(3)
C(7)-C(6)-N(1)	120.5(3)	C(23)-C(24)-C(26)	111.2(3)
C(11)-C(6)-N(1)	117.7(3)	C(23)-C(24)-C(25)	111.4(3)
C(6)-C(7)-C(8)	117.9(3)	C(26)-C(24)-C(25)	109.0(3)
C(6)-C(7)-C(12)	123.7(3)	C(28)-C(27)-C(19)	112.5(4)
C(8)-C(7)-C(12)	118.5(3)	C(28)-C(27)-C(29)	110.4(3)
C(9)-C(8)-C(7)	121.3(4)	C(19)-C(27)-C(29)	110.1(4)

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

Compound ***1b***

Table 1: Crystal structure data

Identification code	**cg_015m**
Empirical formula	$C_{61.50}\ H_{86}\ Ga_2\ N_4\ Te_2$
Formula weight	1275.98
Density (calculated)	1.336 $g \cdot cm^{-1}$
F(000)	2596
Temperature	100(1) K
Crystal size	0.220 × 0.180 × 0.130 mm
Crystal colour	pale yellow
Crystal description	block
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	*C 2/m*
Unit cell dimensions	
a [Å]	18.6322(4)
b [Å]	20.9742(5)
c [Å]	16.4363(4)
α [°]	90
β [°]	98.9820(10)
γ [°]	90
Volume	6344.5(3) $Å^3$
Z	4
Cell measurement reflections used	35084
Cell measurement ϑ min/max	2.51°/32.14°
Diffractometer control software	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Diffractometer measurement device	Bruker D8 KAPPA series II with APEX II area detector system
Diffractometer measurement method	Data collection strategy APEX 2/COSMO
ϑ range for data collection	1.819°- 32.155°
Completeness to ϑ = 25.242°	99.7%
Completeness to ϑ_{max} = 32.155°	99.5%
Index ranges	$-27 \le h \le 27$
	$-28 \le k \le 31$
	$-24 \le l \le 24$
Computing data reduction	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Absorption coefficient	1.788 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Computation absorption correction	BRUKER AXS SMART APEX 2 Vers. 3.0-2009
Max./min. Transmission	0.75/0.68
R_{merg} before/after correction	0.0660 / 0.0423
Computing structure solution	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Computing structure refinement	BRUKER AXS Inc. 2013 Vers. 2013/4
Refinement method	Full-matrix least-squares on F^2
Reflections collected	86728
Independent reflections	11354
R_{int}	0.0319
Reflections with $I > 2\sigma(I)$	9852
Restraints	0
Parameter	342
GooF	1.072
Weighting details	$w = 1/[\sigma^2(F_{obs}^2) + (0.0342P)^2 + 3.2989P]$
	where $P = (F_{obs}^2 + 2F_{calc}^2)/3$
R_1 [$I > 2\sigma(I)$]	0.0223

wR_2 [$I > 2\sigma(I)$]	0.0576
R_1 [all data]	0.0293
wR_2 [all data]	0.0606
Absolute structure parameter	
Largest diff. peak and hole	0.986/-0.453

Table 2: Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for cg_015m. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	U_{eq}
Te(1)	-352(1)	5000	8795(1)	12(1)
Ga(1)	849(1)	5000	9818(1)	9(1)
N(1)	1550(1)	4298(1)	9719(1)	12(1)
C(1)	2262(1)	4398(1)	9940(1)	14(1)
C(2)	2573(1)	5000	10118(1)	16(1)
H(2)	3059	5000	10399	19
C(3)	2796(1)	3851(1)	9980(1)	19(1)
H(3A)	2852	3655	10528	28
H(3B)	3267	4011	9876	28
H(3C)	2613	3532	9563	28
C(4)	1320(1)	3667(1)	9423(1)	13(1)
C(5)	1260(1)	3165(1)	9978(1)	14(1)
C(6)	1066(1)	2560(1)	9650(1)	18(1)
H(6)	1019	2216	10014	21
C(7)	946(1)	2451(1)	8808(1)	20(1)
H(7)	822	2036	8601	24
C(8)	1004(1)	2950(1)	8272(1)	21(1)
H(8)	914	2873	7695	25
C(9)	1189(1)	3563(1)	8564(1)	18(1)
C(10)	1413(1)	3237(1)	10910(1)	14(1)
H(10)	1611	3674	11044	17
C(11)	1975(1)	2745(1)	11306(1)	18(1)
H(11A)	1771	2315	11223	28
H(11B)	2098	2832	11897	28
H(11C)	2415	2776	11049	28
C(12)	713(1)	3157(1)	11279(1)	19(1)
H(12A)	342	3451	11006	29
H(12B)	810	3252	11870	29
H(12C)	538	2718	11197	29
C(13)	1291(1)	4085(1)	7958(1)	33(1)
H(13)	1263	4503	8245	40
C(14)	2043(1)	4036(1)	7706(1)	51(1)
H(14A)	2415	4086	8193	76
H(14B)	2100	4371	7306	76
H(14C)	2097	3617	7456	76
C(15)	696(1)	4083(1)	7197(1)	45(1)
H(15A)	721	3685	6892	68
H(15B)	769	4445	6842	68
H(15C)	218	4119	7372	68
Te(2)	5143(1)	5000	6226(1)	12(1)
Ga(2)	5886(1)	5000	5030(1)	10(1)
N(2)	6609(1)	5693(1)	5020(1)	12(1)
C(21)	7224(1)	5598(1)	4714(1)	14(1)
C(22)	7471(1)	5000	4500(1)	16(1)

H(22)	7848	5000	4173	19
C(23)	7719(1)	6154(1)	4607(1)	22(1)
H(23A)	7502	6412	4136	33
H(23B)	8193	5993	4511	33
H(23C)	7784	6416	5107	33
C(24)	6494(1)	6325(1)	5327(1)	13(1)
C(25)	6219(1)	6817(1)	4783(1)	16(1)
C(26)	6164(1)	7428(1)	5112(1)	20(1)
H(26)	5977	7767	4757	23
C(27)	6377(1)	7550(1)	5940(1)	21(1)
H(27)	6344	7970	6147	25
C(28)	6641(1)	7058(1)	6471(1)	19(1)
H(28)	6782	7145	7041	22
C(29)	6701(1)	6439(1)	6178(1)	15(1)
C(30)	5989(1)	6721(1)	3861(1)	18(1)
H(30)	6096	6271	3721	21
C(31)	5172(1)	6840(1)	3622(1)	24(1)
H(31A)	4904	6562	3948	36
H(31B)	5026	6748	3035	36
H(31C)	5064	7287	3729	36
C(32)	6397(1)	7171(1)	3350(1)	29(1)
H(32A)	6230	7610	3405	44
H(32B)	6300	7044	2769	44
H(32C)	6920	7146	3549	44
C(33)	7017(1)	5918(1)	6769(1)	21(1)
H(33)	6850	5501	6511	25
C(34)	6746(1)	5953(1)	7601(1)	27(1)
H(34A)	6919	6348	7883	41
H(34B)	6933	5587	7940	41
H(34C)	6214	5945	7513	41
C(35)	7850(1)	5924(1)	6885(1)	31(1)
H(35A)	8029	6344	7083	47
H(35B)	8012	5832	6358	47
H(35C)	8042	5598	7289	47
C(41)	0	3977(2)	5000	56(1)
H(41)	0	3521	5000	67
C(42)	433(2)	4305(2)	4543(3)	38(1)
H(42)	732	4074	4223	45
C(43)	430(2)	5000	4550(2)	47(1)
H(43)	727	5234	4237	57
C(44)	0	5311(3)	5000	47(2)
C(41A)	0	6045	5000	48
H(41B)	-331	6198	5348	72
H(41C)	480	6198	5203	72
H(41D)	-149	6198	4449	72

Table 3: Anisotropic displacement parameters ($Å^2 \times 10^3$) for cg_015m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Te(1)	10(1)	16(1)	9(1)	0	0(1)	0
Ga(1)	9(1)	10(1)	9(1)	0	1(1)	0
N(1)	11(1)	12(1)	11(1)	-1(1)	1(1)	0(1)
C(1)	13(1)	15(1)	14(1)	1(1)	2(1)	3(1)

C(2)	10(1)	17(1)	19(1)	0	0(1)	0
C(3)	13(1)	18(1)	26(1)	1(1)	2(1)	5(1)
C(4)	12(1)	12(1)	14(1)	-2(1)	1(1)	2(1)
C(5)	10(1)	13(1)	16(1)	-2(1)	0(1)	1(1)
C(6)	15(1)	13(1)	23(1)	-2(1)	1(1)	-1(1)
C(7)	16(1)	17(1)	26(1)	-9(1)	-1(1)	1(1)
C(8)	21(1)	22(1)	17(1)	-8(1)	-2(1)	4(1)
C(9)	20(1)	18(1)	14(1)	-3(1)	0(1)	5(1)
C(10)	13(1)	13(1)	15(1)	0(1)	0(1)	-1(1)
C(11)	16(1)	18(1)	20(1)	2(1)	-2(1)	2(1)
C(12)	16(1)	19(1)	23(1)	2(1)	5(1)	1(1)
C(13)	68(1)	21(1)	12(1)	-2(1)	5(1)	5(1)
C(14)	62(2)	69(2)	22(1)	8(1)	5(1)	-33(1)
C(15)	75(2)	44(1)	15(1)	0(1)	2(1)	33(1)
Te(2)	10(1)	17(1)	9(1)	0	1(1)	0
Ga(2)	9(1)	10(1)	10(1)	0	1(1)	0
N(2)	12(1)	12(1)	13(1)	0(1)	2(1)	-1(1)
C(21)	12(1)	16(1)	14(1)	2(1)	2(1)	-2(1)
C(22)	14(1)	18(1)	16(1)	0	6(1)	0
C(23)	17(1)	19(1)	31(1)	3(1)	9(1)	-4(1)
C(24)	11(1)	11(1)	17(1)	0(1)	3(1)	-1(1)
C(25)	14(1)	14(1)	19(1)	4(1)	5(1)	-1(1)
C(26)	20(1)	13(1)	27(1)	3(1)	7(1)	1(1)
C(27)	21(1)	13(1)	31(1)	-3(1)	8(1)	-2(1)
C(28)	18(1)	17(1)	22(1)	-5(1)	3(1)	-4(1)
C(29)	14(1)	13(1)	17(1)	-1(1)	1(1)	-3(1)
C(30)	17(1)	19(1)	18(1)	6(1)	4(1)	1(1)
C(31)	17(1)	26(1)	27(1)	7(1)	0(1)	2(1)
C(32)	26(1)	36(1)	26(1)	14(1)	8(1)	-3(1)
C(33)	28(1)	15(1)	16(1)	-1(1)	-5(1)	-1(1)
C(34)	38(1)	25(1)	18(1)	0(1)	-2(1)	-8(1)
C(35)	29(1)	36(1)	26(1)	-3(1)	-5(1)	11(1)
C(41)	54(2)	35(2)	65(2)	0	-32(2)	0
C(42)	22(2)	46(2)	42(2)	-2(2)	-7(1)	3(2)
C(43)	36(2)	54(2)	43(2)	0	-20(1)	0
C(44)	51(4)	34(3)	44(3)	0	-34(3)	0
C(41A)	48	48	48	0	8	0

Table 4: Bond lengths [Å] for cg_015m.

Te(1)-Ga(1)	2.5809(2)	Ga(2)-N(2)	1.9836(11)
Ga(1)-N(1)	1.9922(11)	N(2)-C(21)	1.3369(16)
Ga(1)-Te(1)#1	2.5909(2)	N(2)-C(24)	1.4459(16)
N(1)-C(1)	1.3365(17)	C(21)-C(22)	1.3980(15)
N(1)-C(4)	1.4509(16)	C(21)-C(23)	1.5141(18)
C(1)-C(2)	1.4008(15)	C(22)-C(21)#2	1.3980(15)
C(1)-C(3)	1.5126(18)	C(24)-C(25)	1.4091(18)
C(2)-C(1)#2	1.4007(15)	C(24)-C(29)	1.4123(17)
C(4)-C(5)	1.4096(18)	C(25)-C(26)	1.4004(19)
C(4)-C(9)	1.4117(17)	C(25)-C(30)	1.5226(19)
C(5)-C(6)	1.4024(18)	C(26)-C(27)	1.382(2)
C(5)-C(10)	1.5208(17)	C(27)-C(28)	1.390(2)
C(6)-C(7)	1.3856(19)	C(28)-C(29)	1.3961(18)
C(7)-C(8)	1.382(2)	C(29)-C(33)	1.5179(19)

C(8)-C(9)	1.398(2)	C(30)-C(31)	1.532(2)
C(9)-C(13)	1.512(2)	C(30)-C(32)	1.5405(19)
C(10)-C(12)	1.5308(18)	C(33)-C(34)	1.532(2)
C(10)-C(11)	1.5410(19)	C(33)-C(35)	1.535(2)
C(13)-C(14)	1.525(3)	C(41)-C(42)	1.371(4)
C(13)-C(15)	1.537(3)	C(42)-C(43)	1.459(4)
Te(2)-Ga(2)	2.5755(2)	C(43)-C(44)	1.341(4)
Te(2)-Ga(2)#3	2.5887(2)		

#1 -x,-y+1,-z+2 #2 x,-y+1,z #3 -x+1,-y+1,-z+1

Table 5: Bond angles [°] for cg_015m.

Ga(1)-Te(1)-Ga(1)#1	79.609(7)	N(2)-Ga(2)-Te(2)	116.92(3)
N(1)-Ga(1)-N(1)#2	95.38(6)	N(2)-Ga(2)-Te(2)#3	114.41(3)
N(1)-Ga(1)-Te(1)	117.34(3)	Te(2)-Ga(2)-Te(2)#3	100.944(7)
N(1)-Ga(1)-Te(1)#1	113.66(3)	C(21)-N(2)-C(24)	116.77(11)
Te(1)-Ga(1)-Te(1)#1	100.393(7)	C(21)-N(2)-Ga(2)	121.15(9)
C(1)-N(1)-C(4)	117.62(11)	C(24)-N(2)-Ga(2)	122.08(8)
C(1)-N(1)-Ga(1)	119.81(9)	N(2)-C(21)-C(22)	124.25(13)
C(4)-N(1)-Ga(1)	122.57(8)	N(2)-C(21)-C(23)	120.12(12)
N(1)-C(1)-C(2)	123.95(13)	C(22)-C(21)-C(23)	115.60(12)
N(1)-C(1)-C(3)	120.69(12)	C(21)#2-C(22)-C(21)	127.36(16)
C(2)-C(1)-C(3)	115.32(12)	C(25)-C(24)-C(29)	121.33(12)
C(1)#2-C(2)-C(1)	128.75(17)	C(25)-C(24)-N(2)	120.68(11)
C(5)-C(4)-C(9)	120.87(12)	C(29)-C(24)-N(2)	117.91(11)
C(5)-C(4)-N(1)	120.88(11)	C(26)-C(25)-C(24)	117.89(12)
C(9)-C(4)-N(1)	118.18(11)	C(26)-C(25)-C(30)	118.61(12)
C(6)-C(5)-C(4)	117.93(11)	C(24)-C(25)-C(30)	123.50(12)
C(6)-C(5)-C(10)	118.31(11)	C(27)-C(26)-C(25)	121.45(13)
C(4)-C(5)-C(10)	123.74(11)	C(26)-C(27)-C(28)	120.05(13)
C(7)-C(6)-C(5)	121.70(13)	C(27)-C(28)-C(29)	120.90(13)
C(8)-C(7)-C(6)	119.64(13)	C(28)-C(29)-C(24)	118.36(12)
C(7)-C(8)-C(9)	121.17(12)	C(28)-C(29)-C(33)	119.54(12)
C(8)-C(9)-C(4)	118.68(13)	C(24)-C(29)-C(33)	122.04(12)
C(8)-C(9)-C(13)	119.39(12)	C(25)-C(30)-C(31)	110.34(11)
C(4)-C(9)-C(13)	121.81(13)	C(25)-C(30)-C(32)	112.10(12)
C(5)-C(10)-C(12)	110.57(11)	C(31)-C(30)-C(32)	108.36(12)
C(5)-C(10)-C(11)	111.50(11)	C(29)-C(33)-C(34)	112.84(13)
C(12)-C(10)-C(11)	108.92(11)	C(29)-C(33)-C(35)	110.96(13)
C(9)-C(13)-C(14)	110.14(15)	C(34)-C(33)-C(35)	110.83(13)
C(9)-C(13)-C(15)	112.68(17)	C(42)-C(41)-C(42)#4	119.8(4)
C(14)-C(13)-C(15)	110.81(14)	C(41)-C(42)-C(43)	119.5(4)
Ga(2)-Te(2)-Ga(2)#3	79.056(7)	C(44)-C(43)-C(42)	119.6(4)
N(2)#2-Ga(2)-N(2)	94.20(6)		

#1 -x,-y+1,-z+2 #2 x,-y+1,z #3 -x+1,-y+1,-z+1 #4 -x,y,-z+1

Compound **2**

Table 1: Crystal structure data

Identification code	**cg_005m**
Empirical formula	C_{41} H_{51} Ga N_2 Te_2
Formula weight	896.75
Density (calculated)	1.552 g · cm^{-1}
F(000)	3568
Temperature	100(1) K
Crystal size	0.415 × 0.326 × 0.198 mm
Crystal colour	yellow
Crystal description	plate
Wavelength	0.71073 Å
Crystal system	orthorhombic
Space group	*P b c a*
Unit cell dimensions	
a [Å]	19.1512(8)
b [Å]	19.7070(8)
c [Å]	20.3343(8)
α [°]	90
β [°]	90
γ [°]	90
Volume	7674.4(5) $Å^3$
Z	8
Cell measurement reflections used	46638
Cell measurement ϑ min/max	2.27°/30.20°
Diffractometer control software	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Diffractometer measurement device	Bruker D8 KAPPA series II with APEX II area detector system
Diffractometer measurement method	Data collection strategy APEX 2/COSMO
ϑ range for data collection	2.003°- 30.255°
Completeness to ϑ = 25.242°	99.3%
Completeness to ϑ_{max} = 30.255°	98.4%
Index ranges	-27 ≤ *h* ≤ 27
	-27 ≤ *k* ≤ 26
	-26 ≤ *l* ≤ 28
Computing data reduction	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Absorption coefficient	2.237 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Computation absorption correction	BRUKER AXS SMART APEX 2 Vers. 3.0-2009
Max./min. Transmission	0.75/0.52
R_{merg} before/after correction	0.0902 / 0.0554
Computing structure solution	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Computing structure refinement	BRUKER AXS Inc. 2013 Vers. 2013/4
Refinement method	Full-matrix least-squares on F^2
Reflections collected	131905
Independent reflections	11268
R_{int}	0.0446
Reflections with $I > 2\sigma(I)$	7726
Restraints	0
Parameter	415
GooF	1.127
Weighting details	$w = 1/[\sigma^2(F_{obs}^2) + (0.0247P)^2 + 63.1295P]$
	where $P = (F_{obs}^2 + 2F_{calc}^2)/3$
R_1 [$I > 2\sigma(I)$]	0.0469

wR_2 [$I > 2\sigma(I)$]	0.0941
R_1 [all data]	0.0870
wR_2 [all data]	0.1249
Absolute structure parameter	
Largest diff. peak and hole	2.287/-1.586

Table 2: Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for cg_005m. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	U_{eq}
Ga(1)	3542(1)	6301(1)	2973(1)	16(1)
Te(1)	2286(1)	6266(1)	2546(1)	27(1)
Te(2)	3630(1)	6295(1)	4253(1)	21(1)
N(1)	4091(2)	5566(2)	2593(2)	20(1)
N(2)	4099(2)	7061(2)	2626(2)	17(1)
C(1)	4783(2)	5673(2)	2561(2)	22(1)
C(2)	5084(2)	6305(2)	2603(2)	14(1)
H(2)	5575	6302	2670	17
C(3)	4785(2)	6955(2)	2567(2)	18(1)
C(4)	5267(2)	5074(3)	2482(3)	30(1)
H(4A)	5231	4779	2868	44
H(4B)	5748	5238	2440	44
H(4C)	5139	4818	2087	44
C(5)	5274(2)	7533(2)	2452(3)	25(1)
H(5A)	5010	7934	2313	37
H(5B)	5608	7408	2107	37
H(5C)	5527	7635	2859	37
C(6)	3818(2)	4909(2)	2383(3)	28(1)
C(7)	3732(2)	4382(2)	2834(3)	31(1)
C(8)	3507(2)	3755(3)	2585(3)	36(1)
H(8)	3440	3389	2883	43
C(9)	3382(3)	3651(3)	1937(4)	46(2)
H(9)	3243	3215	1787	55
C(10)	3453(3)	4176(3)	1501(4)	44(2)
H(10)	3361	4103	1047	53
C(11)	3661(3)	4822(3)	1715(3)	35(1)
C(12)	3861(3)	4459(2)	3561(3)	32(1)
H(12)	4053	4923	3641	39
C(13)	3174(3)	4393(3)	3939(4)	48(2)
H(13A)	2826	4696	3742	72
H(13B)	3247	4519	4400	72
H(13C)	3009	3924	3914	72
C(14)	4393(3)	3936(3)	3821(3)	37(1)
H(14A)	4195	3479	3787	56
H(14B)	4502	4035	4282	56
H(14C)	4822	3961	3559	56
C(15)	3708(4)	5386(3)	1217(3)	51(2)
H(15)	3684	5825	1461	61
C(16)	4403(4)	5375(5)	840(4)	67(2)
H(16A)	4790	5425	1151	101
H(16B)	4413	5750	523	101
H(16C)	4449	4943	605	101
C(17)	3101(4)	5378(4)	727(4)	66(2)
H(17A)	3142	4979	442	99

H(17B)	3114	5790	458	99
H(17C)	2658	5358	968	99
C(18)	3819(2)	7726(2)	2466(2)	20(1)
C(19)	3603(3)	7855(2)	1819(3)	26(1)
C(20)	3369(3)	8501(3)	1656(3)	31(1)
H(20)	3245	8596	1213	38
C(21)	3317(3)	9007(2)	2121(3)	31(1)
H(21)	3145	9441	2001	37
C(22)	3510(2)	8878(2)	2761(3)	27(1)
H(22)	3468	9226	3082	32
C(23)	3769(2)	8242(2)	2944(2)	20(1)
C(24)	3625(3)	7311(3)	1296(3)	36(1)
H(24)	3663	6862	1522	44
C(25)	4271(3)	7395(4)	854(3)	53(2)
H(25A)	4219	7805	586	80
H(25B)	4315	6999	566	80
H(25C)	4690	7435	1128	80
C(26)	2962(3)	7304(3)	876(3)	41(1)
H(26A)	2551	7290	1163	61
H(26B)	2965	6903	592	61
H(26C)	2946	7714	604	61
C(27)	4002(2)	8143(2)	3647(3)	25(1)
H(27)	4164	7664	3696	30
C(28)	4614(3)	8612(3)	3827(3)	32(1)
H(28A)	4981	8571	3493	48
H(28B)	4802	8480	4256	48
H(28C)	4450	9082	3845	48
C(29)	3414(3)	8261(3)	4142(3)	37(1)
H(29A)	3286	8742	4143	56
H(29B)	3571	8128	4582	56
H(29C)	3007	7988	4017	56
C(31)	4747(2)	6229(2)	4285(2)	22(1)
C(32)	5081(3)	5603(3)	4316(4)	42(2)
C(33)	5806(3)	5554(3)	4294(4)	52(2)
C(34)	6191(3)	6125(4)	4246(4)	58(2)
C(35)	5884(3)	6760(3)	4241(3)	37(1)
C(36)	5162(2)	6807(3)	4268(3)	28(1)
H(32)	4812	5200	4355	34
H(33)	6029	5123	4309	34
H(34)	6682	6091	4209	34
H(35)	6163	7156	4221	34
H(36)	4949	7242	4276	34
C(41)	1832(2)	6414(3)	3483(2)	25(1)
C(42)	1524(3)	5894(4)	3820(3)	46(2)
H(42)	1522	5446	3648	56
C(43)	1238(4)	6027(4)	4382(4)	54(2)
H(43)	1025	5659	4607	65
C(44)	1202(3)	6644(5)	4685(4)	66(3)
H(44)	976	6704	5097	79
C(45)	1516(4)	7183(4)	4363(4)	57(2)
H(45)	1522	7624	4551	68
C(46)	1822(3)	7065(3)	3759(3)	39(1)
H(46)	2031	7431	3527	47

Table 3: Anisotropic displacement parameters ($Å^2 \times 10^3$) for cg_005m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ga(1)	10(1)	16(1)	22(1)	-2(1)	1(1)	0(1)
Te(1)	11(1)	44(1)	27(1)	-5(1)	-2(1)	-1(1)
Te(2)	16(1)	24(1)	24(1)	1(1)	1(1)	-1(1)
N(1)	13(2)	16(2)	31(2)	-5(1)	1(2)	2(1)
N(2)	11(2)	18(2)	23(2)	-2(1)	0(1)	-1(1)
C(1)	14(2)	24(2)	28(3)	-4(2)	-2(2)	4(2)
C(2)	14(2)	21(2)	8(2)	-9(2)	-1(1)	2(1)
C(3)	13(2)	25(2)	17(2)	-1(2)	0(2)	-3(2)
C(4)	17(2)	29(2)	43(3)	-6(2)	3(2)	7(2)
C(5)	14(2)	29(2)	31(3)	2(2)	2(2)	-7(2)
C(6)	16(2)	18(2)	48(3)	-11(2)	-3(2)	3(2)
C(7)	14(2)	20(2)	58(4)	-8(2)	-4(2)	2(2)
C(8)	19(2)	19(2)	70(4)	-6(2)	-5(2)	2(2)
C(9)	25(2)	27(3)	86(5)	-23(3)	-22(3)	4(2)
C(10)	35(3)	34(3)	64(4)	-26(3)	-24(3)	14(2)
C(11)	32(3)	24(2)	50(4)	-14(2)	-9(2)	9(2)
C(12)	27(2)	17(2)	53(4)	-1(2)	5(2)	-1(2)
C(13)	39(3)	31(3)	75(5)	1(3)	18(3)	-4(2)
C(14)	40(3)	26(2)	46(4)	-1(2)	-1(3)	4(2)
C(15)	78(5)	33(3)	42(4)	-14(3)	-13(4)	9(3)
C(16)	67(5)	86(6)	50(5)	10(4)	-27(4)	-26(4)
C(17)	61(5)	72(5)	64(5)	4(4)	-6(4)	36(4)
C(18)	12(2)	20(2)	28(2)	5(2)	-1(2)	-2(1)
C(19)	26(2)	23(2)	29(3)	3(2)	-5(2)	-4(2)
C(20)	34(3)	29(2)	30(3)	9(2)	-12(2)	-9(2)
C(21)	25(2)	21(2)	47(3)	3(2)	-13(2)	0(2)
C(22)	20(2)	19(2)	41(3)	0(2)	-2(2)	2(2)
C(23)	15(2)	16(2)	29(3)	3(2)	0(2)	-2(1)
C(24)	53(3)	29(3)	28(3)	2(2)	-7(3)	-1(2)
C(25)	38(3)	85(5)	37(4)	-23(3)	-11(3)	14(3)
C(26)	40(3)	51(4)	30(3)	-6(3)	-2(3)	-14(3)
C(27)	24(2)	21(2)	29(3)	-2(2)	1(2)	0(2)
C(28)	38(3)	31(3)	27(3)	-1(2)	-4(2)	-3(2)
C(29)	35(3)	34(3)	42(3)	1(2)	11(3)	5(2)
C(31)	17(2)	33(2)	16(2)	-5(2)	-4(2)	1(2)
C(32)	31(3)	29(3)	67(4)	-12(3)	-20(3)	6(2)
C(33)	36(3)	46(4)	75(5)	-25(3)	-24(3)	18(3)
C(34)	22(3)	83(5)	70(5)	-32(4)	-1(3)	4(3)
C(35)	24(2)	56(4)	30(3)	3(3)	-5(2)	-7(2)
C(36)	21(2)	32(3)	32(3)	1(2)	-5(2)	0(2)
C(41)	9(2)	37(3)	28(3)	6(2)	-4(2)	0(2)
C(42)	46(4)	52(4)	42(4)	8(3)	-5(3)	-20(3)
C(43)	50(4)	51(4)	63(5)	4(3)	-26(4)	-21(3)
C(44)	28(3)	133(8)	37(4)	20(5)	7(3)	9(4)
C(45)	57(4)	64(5)	51(4)	-10(3)	3(4)	24(4)
C(46)	44(3)	34(3)	39(3)	2(2)	2(3)	12(2)

Table 4: Bond lengths [Å] for cg_005m.

Ga(1)-N(1)	1.950(4)	C(15)-C(17)	1.530(10)
Ga(1)-N(2)	1.971(4)	C(18)-C(19)	1.402(7)

Ga(1)-Te(1)	2.5586(5)	C(18)-C(23)	1.411(7)
Ga(1)-Te(2)	2.6076(6)	C(19)-C(20)	1.390(7)
Te(1)-C(41)	2.114(5)	C(19)-C(24)	1.509(7)
Te(2)-C(31)	2.144(4)	C(20)-C(21)	1.378(8)
N(1)-C(1)	1.342(6)	C(21)-C(22)	1.376(8)
N(1)-C(6)	1.461(6)	C(22)-C(23)	1.399(6)
N(2)-C(3)	1.334(5)	C(23)-C(27)	1.509(7)
N(2)-C(18)	1.453(5)	C(24)-C(26)	1.531(8)
C(1)-C(2)	1.377(6)	C(24)-C(25)	1.539(9)
C(1)-C(4)	1.509(6)	C(27)-C(29)	1.529(7)
C(2)-C(3)	1.406(6)	C(27)-C(28)	1.536(7)
C(3)-C(5)	1.494(6)	C(31)-C(36)	1.389(7)
C(6)-C(7)	1.394(8)	C(31)-C(32)	1.392(7)
C(6)-C(11)	1.401(8)	C(32)-C(33)	1.393(8)
C(7)-C(8)	1.404(7)	C(33)-C(34)	1.348(11)
C(7)-C(12)	1.506(9)	C(34)-C(35)	1.382(10)
C(8)-C(9)	1.356(9)	C(35)-C(36)	1.387(7)
C(9)-C(10)	1.370(10)	C(41)-C(42)	1.366(8)
C(10)-C(11)	1.402(7)	C(41)-C(46)	1.402(8)
C(11)-C(15)	1.507(9)	C(42)-C(43)	1.294(11)
C(12)-C(13)	1.528(8)	C(43)-C(44)	1.364(12)
C(12)-C(14)	1.544(7)	C(44)-C(45)	1.384(12)
C(15)-C(16)	1.535(11)	C(45)-C(46)	1.380(9)

Table 5: Bond angles [°] for cg_005m.

N(1)-Ga(1)-N(2)	97.45(15)	C(11)-C(15)-C(16)	112.2(6)
N(1)-Ga(1)-Te(1)	110.65(11)	C(17)-C(15)-C(16)	109.5(6)
N(2)-Ga(1)-Te(1)	114.06(11)	C(19)-C(18)-C(23)	119.8(4)
N(1)-Ga(1)-Te(2)	110.98(12)	C(19)-C(18)-N(2)	118.9(4)
N(2)-Ga(1)-Te(2)	109.00(11)	C(23)-C(18)-N(2)	121.3(4)
Te(1)-Ga(1)-Te(2)	113.587(19)	C(20)-C(19)-C(18)	119.0(5)
C(41)-Te(1)-Ga(1)	94.39(12)	C(20)-C(19)-C(24)	119.4(5)
C(31)-Te(2)-Ga(1)	95.44(12)	C(18)-C(19)-C(24)	121.6(4)
C(1)-N(1)-C(6)	118.5(4)	C(21)-C(20)-C(19)	121.5(5)
C(1)-N(1)-Ga(1)	115.8(3)	C(22)-C(21)-C(20)	119.8(5)
C(6)-N(1)-Ga(1)	125.5(3)	C(21)-C(22)-C(23)	120.8(5)
C(3)-N(2)-C(18)	118.9(4)	C(22)-C(23)-C(18)	119.1(4)
C(3)-N(2)-Ga(1)	116.5(3)	C(22)-C(23)-C(27)	118.2(4)
C(18)-N(2)-Ga(1)	124.5(3)	C(18)-C(23)-C(27)	122.7(4)
N(1)-C(1)-C(2)	123.5(4)	C(19)-C(24)-C(26)	112.1(5)
N(1)-C(1)-C(4)	119.3(4)	C(19)-C(24)-C(25)	110.9(5)
C(2)-C(1)-C(4)	117.2(4)	C(26)-C(24)-C(25)	110.0(5)
C(1)-C(2)-C(3)	130.5(4)	C(23)-C(27)-C(29)	112.7(4)
N(2)-C(3)-C(2)	122.7(4)	C(23)-C(27)-C(28)	111.9(4)
N(2)-C(3)-C(5)	120.8(4)	C(29)-C(27)-C(28)	108.4(4)
C(2)-C(3)-C(5)	116.5(4)	C(36)-C(31)-C(32)	117.7(4)
C(7)-C(6)-C(11)	121.4(5)	C(36)-C(31)-Te(2)	121.4(3)
C(7)-C(6)-N(1)	120.6(5)	C(32)-C(31)-Te(2)	120.9(4)
C(11)-C(6)-N(1)	117.9(5)	C(31)-C(32)-C(33)	121.2(6)
C(6)-C(7)-C(8)	117.0(5)	C(34)-C(33)-C(32)	119.3(6)
C(6)-C(7)-C(12)	123.5(4)	C(33)-C(34)-C(35)	121.6(5)
C(8)-C(7)-C(12)	119.5(5)	C(34)-C(35)-C(36)	118.9(5)
C(9)-C(8)-C(7)	122.5(6)	C(35)-C(36)-C(31)	121.1(5)

C(8)-C(9)-C(10)	119.9(5)	C(42)-C(41)-C(46)	118.6(6)
C(9)-C(10)-C(11)	120.8(6)	C(42)-C(41)-Te(1)	121.8(5)
C(6)-C(11)-C(10)	118.3(6)	C(46)-C(41)-Te(1)	119.5(4)
C(6)-C(11)-C(15)	123.3(5)	C(43)-C(42)-C(41)	118.3(7)
C(10)-C(11)-C(15)	118.5(6)	C(42)-C(43)-C(44)	126.9(7)
C(7)-C(12)-C(13)	110.2(5)	C(43)-C(44)-C(45)	116.6(7)
C(7)-C(12)-C(14)	112.2(4)	C(46)-C(45)-C(44)	118.4(7)
C(13)-C(12)-C(14)	109.8(5)	C(45)-C(46)-C(41)	121.1(6)
C(11)-C(15)-C(17)	112.6(6)		

Compound **3**

Table 1: Crystal structure data

Identification code	**cg_026m**
Empirical formula	C_{35} H_{55} Ga N_2 Te
Formula weight	701.13
Density (calculated)	1.364 g · cm^{-1}
F(000)	1448
Temperature	100(1) K
Crystal size	0.200 × 0.190 × 0.100 mm
Crystal colour	pale yellow
Crystal description	block
Wavelength	0.71073 Å
Crystal system	orthorhombic
Space group	*P n m a*
Unit cell dimensions	
a [Å]	16.888(3)
b [Å]	19.798(3)
c [Å]	10.2125(15)
α [°]	90
β [°]	90
γ [°]	90
Volume	3414.5(9) $Å^3$
Z	4
Cell measurement reflections used	9495
Cell measurement ϑ min/max	2.244°/33.097°
Diffractometer control software	BRUKER D8 KAPPA APEX 2 (3.0-2009)
Diffractometer measurement device	Bruker D8 KAPPA series II with APEX II area detector system
Diffractometer measurement method	Data collection strategy APEX 2/COSMO
ϑ range for data collection	2.057°- 33.202°
Completeness to ϑ = 25.242°	100.0%
Completeness to ϑ_{max} = 33.202°	99.5%
Index ranges	-25 ≤ *h* ≤ 23
	-30 ≤ *k* ≤ 26
	-15 ≤ *l* ≤ 15
Computing data reduction	BRUKER D8 KAPPA APEX 2 (3.0-2009)
Absorption coefficient	1.668 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Computation absorption correction	BRUKER AXS SMART APEX 2 Vers. 3.0-2009
Max./min. Transmission	0.75/0.63
R_{merg} before/after correction	0.0779/0.0415
Computing structure solution	BRUKER D8 KAPPA APEX 2 (3.0-2009)
Computing structure refinement	SHELXL-2014/7 (Sheldrick, 2014)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	77225
Independent reflections	6666
R_{int}	0.0307
Reflections with $I > 2\sigma(I)$	5699
Restraints	0
Parameter	193
GooF	1.046
Weighting details	$w = 1/[\sigma^2(F_{obs}^2) + (0.0288P)^2 + 1.4412P]$
	where $P = (F_{obs}^2 + 2F_{calc}^2)/3$
R_1 [$I > 2\sigma(I)$]	0.0225

wR_2 [$I > 2\sigma(I)$]	0.0534
R_1 [all data]	0.0314
wR_2 [all data]	0.0578
Absolute structure parameter	
Largest diff. peak and hole	0.677/-0.358

Table 2: Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for cg_026m. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	U_{eq}
Te(1)	3342(1)	2500	6506(1)	18(1)
Ga(2)	3842(1)	2500	4106(1)	13(1)
N(1)	3370(1)	3239(1)	3069(1)	14(1)
C(1)	2683(1)	3138(1)	2458(1)	14(1)
C(2)	2330(1)	2500	2311(2)	16(1)
H(2)	1825(13)	2500	1880(20)	19
C(3)	2250(1)	3717(1)	1826(1)	23(1)
H(3A)	2541	4138	1986	34
H(3B)	1718	3753	2201	34
H(3C)	2211	3638	881	34
C(4)	3746(1)	3896(1)	2995(1)	17(1)
C(5)	3557(1)	4402(1)	3909(1)	21(1)
C(6)	3933(1)	5030(1)	3792(2)	31(1)
H(6)	3807	5379	4395	37
C(7)	4482(1)	5151(1)	2816(2)	33(1)
H(7)	4729	5581	2751	40
C(8)	4671(1)	4647(1)	1936(1)	28(1)
H(8)	5053	4732	1274	34
C(9)	4310(1)	4013(1)	2001(1)	20(1)
C(10)	2962(1)	4306(1)	5011(1)	22(1)
H(10)	2782	3825	4998	27
C(11)	2231(1)	4758(1)	4821(1)	29(1)
H(11A)	1872	4702	5566	44
H(11B)	1958	4630	4012	44
H(11C)	2398	5231	4764	44
C(12)	3345(1)	4445(1)	6347(1)	30(1)
H(12A)	3791	4136	6478	45
H(12B)	2953	4375	7042	45
H(12C)	3534	4913	6376	45
C(13)	4516(1)	3485(1)	981(1)	25(1)
H(13)	4329	3037	1311	30
C(14)	5403(1)	3434(1)	736(2)	50(1)
H(14A)	5508	3068	115	75
H(14B)	5676	3341	1563	75
H(14C)	5596	3862	371	75
C(15)	4096(1)	3625(1)	-309(2)	51(1)
H(15A)	3522	3625	-167	76
H(15B)	4233	3274	-945	76
H(15C)	4261	4067	-645	76
C(16)	5019(1)	2500	4213(2)	22(1)
H(16)	5238	2500	3303	26
C(17)	5311(1)	1865(1)	4920(1)	30(1)
H(17A)	5888	1884	5011	46
H(17B)	5164	1464	4411	46

H(17C)	5068	1840	5790	46
C(18)	2041(1)	2500	6449(2)	28(1)
H(18)	1862	2500	5516	34
C(19)	1732(1)	3131(1)	7122(2)	40(1)
H(19A)	1152	3116	7156	61
H(19B)	1900	3531	6630	61
H(19C)	1944	3154	8014	61

Table 3: Anisotropic displacement parameters ($Å^2 \times 10^3$) for cg_026m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Te(1)	20(1)	23(1)	12(1)	0	-1(1)	0
Ga(2)	12(1)	14(1)	12(1)	0	-2(1)	0
N(1)	14(1)	13(1)	14(1)	0(1)	-2(1)	-1(1)
C(1)	15(1)	14(1)	14(1)	1(1)	-1(1)	1(1)
C(2)	14(1)	13(1)	20(1)	0	-3(1)	0
C(3)	23(1)	14(1)	31(1)	4(1)	-10(1)	-1(1)
C(4)	18(1)	13(1)	18(1)	1(1)	-4(1)	-3(1)
C(5)	26(1)	16(1)	22(1)	-2(1)	-4(1)	-4(1)
C(6)	39(1)	19(1)	34(1)	-6(1)	-4(1)	-9(1)
C(7)	37(1)	21(1)	41(1)	1(1)	-3(1)	-15(1)
C(8)	27(1)	24(1)	34(1)	5(1)	0(1)	-9(1)
C(9)	20(1)	18(1)	23(1)	3(1)	-1(1)	-4(1)
C(10)	30(1)	18(1)	20(1)	-5(1)	-2(1)	0(1)
C(11)	33(1)	24(1)	31(1)	-5(1)	-2(1)	4(1)
C(12)	40(1)	24(1)	24(1)	-8(1)	-6(1)	4(1)
C(13)	27(1)	20(1)	29(1)	3(1)	9(1)	-2(1)
C(14)	31(1)	72(1)	47(1)	-7(1)	14(1)	6(1)
C(15)	54(1)	58(1)	41(1)	-25(1)	-14(1)	8(1)
C(16)	13(1)	35(1)	17(1)	0	-2(1)	0
C(17)	21(1)	39(1)	31(1)	0(1)	-7(1)	10(1)
C(18)	20(1)	44(1)	20(1)	0	4(1)	0
C(19)	30(1)	51(1)	40(1)	2(1)	12(1)	10(1)

Table 4: Bond lengths [Å] for cg_026m.

Te(1)-C(18)	2.1983(19)	C(5)-C(10)	1.5209(18)
Te(1)-Ga(2)	2.5929(4)	C(6)-C(7)	1.383(2)
Ga(2)-N(1)	1.9739(10)	C(7)-C(8)	1.381(2)
Ga(2)-N(1)#1	1.9739(10)	C(8)-C(9)	1.3970(17)
Ga(2)-C(16)	1.9902(17)	C(9)-C(13)	1.5162(18)
N(1)-C(1)	1.3321(13)	C(10)-C(12)	1.5353(18)
N(1)-C(4)	1.4502(14)	C(10)-C(11)	1.5366(19)
C(1)-C(2)	1.4044(13)	C(13)-C(15)	1.521(2)
C(1)-C(3)	1.5059(16)	C(13)-C(14)	1.523(2)
C(2)-C(1)#1	1.4044(13)	C(16)-C(17)	1.5313(17)
C(4)-C(5)	1.4050(17)	C(16)-C(17)#1	1.5313(17)
C(4)-C(9)	1.4108(16)	C(18)-C(19)	1.519(2)
C(5)-C(6)	1.4001(18)	C(18)-C(19)#1	1.519(2)

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

Table 5: Bond angles [°] for cg_026m.

C(18)-Te(1)-Ga(2)	107.47(5)	C(4)-C(5)-C(10)	123.54(11)
N(1)-Ga(2)-N(1)#1	95.66(5)	C(7)-C(6)-C(5)	121.35(13)
N(1)-Ga(2)-C(16)	115.64(4)	C(8)-C(7)-C(6)	119.86(13)
N(1)#1-Ga(2)-C(16)	115.64(4)	C(7)-C(8)-C(9)	121.18(13)
N(1)-Ga(2)-Te(1)	112.07(3)	C(8)-C(9)-C(4)	118.41(12)
N(1)#1-Ga(2)-Te(1)	112.07(3)	C(8)-C(9)-C(13)	119.09(11)
C(16)-Ga(2)-Te(1)	105.84(5)	C(4)-C(9)-C(13)	122.46(11)
C(1)-N(1)-C(4)	119.45(9)	C(5)-C(10)-C(12)	110.91(11)
C(1)-N(1)-Ga(2)	119.41(8)	C(5)-C(10)-C(11)	111.40(11)
C(4)-N(1)-Ga(2)	121.11(7)	C(12)-C(10)-C(11)	110.22(10)
N(1)-C(1)-C(2)	123.73(11)	C(9)-C(13)-C(15)	111.21(12)
N(1)-C(1)-C(3)	120.57(10)	C(9)-C(13)-C(14)	112.61(13)
C(2)-C(1)-C(3)	115.66(10)	C(15)-C(13)-C(14)	109.20(14)
C(1)-C(2)-C(1)#1	128.03(14)	C(17)-C(16)-C(17)#1	110.34(15)
C(5)-C(4)-C(9)	120.98(11)	C(17)-C(16)-Ga(2)	110.35(9)
C(5)-C(4)-N(1)	120.35(10)	C(17)#1-C(16)-Ga(2)	110.35(9)
C(9)-C(4)-N(1)	118.66(10)	C(19)-C(18)-C(19)#1	110.74(17)
C(6)-C(5)-C(4)	118.20(12)	C(19)-C(18)-Te(1)	109.38(10)
C(6)-C(5)-C(10)	118.26(12)	C(19)#1-C(18)-Te(1)	109.38(10)

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