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Bis{(*E*)-1-[1-(2-pyridyl)ethylidene]thiosemicarbazonato-κ^3N,N',S}gallium(III) nitrate

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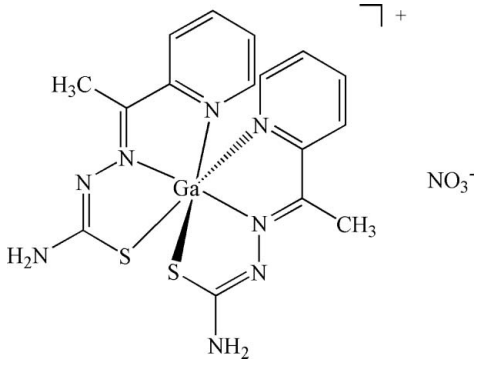
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; disorder in solvent or counterion; R factor = 0.029; wR factor = 0.080; data-to-parameter ratio = 12.3.

Reaction of gallium(III) nitrate with (*E*)-1-[1-(2-pyridyl)ethylidene]thiosemicarbazide (petc) afforded the title complex, $[Ga(C_8H_9N_4S)_2]NO_3$. The title complex contains one Ga^{III} cation and two enol-form petc anions, accompanied by one charge-balancing disordered nitrate anion. The petc is in the enol form, coordinating to the Ga^{III} centre *via* one S atom and two N atoms. Thus, the Ga^{III} centre assumes a distorted octahedral coordination geometry.

Related literature

For related literature, see: Klayman *et al.* (1979); Abram *et al.* (1998).



Experimental

Crystal data

$[Ga(C_8H_9N_4S)_2]NO_3$
M_r = 518.23
Monoclinic, $P2_1/c$
a = 11.715 (2) Å
b = 9.7852 (17) Å
c = 18.079 (3) Å
β = 95.631 (2)°
V = 2062.4 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.58 mm^{-1}
T = 298 (2) K
0.48 × 0.39 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.518, T_{max} = 0.649
10446 measured reflections
3809 independent reflections
3377 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.080
S = 1.02
3809 reflections
310 parameters
36 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL* (Bruker, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2067).

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supplementary materials

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Bis{(*E*)-1-[1-(2-pyridyl)ethylidene]thiosemicarbazonato-κ^3N,N',S}gallium(III) nitrate

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Comment

Heterocyclic thiosemicarbazones, as well as their metal complexes, are currently under discussion. This is due to their complex properties and biological activities (Klayman *et al.*, 1979). We synthesized a new schiff-base ligand (*E*)-1-(1-(pyridin-2-yl)ethylidene)thiosemicarbazide (petc) from 1-(pyridin-2-yl)ethanone and thiosemicarbazide in the lab. Our interest in understanding the relationship between the metal coordination modes with such ligands and their extended structures led us to synthesize the title Ga^{III} complex, (I), and we report its structure here (Fig. 1).

Compound I contains a complex ion made up from the unusual combination of one metal ion and two enol-formed petc molecules. In the petc ligand, the C14—N1 and C6—N4 bond distances clearly show the double bond character for the Schiff base compound, the C16—N2 and C8—N5 bond distances are significantly short while the C16—S1 and C8—S2 bond distance are relatively long (Table 1). This indicates the two coordinated pmtcs are deprotonated enols (Abram *et al.*, 1998). The petc anion chelates the gallium(III) ion with one S atom and two N atoms as a trident ligand (Table 1, Figure 1). Thus the Ga^{III} centre adopts a very distorted hexahedral coordination geometry. A non-coordinated disordered $NO3^{-}$ counter-ion occupys a general position completeing the structure of (I).

Experimental

An methanol solution (10 ml) of Ga(NO3)3 (25.7 mg, 0.10 mmol) was slowly diffused into a dichloromethane solution (10 ml) of (*E*)-1-(1-(pyridin-2-yl)ethylidene)thiosemicarbazide (19.4 mg, 0.10 mmol). Yellow single crystals of (I) were obtained after the solution was allowed to stand at room temperature for ten days.

Refinement

Methyl H atoms were placed in calculated positions with C—H = 0.96 Å and torsion angle was refined to fit the electron density, U_{iso}(H) = 1.5 U_{eq}(C). Other H atoms were placed in calculated positions with N—H = 0.86, C—H = 0.93 (aromatic) or 0.97 Å (methylene), and refined in riding mode with U_{iso}(H) = 1.2U_{eq}(N,*C*).

Figures

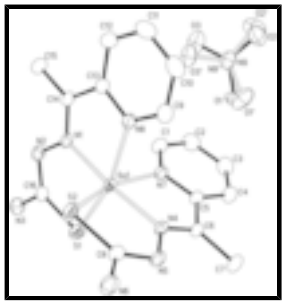


Fig. 1. The diagram of the complex with atom numbering, showing 30% probability displacement ellipsoids.

Bis{(*E*)-1-[1-(2-pyridyl)ethylidene]thiosemicarbazonato-κ^3*N*,*N*',*S*}gallium(III) nitrate

Crystal data

$[Ga(C_8H_9N_4S)_2]NO_3$	F_{000} = 1056
M_r = 518.23	D_x = 1.669 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P2ybc	Cell parameters from 5965 reflections
a = 11.715 (2) Å	θ = 2.4–28.0º
b = 9.7852 (17) Å	μ = 1.58 mm^{-1}
c = 18.079 (3) Å	T = 298 (2) K
β = 95.631 (2)º	Block, yellow
V = 2062.4 (6) Å^3	0.48 × 0.39 × 0.30 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	3809 independent reflections
Radiation source: fine-focus sealed tube	3377 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
T = 298(2) K	θ_{max} = 25.5º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	h = −13→14
T_{min} = 0.518, T_{max} = 0.649	k = −11→9
10446 measured reflections	l = −18→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.029	H-atom parameters constrained

$wR(F^2) = 0.080$	$w = 1/[\sigma^2(F_o^2) + (0.0477P)^2 + 0.6604P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
3809 reflections	$\Delta\rho_{max} = 0.45$ e Å^{-3}
310 parameters	$\Delta\rho_{min} = -0.24$ e Å^{-3}
36 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
N9	0.76005 (18)	0.4989 (2)	0.00088 (11)	0.0411 (5)	0.28 (4)
Ga1	0.752980 (18)	0.03945 (2)	0.146440 (13)	0.03113 (10)	
N1	0.92502 (14)	0.07027 (18)	0.17420 (10)	0.0313 (4)	
N2	0.97719 (15)	0.04506 (18)	0.24397 (11)	0.0363 (4)	
N3	0.94848 (19)	−0.0206 (2)	0.36079 (11)	0.0463 (5)	
H3A	1.0211	−0.0121	0.3725	0.056*	
H3B	0.9047	−0.0462	0.3937	0.056*	
N4	0.57918 (15)	0.03314 (17)	0.11765 (10)	0.0301 (4)	
N5	0.52407 (15)	−0.08256 (18)	0.09147 (10)	0.0352 (4)	
N6	0.54554 (17)	−0.29879 (19)	0.05166 (12)	0.0475 (5)	
H6A	0.4722	−0.3032	0.0424	0.057*	
H6B	0.5873	−0.3681	0.0429	0.057*	
N7	0.70013 (14)	0.24269 (18)	0.16733 (9)	0.0326 (4)	
N8	0.80922 (15)	0.11875 (18)	0.04776 (9)	0.0327 (4)	
N9'	0.76005 (18)	0.4989 (2)	0.00088 (11)	0.0411 (5)	0.72 (4)
C1	0.7672 (2)	0.3470 (2)	0.19012 (13)	0.0415 (5)	
H1	0.8460	0.3332	0.1979	0.050*	
C2	0.7239 (2)	0.4746 (2)	0.20264 (14)	0.0489 (6)	
H2	0.7726	0.5466	0.2176	0.059*	
C3	0.6075 (2)	0.4938 (3)	0.19265 (14)	0.0494 (6)	
H3	0.5762	0.5788	0.2019	0.059*	
C4	0.5367 (2)	0.3863 (2)	0.16880 (13)	0.0424 (5)	
H4	0.4576	0.3981	0.1613	0.051*	
C5	0.58585 (17)	0.2608 (2)	0.15625 (11)	0.0316 (4)	

C6	0.51925 (17)	0.1400 (2)	0.12995 (11)	0.0314 (4)	
C7	0.39180 (18)	0.1432 (3)	0.11965 (14)	0.0435 (5)	
H7A	0.3669	0.1744	0.0704	0.065*	
H7B	0.3639	0.2043	0.1553	0.065*	
H7C	0.3624	0.0531	0.1266	0.065*	
C8	0.59460 (18)	−0.1841 (2)	0.07969 (12)	0.0351 (5)	
C9	0.7436 (2)	0.1406 (2)	−0.01599 (13)	0.0411 (5)	
H9	0.6652	0.1239	−0.0179	0.049*	
C10	0.7888 (2)	0.1868 (3)	−0.07851 (14)	0.0504 (6)	
H10	0.7416	0.2028	−0.1221	0.061*	
C11	0.9046 (2)	0.2092 (3)	−0.07581 (14)	0.0511 (6)	
H11	0.9369	0.2386	−0.1180	0.061*	
C12	0.9732 (2)	0.1881 (2)	−0.01042 (13)	0.0437 (6)	
H12	1.0518	0.2041	−0.0078	0.052*	
C13	0.92311 (18)	0.1427 (2)	0.05134 (12)	0.0330 (5)	
C14	0.98647 (17)	0.1166 (2)	0.12423 (12)	0.0330 (5)	
C15	1.11177 (18)	0.1423 (3)	0.13887 (15)	0.0467 (6)	
H15A	1.1260	0.2005	0.1815	0.070*	
H15B	1.1391	0.1858	0.0964	0.070*	
H15C	1.1511	0.0570	0.1481	0.070*	
C16	0.90376 (19)	0.0060 (2)	0.29146 (12)	0.0350 (5)	
O1	0.681 (3)	0.452 (3)	0.0281 (15)	0.053 (5)	0.28 (4)
O2	0.741 (2)	0.555 (4)	−0.0570 (13)	0.066 (5)	0.28 (4)
O3	0.860 (2)	0.494 (4)	0.0255 (16)	0.077 (6)	0.28 (4)
O1'	0.6636 (9)	0.4511 (11)	0.0137 (7)	0.066 (2)	0.72 (4)
O2'	0.7652 (12)	0.5916 (10)	−0.0457 (6)	0.068 (2)	0.72 (4)
O3'	0.8478 (8)	0.4523 (13)	0.0357 (5)	0.0607 (19)	0.72 (4)
S1	0.75666 (5)	−0.01447 (8)	0.27308 (4)	0.04748 (17)	
S2	0.74308 (5)	−0.18390 (6)	0.09624 (4)	0.04411 (16)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N9	0.0389 (13)	0.0413 (11)	0.0430 (12)	0.0060 (10)	0.0030 (10)	−0.0085 (10)
Ga1	0.01671 (15)	0.03590 (15)	0.04012 (16)	−0.00090 (9)	−0.00051 (10)	0.00223 (9)
N1	0.0195 (9)	0.0330 (9)	0.0405 (10)	0.0011 (7)	−0.0013 (7)	0.0027 (8)
N2	0.0244 (10)	0.0404 (10)	0.0422 (10)	−0.0001 (8)	−0.0064 (8)	0.0035 (8)
N3	0.0412 (12)	0.0544 (12)	0.0414 (11)	0.0025 (10)	−0.0051 (9)	0.0062 (9)
N4	0.0196 (9)	0.0330 (9)	0.0372 (9)	−0.0021 (7)	−0.0005 (7)	0.0009 (7)
N5	0.0216 (9)	0.0338 (9)	0.0494 (10)	−0.0042 (7)	−0.0013 (7)	−0.0016 (8)
N6	0.0320 (11)	0.0355 (10)	0.0738 (14)	−0.0022 (8)	−0.0010 (10)	−0.0076 (10)
N7	0.0253 (9)	0.0344 (9)	0.0380 (9)	−0.0011 (7)	0.0022 (7)	−0.0003 (8)
N8	0.0269 (9)	0.0320 (9)	0.0386 (9)	0.0019 (7)	0.0009 (7)	0.0000 (7)
N9'	0.0389 (13)	0.0413 (11)	0.0430 (12)	0.0060 (10)	0.0030 (10)	−0.0085 (10)
C1	0.0316 (12)	0.0466 (13)	0.0454 (13)	−0.0059 (10)	−0.0014 (10)	−0.0036 (10)
C2	0.0570 (17)	0.0406 (14)	0.0476 (14)	−0.0112 (12)	−0.0025 (12)	−0.0081 (11)
C3	0.0567 (18)	0.0384 (13)	0.0526 (15)	0.0059 (12)	0.0036 (12)	−0.0087 (11)
C4	0.0362 (13)	0.0420 (13)	0.0494 (13)	0.0065 (10)	0.0067 (10)	−0.0037 (10)

C5	0.0250 (11)	0.0365 (11)	0.0332 (10)	0.0008 (9)	0.0020 (8)	0.0005 (9)
C6	0.0202 (10)	0.0388 (11)	0.0353 (11)	0.0017 (9)	0.0027 (8)	0.0028 (9)
C7	0.0224 (11)	0.0507 (14)	0.0569 (14)	0.0033 (10)	0.0011 (10)	−0.0018 (11)
C8	0.0254 (11)	0.0370 (12)	0.0423 (12)	−0.0040 (9)	0.0005 (9)	0.0014 (9)
C9	0.0366 (13)	0.0417 (12)	0.0431 (13)	0.0012 (10)	−0.0060 (10)	−0.0030 (10)
C10	0.0650 (18)	0.0446 (14)	0.0398 (13)	0.0040 (12)	−0.0048 (12)	0.0021 (11)
C11	0.0681 (19)	0.0427 (14)	0.0444 (14)	−0.0028 (12)	0.0145 (12)	0.0043 (11)
C12	0.0397 (13)	0.0390 (12)	0.0542 (14)	−0.0011 (10)	0.0141 (11)	0.0039 (11)
C13	0.0278 (11)	0.0275 (10)	0.0440 (12)	0.0006 (8)	0.0053 (9)	0.0008 (9)
C14	0.0191 (10)	0.0309 (10)	0.0487 (12)	0.0006 (8)	0.0018 (9)	0.0012 (9)
C15	0.0227 (12)	0.0501 (14)	0.0667 (16)	−0.0052 (10)	0.0012 (10)	0.0078 (12)
C16	0.0302 (12)	0.0330 (11)	0.0404 (12)	0.0039 (9)	−0.0027 (9)	0.0020 (9)
O1	0.061 (9)	0.054 (7)	0.048 (7)	0.000 (6)	0.027 (6)	0.013 (5)
O2	0.070 (8)	0.078 (10)	0.049 (6)	0.017 (7)	0.003 (5)	0.019 (7)
O3	0.052 (7)	0.086 (10)	0.091 (8)	0.016 (7)	−0.005 (6)	−0.007 (7)
O1'	0.040 (3)	0.067 (3)	0.091 (5)	−0.010 (2)	0.007 (3)	−0.024 (3)
O2'	0.093 (4)	0.052 (3)	0.063 (3)	0.002 (3)	0.026 (3)	0.006 (2)
O3'	0.047 (3)	0.063 (4)	0.068 (3)	0.010 (2)	−0.0153 (19)	−0.005 (2)
S1	0.0280 (3)	0.0696 (4)	0.0447 (3)	−0.0017 (3)	0.0028 (3)	0.0159 (3)
S2	0.0245 (3)	0.0361 (3)	0.0712 (4)	0.0020 (2)	0.0023 (3)	−0.0050 (3)

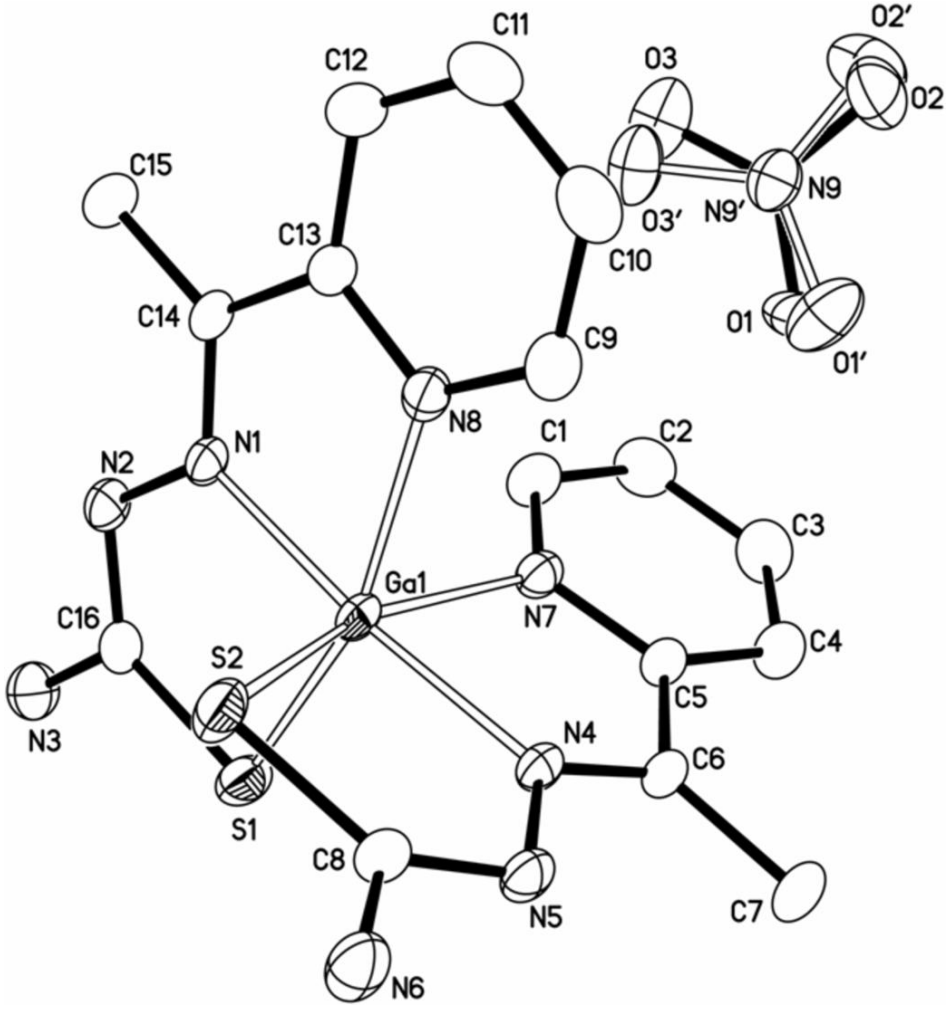
Geometric parameters (Å, °)

N9—O1	1.18 (2)	C2—C3	1.371 (4)
N9—O2	1.18 (2)	C2—H2	0.9300
N9—O3	1.21 (3)	C3—C4	1.381 (4)
Ga1—N1	2.0509 (17)	C3—H3	0.9300
Ga1—N4	2.0523 (17)	C4—C5	1.384 (3)
Ga1—N8	2.1094 (18)	C4—H4	0.9300
Ga1—N7	2.1276 (18)	C5—C6	1.470 (3)
Ga1—S1	2.3458 (8)	C6—C7	1.487 (3)
Ga1—S2	2.3649 (7)	C7—H7A	0.9600
N1—C14	1.291 (3)	C7—H7B	0.9600
N1—N2	1.369 (3)	C7—H7C	0.9600
N2—C16	1.330 (3)	C8—S2	1.736 (2)
N3—C16	1.336 (3)	C9—C10	1.372 (4)
N3—H3A	0.8600	C9—H9	0.9300
N3—H3B	0.8600	C10—C11	1.370 (4)
N4—C6	1.291 (3)	C10—H10	0.9300
N4—N5	1.365 (2)	C11—C12	1.378 (4)
N5—C8	1.323 (3)	C11—H11	0.9300
N6—C8	1.338 (3)	C12—C13	1.385 (3)
N6—H6A	0.8600	C12—H12	0.9300
N6—H6B	0.8600	C13—C14	1.470 (3)
N7—C1	1.328 (3)	C14—C15	1.487 (3)
N7—C5	1.346 (3)	C15—H15A	0.9600
N8—C9	1.338 (3)	C15—H15B	0.9600
N8—C13	1.350 (3)	C15—H15C	0.9600
C1—C2	1.376 (4)	C16—S1	1.734 (2)

C1—H1	0.9300		
O1—N9—O2	117.4 (15)	C3—C4—C5	118.7 (2)
O1—N9—O3	126.8 (17)	C3—C4—H4	120.7
O2—N9—O3	115.8 (16)	C5—C4—H4	120.7
N1—Ga1—N4	173.26 (7)	N7—C5—C4	121.1 (2)
N1—Ga1—N8	76.82 (7)	N7—C5—C6	115.52 (18)
N4—Ga1—N8	100.42 (7)	C4—C5—C6	123.41 (19)
N1—Ga1—N7	96.61 (7)	N4—C6—C5	115.28 (17)
N4—Ga1—N7	76.97 (7)	N4—C6—C7	123.5 (2)
N8—Ga1—N7	85.80 (7)	C5—C6—C7	121.21 (19)
N1—Ga1—S1	82.57 (5)	C6—C7—H7A	109.5
N4—Ga1—S1	99.41 (5)	C6—C7—H7B	109.5
N8—Ga1—S1	158.57 (5)	H7A—C7—H7B	109.5
N7—Ga1—S1	90.85 (5)	C6—C7—H7C	109.5
N1—Ga1—S2	103.87 (5)	H7A—C7—H7C	109.5
N4—Ga1—S2	82.23 (5)	H7B—C7—H7C	109.5
N8—Ga1—S2	91.32 (5)	N5—C8—N6	116.06 (19)
N7—Ga1—S2	158.09 (5)	N5—C8—S2	127.06 (16)
S1—Ga1—S2	99.33 (3)	N6—C8—S2	116.88 (17)
C14—N1—N2	118.61 (18)	N8—C9—C10	121.8 (2)
C14—N1—Ga1	118.83 (14)	N8—C9—H9	119.1
N2—N1—Ga1	122.55 (13)	C10—C9—H9	119.1
C16—N2—N1	112.84 (18)	C11—C10—C9	119.0 (2)
C16—N3—H3A	120.0	C11—C10—H10	120.5
C16—N3—H3B	120.0	C9—C10—H10	120.5
H3A—N3—H3B	120.0	C10—C11—C12	119.9 (2)
C6—N4—N5	119.01 (17)	C10—C11—H11	120.1
C6—N4—Ga1	118.34 (14)	C12—C11—H11	120.1
N5—N4—Ga1	122.46 (13)	C11—C12—C13	118.8 (2)
C8—N5—N4	113.40 (17)	C11—C12—H12	120.6
C8—N6—H6A	120.0	C13—C12—H12	120.6
C8—N6—H6B	120.0	N8—C13—C12	120.8 (2)
H6A—N6—H6B	120.0	N8—C13—C14	114.99 (18)
C1—N7—C5	119.63 (19)	C12—C13—C14	124.2 (2)
C1—N7—Ga1	126.83 (15)	N1—C14—C13	114.91 (18)
C5—N7—Ga1	113.54 (14)	N1—C14—C15	122.9 (2)
C9—N8—C13	119.67 (19)	C13—C14—C15	122.21 (19)
C9—N8—Ga1	125.90 (15)	C14—C15—H15A	109.5
C13—N8—Ga1	114.37 (14)	C14—C15—H15B	109.5
N7—C1—C2	122.1 (2)	H15A—C15—H15B	109.5
N7—C1—H1	118.9	C14—C15—H15C	109.5
C2—C1—H1	118.9	H15A—C15—H15C	109.5
C3—C2—C1	118.7 (2)	H15B—C15—H15C	109.5
C3—C2—H2	120.6	N2—C16—N3	116.3 (2)
C1—C2—H2	120.6	N2—C16—S1	127.09 (17)
C2—C3—C4	119.7 (2)	N3—C16—S1	116.62 (18)
C2—C3—H3	120.1	C16—S1—Ga1	94.80 (8)
C4—C3—H3	120.1	C8—S2—Ga1	94.46 (8)

N8—Ga1—N1—C14	−1.44 (16)	Ga1—N7—C5—C6	−1.7 (2)
N7—Ga1—N1—C14	−85.53 (16)	C3—C4—C5—N7	0.4 (3)
S1—Ga1—N1—C14	−175.53 (16)	C3—C4—C5—C6	−179.2 (2)
S2—Ga1—N1—C14	86.64 (16)	N5—N4—C6—C5	−178.52 (17)
N8—Ga1—N1—N2	177.81 (17)	Ga1—N4—C6—C5	6.4 (2)
N7—Ga1—N1—N2	93.72 (16)	N5—N4—C6—C7	2.2 (3)
S1—Ga1—N1—N2	3.72 (15)	Ga1—N4—C6—C7	−172.84 (17)
S2—Ga1—N1—N2	−94.11 (15)	N7—C5—C6—N4	−2.9 (3)
C14—N1—N2—C16	176.00 (19)	C4—C5—C6—N4	176.7 (2)
Ga1—N1—N2—C16	−3.2 (2)	N7—C5—C6—C7	176.38 (19)
N8—Ga1—N4—C6	−88.82 (16)	C4—C5—C6—C7	−4.0 (3)
N7—Ga1—N4—C6	−5.66 (15)	N4—N5—C8—N6	−177.87 (19)
S1—Ga1—N4—C6	83.03 (15)	N4—N5—C8—S2	1.8 (3)
S2—Ga1—N4—C6	−178.74 (16)	C13—N8—C9—C10	0.1 (3)
N8—Ga1—N4—N5	96.31 (16)	Ga1—N8—C9—C10	−176.99 (17)
N7—Ga1—N4—N5	179.47 (17)	N8—C9—C10—C11	1.0 (4)
S1—Ga1—N4—N5	−91.84 (15)	C9—C10—C11—C12	−1.5 (4)
S2—Ga1—N4—N5	6.40 (15)	C10—C11—C12—C13	0.8 (4)
C6—N4—N5—C8	178.74 (19)	C9—N8—C13—C12	−0.8 (3)
Ga1—N4—N5—C8	−6.4 (2)	Ga1—N8—C13—C12	176.63 (16)
N1—Ga1—N7—C1	0.73 (19)	C9—N8—C13—C14	179.40 (19)
N4—Ga1—N7—C1	−177.18 (19)	Ga1—N8—C13—C14	−3.2 (2)
N8—Ga1—N7—C1	−75.45 (18)	C11—C12—C13—N8	0.3 (3)
S1—Ga1—N7—C1	83.35 (18)	C11—C12—C13—C14	−179.9 (2)
S2—Ga1—N7—C1	−158.52 (14)	N2—N1—C14—C13	−179.08 (17)
N1—Ga1—N7—C5	−178.36 (14)	Ga1—N1—C14—C13	0.2 (2)
N4—Ga1—N7—C5	3.72 (13)	N2—N1—C14—C15	0.8 (3)
N8—Ga1—N7—C5	105.45 (14)	Ga1—N1—C14—C15	−179.96 (16)
S1—Ga1—N7—C5	−95.74 (13)	N8—C13—C14—N1	2.0 (3)
S2—Ga1—N7—C5	22.4 (2)	C12—C13—C14—N1	−177.8 (2)
N1—Ga1—N8—C9	179.73 (19)	N8—C13—C14—C15	−177.81 (19)
N4—Ga1—N8—C9	−6.55 (19)	C12—C13—C14—C15	2.4 (3)
N7—Ga1—N8—C9	−82.46 (18)	N1—N2—C16—N3	179.94 (18)
S1—Ga1—N8—C9	−164.03 (14)	N1—N2—C16—S1	0.1 (3)
S2—Ga1—N8—C9	75.79 (18)	N2—C16—S1—Ga1	2.2 (2)
N1—Ga1—N8—C13	2.50 (14)	N3—C16—S1—Ga1	−177.58 (17)
N4—Ga1—N8—C13	176.22 (14)	N1—Ga1—S1—C16	−2.54 (9)
N7—Ga1—N8—C13	100.31 (15)	N4—Ga1—S1—C16	−176.03 (9)
S1—Ga1—N8—C13	18.7 (2)	N8—Ga1—S1—C16	−18.47 (17)
S2—Ga1—N8—C13	−101.44 (14)	N7—Ga1—S1—C16	−99.10 (9)
C5—N7—C1—C2	−0.4 (3)	S2—Ga1—S1—C16	100.38 (8)
Ga1—N7—C1—C2	−179.40 (18)	N5—C8—S2—Ga1	2.4 (2)
N7—C1—C2—C3	1.3 (4)	N6—C8—S2—Ga1	−177.88 (17)
C1—C2—C3—C4	−1.5 (4)	N1—Ga1—S2—C8	179.11 (9)
C2—C3—C4—C5	0.6 (4)	N4—Ga1—S2—C8	−3.81 (9)
C1—N7—C5—C4	−0.5 (3)	N8—Ga1—S2—C8	−104.15 (9)
Ga1—N7—C5—C4	178.64 (16)	N7—Ga1—S2—C8	−22.15 (16)
C1—N7—C5—C6	179.09 (19)	S1—Ga1—S2—C8	94.52 (8)

Fig. 1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C8
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