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# (*N*-Phenyl-2-{2′-[(phenylethylcarbamoyl)methoxy]biphenyl-2-yloxy}-*N*-ethylacetamide-$\kappa^4O$)(2,4,6-trinitrophenolato-$\kappa O$)bis(2,4,6-trinitrophenolato-$\kappa^2O,O'$)-gadolinium(III)

**Yan-Ling Guo,[a] Ya-Wen Wang,[a] Wei Dou,[a] Wei-Sheng Liu[a]* and Da-Qi Wang[b]**

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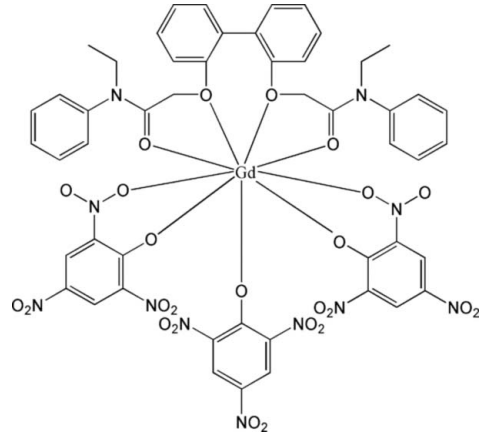
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.008 Å; $R$ factor = 0.036; $wR$ factor = 0.086; data-to-parameter ratio = 12.2.

In the title compound, $[Gd(C_6H_2N_3O_7)_3(C_{32}H_{32}N_2O_4)]$, the $Gd^{III}$ ion is nine-coordinated by four O atoms from the *N*-phenyl-2-{2′-[(phenylethylcarbamoyl)methoxy]biphenyl-2-yloxy}-*N*-ethylacetamide ligand and five from two bidentate and one monodentate 2,4,6-trinitrophenolate (picrate) ligands. The coordination polyhedron around the $Gd^{III}$ ion is a distorted tricapped trigonal prism. The tetradentate ligand wraps around the metal ion with its O atoms and forms a ring-like coordination structure together with the Gd atom. The mean distance between the Gd atom and the coordinated carbonyl O atoms is shorter than that between the Gd atom and the coordinated ether atoms. This suggests that the Gd—O (C═O) bond is stronger than the Gd—O (C—O—C) bond.

## Related literature

For general backgound, see: Lehn, 1995; Steed & Atwood, 2000; Bourne *et al.*, 2001; Evan & Lin, 2002; Janiak, 2003; Carlucci *et al.*, 2003; Gutschke *et al.*, 1996. For related structures, see: Wang *et al.*, 2003.




## Experimental

### *Crystal data*

$[Gd(C_6H_2N_3O_7)_3(C_{32}H_{32}N_2O_4)]$
$M_r$ = 1350.16
Monoclinic, $P2_1/c$
$a$ = 20.125 (2) Å
$b$ = 16.7778 (18) Å
$c$ = 16.6491 (18) Å
$\beta$ = 105.051 (2)°
$V$ = 5428.9 (10) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.32 mm$^{-1}$
$T$ = 298 (2) K
0.40 × 0.37 × 0.29 mm

### *Data collection*

Bruker SMART CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.620, $T_{max}$ = 0.701
28190 measured reflections
9559 independent reflections
6585 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.036

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.087
$S$ = 1.08
9559 reflections
786 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.50 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.58 e Å$^{-3}$

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2162).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, m1619-m1620 [ **doi:10.1107/S160053680702137X** ]

# (*N*-Phenyl-2-{2'-[(phenylethylcarbamoyl)methoxy]biphenyl-2-yloxy}-*N*-ethylacetamide-$\kappa^4O$)(2,4,6-trinitrophenolato-$\kappa O$)bis(2,4,6-trinitrophenolato-$\kappa^2O,O'$)gadolinium(III)

**Y.-L. Guo, Y.-W. Wang, W. Dou, W.-S. Liu and D.-Q. Wang**

## Comment

Metal-directed self-assembly of organic ligands and metal ions, or organometallic moieties, to form well defined structures has been a very attractive field in recent years (Lehn, 1995; Steed & Atwood, 2000; Bourne *et al.*, 2001;), for their fascinating structural diversities and potential application in functional materials, nanotechnology and biological recognition (Evan & Lin, 2002; Janiak, 2003; Carlucci *et al.*, 2003; Gutschke *et al.*, 1996;). We have now investigated the assembly of the ligand *N*-phenyl-2-{2'-[(phenyl- ethyl-carbamoyl)-methoxy]-biphenyl-2-yloxy}-*N*-ethyl-acetamide with gadolinium picrate.

In the title complex I, The Gd(III) ion is coordinated by 9 oxygen donor atoms, five of them belonging to two bidentate and one monodentate picrate groups whereas the remaining four are from the tetradentate ligand *L*(Fig. 1). The coordination polyhedron around Gd(III) ion is a distorted tricapped trigonal prism (Fig. 2) (Wang *et al.*, 2003). The quadridentate ligand wraps around the metal ion with its oxygen atoms and forms a ring-like coordination structure together with the Gd atom. The two phenyl rings about the central bond in the molecule have a drastic twisting, with the dihedral angle between them being 61.18°. The mean distances between the Gd atom and the coordinated ether and carbonyl oxygen atoms are 2.575 Å and 2.3105 Å, respectively. This suggests that the Gd—O (C═O) bond is stronger than the Gd—O (C—O—C) bond.

## Experimental

To a solution of 0.2 mmol gadolinium picrate in 5 ml of ethanol was added dropwise the solution of 0.2 mmol ligand in 10 ml of ethanol. The mixture was stirred at room temperature for 6 h. The precipitated solid complex was filtered, washed with ethanol and dried *in vacuo* over $P_2O_5$ for 72 h. The complex was obtained as yellow powder. Single crystal of the gadolinium complex grew from $CH_3Cl$ and $CH_3CH_2OH$ by slow evaporation at room temperature. After about two weeks, yellow crystal formed from the solution.

## Refinement

All H atoms attached were fixed geometrically and treated as riding with C—H = 0.93 Å ($C_{aromatic}$), 0.97 Å ($C_{methylene}$) and C—H =0.96 Å ($C_{methyl}$) with $U_{iso}(H) = 1.2U_{eq}(C_{aromatic}$ or $C_{methylene})$ and $U_{iso}(H) = 1.5U_{eq}(C_{methyl})$.

**Figures**

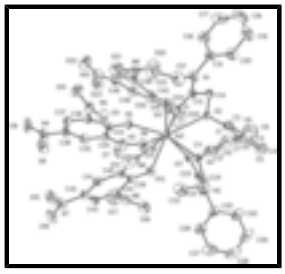


Fig. 1. The independent components of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

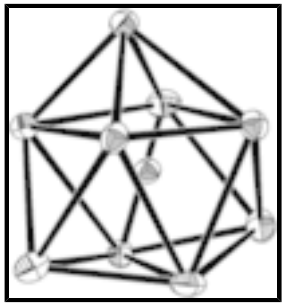


Fig. 2. The coordination polyhedron of (I), showing the distorted tricapped trigonal prism.

**(*N*-Phenyl-2-{2'-[(phenylethylcarbamoyl)methoxy]biphenyl-2-yloxy}- *N*-ethylacetamide-κ$^4$*O*)(2,4,6-trinitrophenolato-κ*O*) bis(2,4,6-trinitrophenolato-κ$^2$*O*,*O*')gadolinium(III)**

*Crystal data*

| | |
|---|---|
| $[Gd(C_6H_2N_3O_7)_3(C_{32}H_{32}N_2O_4)]$ | $F_{000}$ = 2716 |
| $M_r$ = 1350.16 | $D_x$ = 1.652 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 8109 reflections |
| $a$ = 20.125 (2) Å | θ = 2.2–25.3º |
| $b$ = 16.7778 (18) Å | μ = 1.32 mm$^{-1}$ |
| $c$ = 16.6491 (18) Å | $T$ = 298 (2) K |
| β = 105.051 (2)º | Block, yellow |
| $V$ = 5428.9 (10) Å$^3$ | 0.40 × 0.37 × 0.29 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area detector diffractometer | 9559 independent reflections |
| Radiation source: fine-focus sealed tube | 6585 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.036 |
| $T$ = 298(2) K | $\theta_{max}$ = 25.0º |
| phi and ω scans | $\theta_{min}$ = 1.8º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h$ = −16→23 |
| $T_{min}$ = 0.620, $T_{max}$ = 0.701 | $k$ = −19→19 |

28190 measured reflections

$l = -19 \rightarrow 17$

*Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.087$

$S = 1.08$

9559 reflections

786 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0225P)^2 + 8.0112P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.002$

$\Delta\rho_{max} = 1.50$ e Å$^{-3}$

$\Delta\rho_{min} = -0.58$ e Å$^{-3}$

Extinction correction: none

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Gd | 0.749509 (11) | 0.628330 (12) | 0.769967 (14) | 0.03694 (8) |
| N1 | 0.9530 (2) | 0.7437 (2) | 0.8655 (3) | 0.0527 (11) |
| N2 | 0.5485 (2) | 0.7472 (3) | 0.6819 (3) | 0.0604 (12) |
| N3 | 0.6661 (2) | 0.4428 (3) | 0.7896 (3) | 0.0558 (11) |
| N4 | 0.7446 (4) | 0.1794 (3) | 0.7376 (3) | 0.0817 (17) |
| N5 | 0.8962 (2) | 0.4044 (3) | 0.7360 (3) | 0.0580 (11) |
| N6 | 0.8047 (2) | 0.5775 (2) | 0.5830 (3) | 0.0526 (11) |
| N7 | 0.7101 (3) | 0.3392 (3) | 0.4317 (3) | 0.0794 (15) |
| N8 | 0.5725 (2) | 0.4815 (3) | 0.5851 (3) | 0.0649 (13) |
| N9 | 0.9043 (3) | 0.5088 (3) | 0.9422 (3) | 0.0657 (13) |
| N10 | 0.7864 (4) | 0.3033 (3) | 1.0554 (3) | 0.0798 (16) |
| N11 | 0.6777 (3) | 0.5639 (3) | 0.9963 (4) | 0.0712 (14) |
| O1 | 0.85746 (15) | 0.68313 (18) | 0.7941 (2) | 0.0476 (8) |
| O2 | 0.77451 (14) | 0.75760 (16) | 0.85945 (19) | 0.0421 (8) |
| O3 | 0.64424 (14) | 0.69007 (17) | 0.75993 (19) | 0.0411 (7) |
| O4 | 0.72718 (14) | 0.75474 (16) | 0.68295 (18) | 0.0398 (7) |
| O5 | 0.79637 (15) | 0.50497 (16) | 0.7700 (2) | 0.0456 (8) |

| | | | | |
|---|---|---|---|---|
| O6 | 0.66987 (17) | 0.51556 (19) | 0.7911 (2) | 0.0602 (10) |
| O7 | 0.6175 (2) | 0.4090 (2) | 0.8044 (3) | 0.1057 (17) |
| O8 | 0.6861 (3) | 0.1556 (2) | 0.7312 (3) | 0.1065 (17) |
| O9 | 0.7935 (3) | 0.1368 (2) | 0.7345 (3) | 0.1079 (17) |
| O10 | 0.9479 (2) | 0.3659 (2) | 0.7687 (3) | 0.0836 (12) |
| O11 | 0.8964 (2) | 0.4630 (2) | 0.6944 (3) | 0.0776 (12) |
| O12 | 0.68209 (16) | 0.58803 (18) | 0.6408 (2) | 0.0524 (9) |
| O13 | 0.81129 (17) | 0.62156 (19) | 0.6441 (2) | 0.0576 (9) |
| O14 | 0.8431 (2) | 0.5811 (2) | 0.5371 (3) | 0.0747 (11) |
| O15 | 0.7645 (3) | 0.3316 (3) | 0.4143 (3) | 0.1159 (19) |
| O16 | 0.6607 (3) | 0.2947 (3) | 0.4072 (3) | 0.0965 (15) |
| O17 | 0.5489 (2) | 0.4223 (3) | 0.6085 (3) | 0.1105 (17) |
| O18 | 0.5445 (2) | 0.5463 (3) | 0.5762 (3) | 0.0924 (14) |
| O19 | 0.78189 (17) | 0.60133 (18) | 0.9109 (2) | 0.0557 (9) |
| O20 | 0.9221 (2) | 0.5779 (3) | 0.9556 (3) | 0.0882 (13) |
| O21 | 0.9358 (2) | 0.4588 (3) | 0.9138 (3) | 0.0891 (13) |
| O22 | 0.8388 (3) | 0.2635 (3) | 1.0675 (3) | 0.1086 (17) |
| O23 | 0.7321 (3) | 0.2800 (2) | 1.0683 (3) | 0.0938 (14) |
| O24 | 0.6489 (2) | 0.5496 (3) | 1.0510 (3) | 0.0947 (15) |
| O25 | 0.6636 (3) | 0.6196 (3) | 0.9512 (4) | 0.135 (2) |
| C1 | 0.7289 (2) | 0.8213 (3) | 0.8567 (3) | 0.0438 (12) |
| C2 | 0.6850 (3) | 0.8186 (3) | 0.9071 (3) | 0.0571 (14) |
| H2 | 0.6882 | 0.7775 | 0.9455 | 0.069* |
| C3 | 0.6358 (3) | 0.8777 (4) | 0.9003 (4) | 0.0713 (17) |
| H3 | 0.6048 | 0.8759 | 0.9330 | 0.086* |
| C4 | 0.6330 (3) | 0.9391 (4) | 0.8450 (4) | 0.081 (2) |
| H4 | 0.6005 | 0.9792 | 0.8413 | 0.097* |
| C5 | 0.6779 (3) | 0.9420 (3) | 0.7950 (4) | 0.0713 (17) |
| H5 | 0.6759 | 0.9845 | 0.7587 | 0.086* |
| C6 | 0.7264 (2) | 0.8814 (3) | 0.7984 (3) | 0.0495 (12) |
| C7 | 0.7730 (2) | 0.8811 (3) | 0.7422 (3) | 0.0495 (12) |
| C8 | 0.8195 (3) | 0.9428 (3) | 0.7435 (4) | 0.0711 (17) |
| H8 | 0.8203 | 0.9863 | 0.7784 | 0.085* |
| C9 | 0.8642 (3) | 0.9402 (4) | 0.6938 (5) | 0.083 (2) |
| H9 | 0.8956 | 0.9814 | 0.6963 | 0.099* |
| C10 | 0.8633 (3) | 0.8781 (3) | 0.6406 (4) | 0.0692 (16) |
| H10 | 0.8940 | 0.8769 | 0.6074 | 0.083* |
| C11 | 0.8165 (2) | 0.8170 (3) | 0.6364 (3) | 0.0546 (13) |
| H11 | 0.8153 | 0.7745 | 0.6001 | 0.066* |
| C12 | 0.7720 (2) | 0.8196 (3) | 0.6860 (3) | 0.0421 (11) |
| C13 | 0.8865 (2) | 0.7291 (3) | 0.8501 (3) | 0.0404 (11) |
| C14 | 0.8455 (2) | 0.7713 (3) | 0.9012 (3) | 0.0466 (12) |
| H14A | 0.8562 | 0.7498 | 0.9572 | 0.056* |
| H14B | 0.8556 | 0.8279 | 0.9043 | 0.056* |
| C15 | 0.9900 (2) | 0.7912 (3) | 0.9347 (3) | 0.0534 (13) |
| C16 | 1.0082 (3) | 0.7587 (4) | 1.0134 (4) | 0.0774 (18) |
| H16 | 0.9959 | 0.7067 | 1.0226 | 0.093* |
| C17 | 1.0449 (4) | 0.8047 (6) | 1.0778 (5) | 0.112 (3) |
| H17 | 1.0572 | 0.7841 | 1.1314 | 0.135* |

| | | | | |
|---|---|---|---|---|
| C18 | 1.0633 (4) | 0.8798 (6) | 1.0638 (6) | 0.114 (3) |
| H18 | 1.0885 | 0.9100 | 1.1081 | 0.137* |
| C19 | 1.0456 (3) | 0.9123 (4) | 0.9861 (6) | 0.093 (2) |
| H19 | 1.0586 | 0.9641 | 0.9774 | 0.112* |
| C20 | 1.0086 (3) | 0.8675 (3) | 0.9206 (4) | 0.0669 (15) |
| H20 | 0.9962 | 0.8887 | 0.8672 | 0.080* |
| C21 | 0.9901 (3) | 0.7119 (4) | 0.8036 (5) | 0.093 (2) |
| H21A | 0.9609 | 0.7192 | 0.7478 | 0.111* |
| H21B | 1.0317 | 0.7427 | 0.8083 | 0.111* |
| C22 | 1.0076 (4) | 0.6313 (4) | 0.8152 (5) | 0.115 (3) |
| H22A | 1.0355 | 0.6233 | 0.8709 | 0.173* |
| H22B | 1.0329 | 0.6155 | 0.7763 | 0.173* |
| H22C | 0.9665 | 0.5999 | 0.8065 | 0.173* |
| C23 | 0.6152 (2) | 0.7319 (3) | 0.6994 (3) | 0.0406 (11) |
| C24 | 0.6557 (2) | 0.7696 (3) | 0.6443 (3) | 0.0429 (11) |
| H24A | 0.6426 | 0.7462 | 0.5892 | 0.052* |
| H24B | 0.6469 | 0.8265 | 0.6394 | 0.052* |
| C25 | 0.5145 (2) | 0.7904 (3) | 0.6082 (4) | 0.0600 (15) |
| C26 | 0.4971 (3) | 0.7523 (4) | 0.5331 (4) | 0.0774 (18) |
| H26 | 0.5078 | 0.6988 | 0.5295 | 0.093* |
| C27 | 0.4633 (3) | 0.7942 (5) | 0.4619 (5) | 0.097 (2) |
| H27 | 0.4509 | 0.7688 | 0.4105 | 0.117* |
| C28 | 0.4486 (3) | 0.8726 (6) | 0.4686 (5) | 0.102 (3) |
| H28 | 0.4264 | 0.9009 | 0.4212 | 0.122* |
| C29 | 0.4658 (3) | 0.9104 (4) | 0.5432 (5) | 0.096 (2) |
| H29 | 0.4549 | 0.9639 | 0.5466 | 0.115* |
| C30 | 0.4995 (3) | 0.8692 (4) | 0.6143 (4) | 0.0760 (17) |
| H30 | 0.5118 | 0.8950 | 0.6655 | 0.091* |
| C31 | 0.5076 (3) | 0.7199 (4) | 0.7423 (4) | 0.0829 (19) |
| H31A | 0.5353 | 0.7265 | 0.7991 | 0.100* |
| H31B | 0.4666 | 0.7525 | 0.7351 | 0.100* |
| C32 | 0.4882 (4) | 0.6369 (5) | 0.7274 (5) | 0.113 (3) |
| H32A | 0.4636 | 0.6299 | 0.6702 | 0.169* |
| H32B | 0.4592 | 0.6215 | 0.7624 | 0.169* |
| H32C | 0.5288 | 0.6043 | 0.7398 | 0.169* |
| C33 | 0.7823 (2) | 0.4308 (3) | 0.7624 (3) | 0.0403 (11) |
| C34 | 0.7199 (2) | 0.3955 (3) | 0.7704 (3) | 0.0435 (11) |
| C35 | 0.7077 (3) | 0.3137 (3) | 0.7636 (3) | 0.0553 (13) |
| H35 | 0.6665 | 0.2925 | 0.7694 | 0.066* |
| C36 | 0.7573 (3) | 0.2654 (3) | 0.7482 (3) | 0.0585 (15) |
| C37 | 0.8195 (3) | 0.2949 (3) | 0.7425 (3) | 0.0569 (14) |
| H37 | 0.8536 | 0.2605 | 0.7351 | 0.068* |
| C38 | 0.8307 (2) | 0.3745 (3) | 0.7477 (3) | 0.0446 (11) |
| C39 | 0.6896 (2) | 0.5324 (3) | 0.5928 (3) | 0.0420 (11) |
| C40 | 0.7487 (2) | 0.5201 (3) | 0.5628 (3) | 0.0422 (11) |
| C41 | 0.7559 (3) | 0.4577 (3) | 0.5115 (3) | 0.0529 (13) |
| H41 | 0.7957 | 0.4524 | 0.4936 | 0.063* |
| C42 | 0.7036 (3) | 0.4038 (3) | 0.4877 (3) | 0.0548 (14) |
| C43 | 0.6442 (3) | 0.4111 (3) | 0.5133 (3) | 0.0537 (13) |

| | | | | |
|---|---|---|---|---|
| H43 | 0.6092 | 0.3736 | 0.4974 | 0.064* |
| C44 | 0.6373 (2) | 0.4742 (3) | 0.5623 (3) | 0.0463 (12) |
| C45 | 0.7854 (3) | 0.5374 (3) | 0.9522 (3) | 0.0495 (13) |
| C46 | 0.8420 (3) | 0.4827 (3) | 0.9640 (3) | 0.0503 (13) |
| C47 | 0.8420 (3) | 0.4077 (3) | 0.9951 (3) | 0.0576 (14) |
| H47 | 0.8786 | 0.3733 | 0.9974 | 0.069* |
| C48 | 0.7870 (3) | 0.3842 (3) | 1.0228 (3) | 0.0586 (14) |
| C49 | 0.7337 (3) | 0.4356 (3) | 1.0239 (3) | 0.0597 (14) |
| H49 | 0.6985 | 0.4200 | 1.0472 | 0.072* |
| C50 | 0.7336 (3) | 0.5102 (3) | 0.9904 (3) | 0.0539 (13) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Gd | 0.03632 (13) | 0.02908 (11) | 0.04381 (13) | 0.00121 (11) | 0.00754 (9) | −0.00233 (11) |
| N1 | 0.037 (2) | 0.055 (3) | 0.070 (3) | −0.009 (2) | 0.021 (2) | −0.017 (2) |
| N2 | 0.037 (2) | 0.070 (3) | 0.076 (3) | 0.010 (2) | 0.017 (2) | 0.027 (2) |
| N3 | 0.060 (3) | 0.051 (3) | 0.061 (3) | −0.011 (2) | 0.024 (2) | 0.003 (2) |
| N4 | 0.141 (5) | 0.024 (2) | 0.083 (4) | −0.008 (3) | 0.034 (4) | 0.005 (2) |
| N5 | 0.058 (3) | 0.053 (3) | 0.068 (3) | 0.014 (2) | 0.025 (2) | −0.007 (2) |
| N6 | 0.055 (3) | 0.052 (3) | 0.049 (3) | 0.006 (2) | 0.010 (2) | 0.010 (2) |
| N7 | 0.082 (4) | 0.082 (4) | 0.067 (4) | 0.012 (3) | 0.006 (3) | −0.030 (3) |
| N8 | 0.056 (3) | 0.078 (4) | 0.059 (3) | −0.008 (3) | 0.013 (2) | −0.019 (3) |
| N9 | 0.068 (3) | 0.074 (3) | 0.053 (3) | 0.006 (3) | 0.013 (2) | 0.007 (3) |
| N10 | 0.110 (5) | 0.067 (4) | 0.062 (3) | −0.006 (4) | 0.021 (3) | 0.016 (3) |
| N11 | 0.075 (4) | 0.057 (3) | 0.085 (4) | −0.009 (3) | 0.028 (3) | −0.014 (3) |
| O1 | 0.0425 (19) | 0.0457 (18) | 0.055 (2) | −0.0046 (15) | 0.0132 (15) | −0.0132 (16) |
| O2 | 0.0371 (18) | 0.0340 (16) | 0.053 (2) | 0.0047 (13) | 0.0076 (14) | −0.0029 (14) |
| O3 | 0.0390 (18) | 0.0380 (17) | 0.047 (2) | 0.0055 (14) | 0.0124 (15) | 0.0019 (15) |
| O4 | 0.0328 (17) | 0.0326 (16) | 0.053 (2) | 0.0002 (13) | 0.0082 (14) | 0.0022 (14) |
| O5 | 0.0463 (19) | 0.0267 (16) | 0.067 (2) | 0.0026 (14) | 0.0214 (16) | −0.0031 (15) |
| O6 | 0.057 (2) | 0.0381 (19) | 0.093 (3) | 0.0003 (17) | 0.032 (2) | 0.0017 (18) |
| O7 | 0.090 (3) | 0.070 (3) | 0.186 (5) | −0.021 (2) | 0.087 (3) | −0.001 (3) |
| O8 | 0.148 (5) | 0.054 (3) | 0.123 (4) | −0.038 (3) | 0.044 (4) | −0.008 (2) |
| O9 | 0.167 (5) | 0.037 (2) | 0.123 (4) | 0.029 (3) | 0.043 (3) | −0.003 (2) |
| O10 | 0.062 (3) | 0.086 (3) | 0.103 (3) | 0.030 (2) | 0.022 (2) | 0.005 (3) |
| O11 | 0.075 (3) | 0.064 (3) | 0.109 (3) | 0.010 (2) | 0.052 (2) | 0.017 (2) |
| O12 | 0.056 (2) | 0.0490 (19) | 0.048 (2) | 0.0068 (16) | 0.0069 (16) | −0.0169 (16) |
| O13 | 0.061 (2) | 0.048 (2) | 0.060 (2) | −0.0081 (18) | 0.0088 (17) | −0.0074 (19) |
| O14 | 0.077 (3) | 0.084 (3) | 0.070 (3) | −0.011 (2) | 0.032 (2) | 0.004 (2) |
| O15 | 0.089 (4) | 0.146 (5) | 0.108 (4) | 0.025 (3) | 0.018 (3) | −0.072 (3) |
| O16 | 0.111 (4) | 0.080 (3) | 0.091 (3) | −0.011 (3) | 0.013 (3) | −0.047 (3) |
| O17 | 0.102 (4) | 0.116 (4) | 0.132 (5) | −0.034 (3) | 0.064 (3) | −0.001 (3) |
| O18 | 0.058 (3) | 0.103 (4) | 0.114 (4) | 0.010 (3) | 0.019 (2) | −0.039 (3) |
| O19 | 0.076 (2) | 0.0409 (19) | 0.048 (2) | 0.0006 (17) | 0.0120 (17) | 0.0030 (16) |
| O20 | 0.084 (3) | 0.082 (3) | 0.100 (4) | −0.020 (3) | 0.025 (2) | 0.006 (3) |
| O21 | 0.077 (3) | 0.104 (3) | 0.092 (3) | 0.019 (3) | 0.033 (3) | 0.006 (3) |
| O22 | 0.130 (4) | 0.076 (3) | 0.121 (4) | 0.031 (3) | 0.034 (3) | 0.041 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O23 | 0.128 (4) | 0.072 (3) | 0.082 (3) | −0.026 (3) | 0.027 (3) | 0.015 (2) |
| O24 | 0.093 (3) | 0.084 (3) | 0.124 (4) | −0.014 (3) | 0.059 (3) | −0.024 (3) |
| O25 | 0.138 (5) | 0.114 (4) | 0.176 (6) | 0.071 (4) | 0.081 (4) | 0.067 (4) |
| C1 | 0.038 (3) | 0.033 (3) | 0.056 (3) | 0.003 (2) | 0.005 (2) | −0.016 (2) |
| C2 | 0.052 (3) | 0.060 (3) | 0.060 (4) | 0.000 (3) | 0.016 (3) | −0.021 (3) |
| C3 | 0.056 (4) | 0.082 (4) | 0.077 (4) | 0.004 (3) | 0.018 (3) | −0.035 (4) |
| C4 | 0.064 (4) | 0.077 (4) | 0.094 (5) | 0.027 (3) | 0.007 (4) | −0.038 (4) |
| C5 | 0.075 (4) | 0.045 (3) | 0.085 (5) | 0.016 (3) | 0.005 (4) | −0.008 (3) |
| C6 | 0.048 (3) | 0.029 (3) | 0.066 (3) | 0.005 (2) | 0.005 (3) | −0.007 (2) |
| C7 | 0.050 (3) | 0.031 (3) | 0.062 (3) | −0.002 (2) | 0.005 (3) | 0.006 (2) |
| C8 | 0.086 (5) | 0.036 (3) | 0.086 (5) | −0.016 (3) | 0.013 (4) | 0.006 (3) |
| C9 | 0.076 (5) | 0.059 (4) | 0.106 (6) | −0.034 (3) | 0.010 (4) | 0.024 (4) |
| C10 | 0.056 (3) | 0.067 (4) | 0.087 (5) | −0.011 (3) | 0.023 (3) | 0.027 (4) |
| C11 | 0.053 (3) | 0.054 (3) | 0.058 (4) | −0.001 (3) | 0.015 (3) | 0.013 (3) |
| C12 | 0.035 (3) | 0.035 (3) | 0.053 (3) | −0.002 (2) | 0.005 (2) | 0.010 (2) |
| C13 | 0.039 (3) | 0.035 (2) | 0.048 (3) | −0.003 (2) | 0.014 (2) | −0.002 (2) |
| C14 | 0.039 (3) | 0.049 (3) | 0.050 (3) | 0.000 (2) | 0.007 (2) | −0.011 (2) |
| C15 | 0.034 (3) | 0.058 (3) | 0.066 (4) | −0.009 (2) | 0.011 (2) | −0.013 (3) |
| C16 | 0.064 (4) | 0.081 (4) | 0.080 (5) | −0.008 (3) | 0.007 (3) | 0.000 (4) |
| C17 | 0.094 (6) | 0.153 (8) | 0.070 (5) | −0.008 (6) | −0.012 (4) | −0.007 (5) |
| C18 | 0.081 (5) | 0.134 (8) | 0.113 (7) | −0.037 (5) | 0.001 (5) | −0.053 (6) |
| C19 | 0.069 (5) | 0.077 (5) | 0.137 (7) | −0.028 (4) | 0.030 (5) | −0.030 (5) |
| C20 | 0.048 (3) | 0.067 (4) | 0.088 (4) | −0.012 (3) | 0.023 (3) | −0.009 (3) |
| C21 | 0.057 (4) | 0.085 (5) | 0.147 (7) | −0.010 (4) | 0.044 (4) | −0.019 (5) |
| C22 | 0.084 (5) | 0.109 (6) | 0.154 (8) | 0.010 (5) | 0.033 (5) | −0.011 (6) |
| C23 | 0.038 (3) | 0.034 (2) | 0.049 (3) | 0.000 (2) | 0.012 (2) | −0.005 (2) |
| C24 | 0.033 (3) | 0.046 (3) | 0.048 (3) | 0.005 (2) | 0.009 (2) | 0.003 (2) |
| C25 | 0.034 (3) | 0.068 (4) | 0.078 (4) | 0.008 (3) | 0.015 (3) | 0.019 (3) |
| C26 | 0.057 (4) | 0.084 (4) | 0.087 (5) | −0.003 (3) | 0.010 (3) | 0.012 (4) |
| C27 | 0.070 (5) | 0.128 (7) | 0.088 (6) | 0.001 (5) | 0.010 (4) | 0.004 (5) |
| C28 | 0.068 (4) | 0.144 (8) | 0.094 (6) | 0.027 (5) | 0.020 (4) | 0.052 (6) |
| C29 | 0.074 (5) | 0.095 (5) | 0.123 (7) | 0.034 (4) | 0.031 (5) | 0.046 (5) |
| C30 | 0.054 (3) | 0.082 (4) | 0.094 (5) | 0.021 (3) | 0.021 (3) | 0.021 (4) |
| C31 | 0.054 (4) | 0.094 (5) | 0.101 (5) | 0.006 (3) | 0.020 (3) | 0.028 (4) |
| C32 | 0.092 (5) | 0.128 (7) | 0.120 (7) | −0.025 (5) | 0.033 (5) | −0.014 (5) |
| C33 | 0.049 (3) | 0.034 (3) | 0.036 (3) | 0.003 (2) | 0.008 (2) | 0.003 (2) |
| C34 | 0.051 (3) | 0.040 (3) | 0.042 (3) | 0.000 (2) | 0.016 (2) | 0.000 (2) |
| C35 | 0.073 (4) | 0.047 (3) | 0.048 (3) | −0.007 (3) | 0.021 (3) | 0.005 (2) |
| C36 | 0.093 (4) | 0.029 (2) | 0.054 (4) | 0.000 (3) | 0.021 (3) | 0.001 (2) |
| C37 | 0.075 (4) | 0.044 (3) | 0.051 (3) | 0.016 (3) | 0.016 (3) | −0.002 (2) |
| C38 | 0.056 (3) | 0.032 (2) | 0.047 (3) | 0.005 (2) | 0.015 (2) | 0.000 (2) |
| C39 | 0.051 (3) | 0.038 (3) | 0.034 (3) | 0.005 (2) | 0.005 (2) | 0.001 (2) |
| C40 | 0.048 (3) | 0.037 (3) | 0.036 (3) | 0.000 (2) | 0.002 (2) | 0.001 (2) |
| C41 | 0.055 (3) | 0.059 (3) | 0.043 (3) | 0.010 (3) | 0.009 (2) | 0.000 (3) |
| C42 | 0.067 (4) | 0.054 (3) | 0.040 (3) | 0.007 (3) | 0.008 (3) | −0.016 (2) |
| C43 | 0.067 (4) | 0.042 (3) | 0.048 (3) | −0.009 (3) | 0.008 (3) | −0.006 (2) |
| C44 | 0.053 (3) | 0.045 (3) | 0.040 (3) | 0.002 (2) | 0.011 (2) | −0.002 (2) |
| C45 | 0.061 (3) | 0.045 (3) | 0.038 (3) | −0.002 (3) | 0.005 (2) | −0.003 (2) |
| C46 | 0.056 (3) | 0.050 (3) | 0.045 (3) | −0.001 (3) | 0.012 (2) | 0.005 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C47 | 0.069 (4) | 0.055 (3) | 0.047 (3) | 0.010 (3) | 0.011 (3) | 0.010 (3) |
| C48 | 0.075 (4) | 0.049 (3) | 0.049 (3) | 0.003 (3) | 0.011 (3) | 0.015 (3) |
| C49 | 0.063 (4) | 0.064 (4) | 0.052 (3) | −0.008 (3) | 0.016 (3) | 0.004 (3) |
| C50 | 0.060 (3) | 0.048 (3) | 0.052 (3) | 0.000 (3) | 0.010 (3) | −0.003 (3) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Gd—O5 | 2.274 (3) | C10—C11 | 1.380 (7) |
| Gd—O1 | 2.296 (3) | C10—H10 | 0.9300 |
| Gd—O19 | 2.311 (3) | C11—C12 | 1.369 (7) |
| Gd—O3 | 2.325 (3) | C11—H11 | 0.9300 |
| Gd—O12 | 2.326 (3) | C13—C14 | 1.508 (6) |
| Gd—O4 | 2.542 (3) | C14—H14A | 0.9700 |
| Gd—O6 | 2.562 (3) | C14—H14B | 0.9700 |
| Gd—O2 | 2.605 (3) | C15—C20 | 1.370 (7) |
| Gd—O13 | 2.703 (4) | C15—C16 | 1.378 (7) |
| N1—C13 | 1.318 (5) | C16—C17 | 1.371 (9) |
| N1—C15 | 1.440 (6) | C16—H16 | 0.9300 |
| N1—C21 | 1.517 (7) | C17—C18 | 1.350 (10) |
| N2—C23 | 1.321 (5) | C17—H17 | 0.9300 |
| N2—C25 | 1.436 (6) | C18—C19 | 1.363 (10) |
| N2—C31 | 1.527 (7) | C18—H18 | 0.9300 |
| N3—O7 | 1.209 (5) | C19—C20 | 1.373 (8) |
| N3—O6 | 1.223 (5) | C19—H19 | 0.9300 |
| N3—C34 | 1.445 (6) | C20—H20 | 0.9300 |
| N4—O8 | 1.221 (6) | C21—C22 | 1.397 (8) |
| N4—O9 | 1.228 (7) | C21—H21A | 0.9700 |
| N4—C36 | 1.468 (6) | C21—H21B | 0.9700 |
| N5—O11 | 1.203 (5) | C22—H22A | 0.9600 |
| N5—O10 | 1.225 (5) | C22—H22B | 0.9600 |
| N5—C38 | 1.469 (6) | C22—H22C | 0.9600 |
| N6—O14 | 1.221 (5) | C23—C24 | 1.515 (6) |
| N6—O13 | 1.236 (5) | C24—H24A | 0.9700 |
| N6—C40 | 1.454 (6) | C24—H24B | 0.9700 |
| N7—O15 | 1.210 (6) | C25—C26 | 1.365 (8) |
| N7—O16 | 1.224 (6) | C25—C30 | 1.367 (7) |
| N7—C42 | 1.458 (6) | C26—C27 | 1.394 (9) |
| N8—O17 | 1.208 (6) | C26—H26 | 0.9300 |
| N8—O18 | 1.216 (6) | C27—C28 | 1.360 (10) |
| N8—C44 | 1.453 (6) | C27—H27 | 0.9300 |
| N9—O20 | 1.218 (6) | C28—C29 | 1.357 (10) |
| N9—O21 | 1.219 (6) | C28—H28 | 0.9300 |
| N9—C46 | 1.460 (7) | C29—C30 | 1.386 (8) |
| N10—O22 | 1.221 (6) | C29—H29 | 0.9300 |
| N10—O23 | 1.230 (6) | C30—H30 | 0.9300 |
| N10—C48 | 1.462 (7) | C31—C32 | 1.451 (8) |
| N11—O25 | 1.186 (6) | C31—H31A | 0.9700 |
| N11—O24 | 1.223 (6) | C31—H31B | 0.9700 |
| N11—C50 | 1.466 (7) | C32—H32A | 0.9600 |

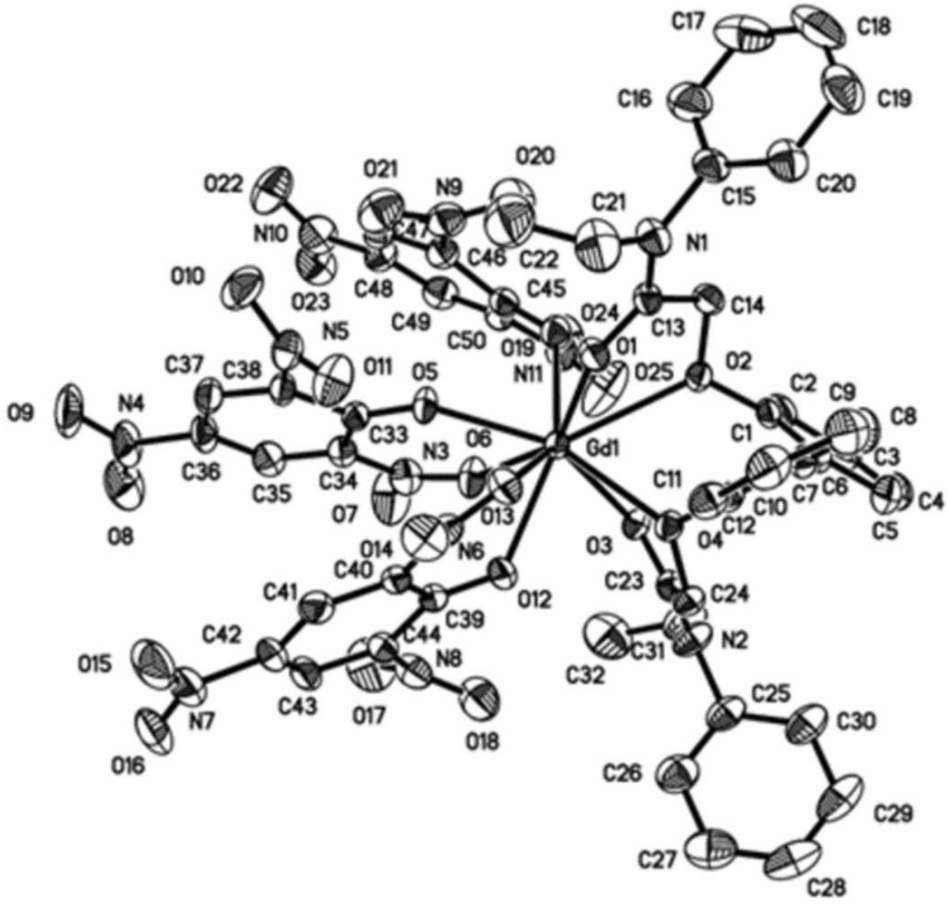
| | | | |
|---|---|---|---|
| O1—C13 | 1.234 (5) | C32—H32B | 0.9600 |
| O2—C1 | 1.402 (5) | C32—H32C | 0.9600 |
| O2—C14 | 1.436 (5) | C33—C38 | 1.424 (6) |
| O3—C23 | 1.243 (5) | C33—C34 | 1.426 (6) |
| O4—C12 | 1.405 (5) | C34—C35 | 1.393 (6) |
| O4—C24 | 1.437 (5) | C35—C36 | 1.360 (7) |
| O5—C33 | 1.275 (5) | C35—H35 | 0.9300 |
| O12—C39 | 1.262 (5) | C36—C37 | 1.372 (7) |
| O19—C45 | 1.266 (5) | C37—C38 | 1.354 (6) |
| C1—C2 | 1.368 (7) | C37—H37 | 0.9300 |
| C1—C6 | 1.391 (7) | C39—C40 | 1.420 (6) |
| C2—C3 | 1.385 (7) | C39—C44 | 1.429 (6) |
| C2—H2 | 0.9300 | C40—C41 | 1.382 (6) |
| C3—C4 | 1.371 (8) | C41—C42 | 1.365 (7) |
| C3—H3 | 0.9300 | C41—H41 | 0.9300 |
| C4—C5 | 1.379 (8) | C42—C43 | 1.375 (7) |
| C4—H4 | 0.9300 | C43—C44 | 1.367 (6) |
| C5—C6 | 1.400 (7) | C43—H43 | 0.9300 |
| C5—H5 | 0.9300 | C45—C50 | 1.429 (7) |
| C6—C7 | 1.487 (7) | C45—C46 | 1.436 (7) |
| C7—C12 | 1.390 (6) | C46—C47 | 1.361 (6) |
| C7—C8 | 1.392 (7) | C47—C48 | 1.363 (7) |
| C8—C9 | 1.373 (8) | C47—H47 | 0.9300 |
| C8—H8 | 0.9300 | C48—C49 | 1.380 (7) |
| C9—C10 | 1.364 (8) | C49—C50 | 1.369 (7) |
| C9—H9 | 0.9300 | C49—H49 | 0.9300 |
| O5—Gd—O1 | 89.48 (10) | C13—C14—H14B | 110.6 |
| O5—Gd—O19 | 79.26 (11) | H14A—C14—H14B | 108.7 |
| O1—Gd—O19 | 84.06 (12) | C20—C15—C16 | 121.0 (5) |
| O5—Gd—O3 | 140.85 (10) | C20—C15—N1 | 119.2 (5) |
| O1—Gd—O3 | 129.59 (10) | C16—C15—N1 | 119.7 (5) |
| O19—Gd—O3 | 99.89 (11) | C17—C16—C15 | 118.4 (6) |
| O5—Gd—O12 | 82.99 (11) | C17—C16—H16 | 120.8 |
| O1—Gd—O12 | 125.18 (12) | C15—C16—H16 | 120.8 |
| O19—Gd—O12 | 145.59 (12) | C18—C17—C16 | 120.5 (8) |
| O3—Gd—O12 | 76.19 (11) | C18—C17—H17 | 119.8 |
| O5—Gd—O4 | 140.48 (10) | C16—C17—H17 | 119.8 |
| O1—Gd—O4 | 77.57 (10) | C17—C18—C19 | 121.4 (7) |
| O19—Gd—O4 | 134.73 (10) | C17—C18—H18 | 119.3 |
| O3—Gd—O4 | 64.17 (10) | C19—C18—H18 | 119.3 |
| O12—Gd—O4 | 74.99 (10) | C18—C19—C20 | 119.2 (7) |
| O5—Gd—O6 | 66.55 (11) | C18—C19—H19 | 120.4 |
| O1—Gd—O6 | 150.32 (11) | C20—C19—H19 | 120.4 |
| O19—Gd—O6 | 74.79 (12) | C15—C20—C19 | 119.5 (6) |
| O3—Gd—O6 | 75.41 (10) | C15—C20—H20 | 120.3 |
| O12—Gd—O6 | 71.14 (12) | C19—C20—H20 | 120.3 |
| O4—Gd—O6 | 132.07 (10) | C22—C21—N1 | 113.4 (6) |
| O5—Gd—O2 | 137.64 (10) | C22—C21—H21A | 108.9 |
| O1—Gd—O2 | 62.18 (10) | N1—C21—H21A | 108.9 |

| | | | |
|---|---|---|---|
| O19—Gd—O2 | 67.72 (10) | C22—C21—H21B | 108.9 |
| O3—Gd—O2 | 72.98 (9) | N1—C21—H21B | 108.9 |
| O12—Gd—O2 | 138.64 (10) | H21A—C21—H21B | 107.7 |
| O4—Gd—O2 | 67.09 (9) | C21—C22—H22A | 109.5 |
| O6—Gd—O2 | 124.83 (10) | C21—C22—H22B | 109.5 |
| O5—Gd—O13 | 71.81 (11) | H22A—C22—H22B | 109.5 |
| O1—Gd—O13 | 63.09 (10) | C21—C22—H22C | 109.5 |
| O19—Gd—O13 | 135.55 (11) | H22A—C22—H22C | 109.5 |
| O3—Gd—O13 | 123.85 (10) | H22B—C22—H22C | 109.5 |
| O12—Gd—O13 | 62.99 (11) | O3—C23—N2 | 121.7 (4) |
| O4—Gd—O13 | 69.02 (10) | O3—C23—C24 | 120.8 (4) |
| O6—Gd—O13 | 120.36 (10) | N2—C23—C24 | 117.4 (4) |
| O2—Gd—O13 | 114.77 (10) | O4—C24—C23 | 106.9 (3) |
| C13—N1—C15 | 123.1 (4) | O4—C24—H24A | 110.3 |
| C13—N1—C21 | 117.1 (4) | C23—C24—H24A | 110.3 |
| C15—N1—C21 | 119.7 (4) | O4—C24—H24B | 110.3 |
| C23—N2—C25 | 121.2 (4) | C23—C24—H24B | 110.3 |
| C23—N2—C31 | 119.1 (4) | H24A—C24—H24B | 108.6 |
| C25—N2—C31 | 119.7 (4) | C26—C25—C30 | 120.8 (6) |
| O7—N3—O6 | 120.9 (5) | C26—C25—N2 | 119.9 (5) |
| O7—N3—C34 | 118.6 (4) | C30—C25—N2 | 119.3 (6) |
| O6—N3—C34 | 120.5 (4) | C25—C26—C27 | 119.7 (7) |
| O8—N4—O9 | 124.7 (5) | C25—C26—H26 | 120.1 |
| O8—N4—C36 | 117.8 (6) | C27—C26—H26 | 120.1 |
| O9—N4—C36 | 117.5 (6) | C28—C27—C26 | 119.1 (7) |
| O11—N5—O10 | 123.9 (5) | C28—C27—H27 | 120.5 |
| O11—N5—C38 | 119.4 (4) | C26—C27—H27 | 120.5 |
| O10—N5—C38 | 116.7 (5) | C29—C28—C27 | 121.2 (7) |
| O14—N6—O13 | 122.4 (5) | C29—C28—H28 | 119.4 |
| O14—N6—C40 | 117.8 (5) | C27—C28—H28 | 119.4 |
| O13—N6—C40 | 119.8 (4) | C28—C29—C30 | 120.1 (7) |
| O15—N7—O16 | 124.3 (5) | C28—C29—H29 | 120.0 |
| O15—N7—C42 | 117.8 (5) | C30—C29—H29 | 120.0 |
| O16—N7—C42 | 117.9 (6) | C25—C30—C29 | 119.2 (7) |
| O17—N8—O18 | 124.4 (6) | C25—C30—H30 | 120.4 |
| O17—N8—C44 | 118.1 (5) | C29—C30—H30 | 120.4 |
| O18—N8—C44 | 117.5 (5) | C32—C31—N2 | 110.0 (6) |
| O20—N9—O21 | 124.6 (6) | C32—C31—H31A | 109.7 |
| O20—N9—C46 | 118.1 (5) | N2—C31—H31A | 109.7 |
| O21—N9—C46 | 117.3 (5) | C32—C31—H31B | 109.7 |
| O22—N10—O23 | 124.4 (6) | N2—C31—H31B | 109.7 |
| O22—N10—C48 | 118.6 (6) | H31A—C31—H31B | 108.2 |
| O23—N10—C48 | 117.0 (6) | C31—C32—H32A | 109.5 |
| O25—N11—O24 | 123.0 (6) | C31—C32—H32B | 109.5 |
| O25—N11—C50 | 120.3 (6) | H32A—C32—H32B | 109.5 |
| O24—N11—C50 | 116.7 (5) | C31—C32—H32C | 109.5 |
| C13—O1—Gd | 128.6 (3) | H32A—C32—H32C | 109.5 |
| C1—O2—C14 | 117.0 (3) | H32B—C32—H32C | 109.5 |
| C1—O2—Gd | 126.1 (2) | O5—C33—C38 | 121.3 (4) |

| | | | |
|---|---|---|---|
| C14—O2—Gd | 115.5 (2) | O5—C33—C34 | 125.1 (4) |
| C23—O3—Gd | 122.6 (3) | C38—C33—C34 | 113.5 (4) |
| C12—O4—C24 | 116.1 (3) | C35—C34—C33 | 122.9 (4) |
| C12—O4—Gd | 127.5 (2) | C35—C34—N3 | 115.7 (4) |
| C24—O4—Gd | 114.1 (2) | C33—C34—N3 | 121.4 (4) |
| C33—O5—Gd | 143.8 (3) | C36—C35—C34 | 118.6 (5) |
| N3—O6—Gd | 140.6 (3) | C36—C35—H35 | 120.7 |
| C39—O12—Gd | 131.5 (3) | C34—C35—H35 | 120.7 |
| N6—O13—Gd | 133.7 (3) | C35—C36—C37 | 121.7 (5) |
| C45—O19—Gd | 132.8 (3) | C35—C36—N4 | 119.6 (6) |
| C2—C1—C6 | 122.7 (4) | C37—C36—N4 | 118.7 (5) |
| C2—C1—O2 | 118.4 (4) | C38—C37—C36 | 119.5 (5) |
| C6—C1—O2 | 118.7 (4) | C38—C37—H37 | 120.2 |
| C1—C2—C3 | 119.1 (6) | C36—C37—H37 | 120.2 |
| C1—C2—H2 | 120.5 | C37—C38—C33 | 123.7 (5) |
| C3—C2—H2 | 120.5 | C37—C38—N5 | 118.0 (4) |
| C4—C3—C2 | 119.8 (6) | C33—C38—N5 | 118.3 (4) |
| C4—C3—H3 | 120.1 | O12—C39—C40 | 125.4 (4) |
| C2—C3—H3 | 120.1 | O12—C39—C44 | 122.1 (4) |
| C3—C4—C5 | 120.8 (6) | C40—C39—C44 | 112.5 (4) |
| C3—C4—H4 | 119.6 | C41—C40—C39 | 124.0 (4) |
| C5—C4—H4 | 119.6 | C41—C40—N6 | 116.5 (5) |
| C4—C5—C6 | 120.6 (6) | C39—C40—N6 | 119.5 (4) |
| C4—C5—H5 | 119.7 | C42—C41—C40 | 119.1 (5) |
| C6—C5—H5 | 119.7 | C42—C41—H41 | 120.5 |
| C1—C6—C5 | 116.9 (5) | C40—C41—H41 | 120.5 |
| C1—C6—C7 | 121.5 (4) | C41—C42—C43 | 121.1 (5) |
| C5—C6—C7 | 121.6 (5) | C41—C42—N7 | 119.3 (5) |
| C12—C7—C8 | 117.1 (5) | C43—C42—N7 | 119.5 (5) |
| C12—C7—C6 | 121.6 (4) | C44—C43—C42 | 119.1 (5) |
| C8—C7—C6 | 121.3 (5) | C44—C43—H43 | 120.5 |
| C9—C8—C7 | 120.7 (6) | C42—C43—H43 | 120.5 |
| C9—C8—H8 | 119.7 | C43—C44—C39 | 124.1 (5) |
| C7—C8—H8 | 119.7 | C43—C44—N8 | 117.3 (5) |
| C10—C9—C8 | 121.0 (5) | C39—C44—N8 | 118.6 (4) |
| C10—C9—H9 | 119.5 | O19—C45—C50 | 124.7 (5) |
| C8—C9—H9 | 119.5 | O19—C45—C46 | 123.1 (5) |
| C9—C10—C11 | 119.7 (6) | C50—C45—C46 | 112.2 (4) |
| C9—C10—H10 | 120.2 | C47—C46—C45 | 124.4 (5) |
| C11—C10—H10 | 120.2 | C47—C46—N9 | 117.2 (5) |
| C12—C11—C10 | 119.4 (5) | C45—C46—N9 | 118.4 (4) |
| C12—C11—H11 | 120.3 | C46—C47—C48 | 118.5 (5) |
| C10—C11—H11 | 120.3 | C46—C47—H47 | 120.8 |
| C11—C12—C7 | 122.1 (4) | C48—C47—H47 | 120.8 |
| C11—C12—O4 | 117.9 (4) | C47—C48—C49 | 121.6 (5) |
| C7—C12—O4 | 119.8 (4) | C47—C48—N10 | 118.7 (5) |
| O1—C13—N1 | 121.4 (4) | C49—C48—N10 | 119.6 (6) |
| O1—C13—C14 | 119.9 (4) | C50—C49—C48 | 119.0 (5) |
| N1—C13—C14 | 118.7 (4) | C50—C49—H49 | 120.5 |

| | | | |
|---|---|---|---|
| O2—C14—C13 | 105.9 (3) | C48—C49—H49 | 120.5 |
| O2—C14—H14A | 110.6 | C49—C50—C45 | 123.3 (5) |
| C13—C14—H14A | 110.6 | C49—C50—N11 | 117.0 (5) |
| O2—C14—H14B | 110.6 | C45—C50—N11 | 119.6 (5) |

**Fig. 1**


C17
C18
C16
C19
O20
O21
O22
N9
C15
C20
C21
N10
C47
C46
C22
N1
O10
O23
C48
C45
C14
C49
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C13
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N4
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C3
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N3
C11
C35
C34
C10
C7
C6
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C44
C31
N2
O15
N8
C32
C25
C43
O17
C30
N7
O18
C26
O16
C29
C27
C28

**Fig. 2**