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# (4′-Allyloxy-2,2′:6′,2″-terpyridine-$\kappa^3N,N',N''$)(dibenzoylmethanido-$\kappa^2O,O'$)bis(nitrato-$\kappa^2O,O'$)-neodymium(III) acetonitrile solvate

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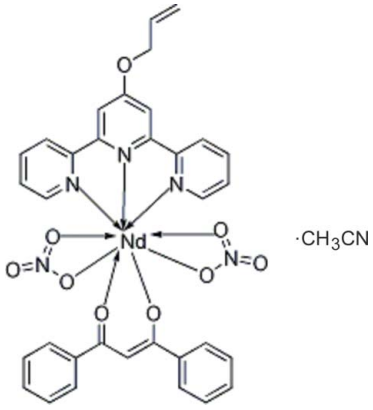
Key indicators: single-crystal X-ray study; $T$ = 569 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.029; $wR$ factor = 0.069; data-to-parameter ratio = 14.2.

The title complex, $[Nd(C_{15}H_{11}O_2)(NO_3)_2(C_{18}H_{15}N_3O)]\cdot CH_3CN$ or $[Nd(altpy)(dbm)(NO_3)_2]\cdot CH_3CN$ (altpy = 4′-allyloxy-2,2′:6′,2″-terpyridine, dbm = dibenzoylmethanide anion), has been synthesized from 4′-allyloxy-2,2′:6′,2″-terpyridine, dibenzoylmethanate and neodymium nitrate. The $Nd^{3+}$ atom is nine-coordinated by two O atoms from the bidentate dbm ligand, three N atoms from the tridentate altpy ligand and four O atoms from two nitrate anions that act as bidentate ligands and occupy mutually *trans* sites in a distorted monocapped square-antiprismatic geometry.

## Related literature

For the use of lanthanide complexes as shift reagents, functional materials and as catalysts, see: Su *et al.* (1999); Sutter *et al.* (1998); Aspinall *et al.* (1998). For related structures, see: Niu *et al.* (1997); Chen *et al.* (1998); Cotton *et al.* (2003); Hunter *et al.* (2007).




## Experimental

### Crystal data

$[Nd(C_{15}H_{11}O_2)(NO_3)_2(C_{18}H_{15}N_3O)]\cdot C_2H_3N$
$M_r$ = 821.88
Monoclinic, $P2_1/n$
$a$ = 13.3711 (16) Å
$b$ = 16.1009 (19) Å
$c$ = 15.9490 (19) Å
$\beta$ = 103.040 (2)°
$V$ = 3345.1 (7) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.62 mm$^{-1}$
$T$ = 569 K
0.41 × 0.36 × 0.25 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan *SADABS* (Bruker, 1997)
$T_{min}$ = 0.557, $T_{max}$ = 0.688
6565 measured reflections
6565 independent reflections
5101 reflections with $I > 2\sigma(I)$

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.069
$S$ = 1.09
6565 reflections
461 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.91 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.46 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Nd1—O2 | 2.343 (2) | Nd1—O5 | 2.571 (3) |
| Nd1—O3 | 2.354 (2) | Nd1—N3 | 2.578 (3) |
| Nd1—O6 | 2.550 (2) | Nd1—N1 | 2.603 (2) |
| Nd1—O9 | 2.558 (2) | Nd1—N2 | 2.605 (2) |
| Nd1—O8 | 2.559 (2) | | |

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: SJ2697).

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# supplementary materials

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# (4'-Allyloxy-2,2':6',2''-terpyridine-$\kappa^3N,N',N''$)(dibenzoylmethanido-$\kappa^2O,O'$)bis(nitrato-$\kappa^2O,O'$)neodymium(III) acetonitrile solvate

**Q. Mei and B. Tong**

## Comment

Lanthanide complexes are often used as shift reagents to probe metal-binding sites in solutions (Su *et al.*, 1999) and they are also used in functional materials (Sutter *et al.*, 1998) or catalysts (Aspinall *et al.*, 1998). The ability of these elements to adopt coordination numbers from six to twelve provides a rich and variable structural chemistry. In the title compound, $[Nd(altpy)(dbm)(NO_3)_2].CH_3CN$(altpy=4'-allyloxy-2, 2':6', 2''-terpyridine, dbm=dibenzoylmethanate), each Nd(III) atom is in a nine coordinate environment comprising two oxygen atoms from the bidentate dbm ligand, three nitrogen atoms from the tridentate altpy ligand and four oxygen atoms from two tertiary nitrate anions that act as bidentate ligands an occupy mutually *trans* sites in the coordination polyhedron. The coordination polyhedron is a distorted monocapped square antiprism. The Nd—O distances lie in two groups, those to the beta-diketone oxygen atoms in the range 2.343 (2)–2.354 (2) Å and those to nitrate O atoms in the range 2.550 (3)–2.573 (3) Å. These are comparable to those [2.485 (19), 2.600 (15) Å] in the nine-coordinate complex $[Nd_2(O_2CMe)_4(NO_3)_2(phen)_2]$ (phen=1,10-phenanthroline) which also contains bidentate chelating nitrate anions (Niu *et al.*, 1997). The O—Nd—O angle (73.64 (8) °) of the beta-diketonate ligand is somewhat higher as compared to those found in the neodymium tris(beta-diketonates) type of complexes (Chen *et al.*, 1998). The average Nd—N distance (2.595 (3) Å) is slightly longer than that in the nine-coordinate complex $[Eu(terpy)(NO_3)_3^-(H_2O)]$ (2.554 Å)(Cotton *et al.* (2003)).The geometrical parameters of the $[NO_3]^-$ anions in the title complex are as expected with normal distances and angles, comparable to those reported by Hunter *et al.*, (2007) for a complex also containing bidentate chelating nitrate anions

## Experimental

The title compound was obtained by refluxing neodymium nitrate, 4'-allyloxy-2, 2':6',2''-terpyridine and dibenzoylmethanate in ethanol to give the title compound as a blue precipitate in 78% yield. Recrystallization from ethanol and acetonitrile (1:1) gave blue block-like crystals suitable for an X-ray diffraction determination. Anal.Calcd. for $C_{35}H_{30}N_6NdO_9$: C, 51.03, H, 3.64, N, 10.21%. Found:*C*, 51.10, H, 3.67, N, 10.12%.

## Refinement

H atoms were positioned geometrically and refined using a riding model (including free rotation about the ethanol C—C bond), with C—H = 0.95–0.99 Å and with $U_{iso}$(H) = 1.2 (1.5 for methyl groups) $U_{eq}$(C).

## Figures

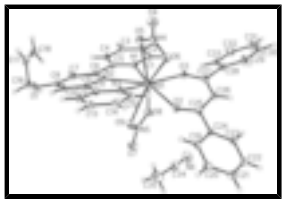


Fig. 1. The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

## (4'-Allyloxy-2,2':6',2''-terpyridine-κ$^3$*N*,*N*',*N*'') (dibenzoylmethanido-κ$^2$*O*,*O*')bis(nitrato-κ$^2$*O*,*O*') neodymium(III) acetonitrile solvate

*Crystal data*

| | |
|---|---|
| $[Nd(C_{15}H_{11}O_2)(NO_3)_2(C_{18}H_{15}N_3O)]\cdot C_2H_3N$ | $F(000) = 1652$ |
| $M_r = 821.88$ | $D_x = 1.632$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2yn | Cell parameters from 4901 reflections |
| $a = 13.3711$ (16) Å | $\theta = 2.2$–$27.1°$ |
| $b = 16.1009$ (19) Å | $\mu = 1.62$ mm$^{-1}$ |
| $c = 15.9490$ (19) Å | $T = 569$ K |
| $\beta = 103.040$ (2)° | Block, blue |
| $V = 3345.1$ (7) Å$^3$ | 0.41 × 0.36 × 0.25 mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 6565 independent reflections |
| Radiation source: fine-focus sealed tube | 5101 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.0000$ |
| φ and ω scans | $\theta_{max} = 26.0°$, $\theta_{min} = 1.8°$ |
| Absorption correction: multi-scan *SADABS* (Bruker, 1997) | $h = -16\rightarrow16$ |
| $T_{min} = 0.557$, $T_{max} = 0.688$ | $k = 0\rightarrow19$ |
| 6565 measured reflections | $l = 0\rightarrow19$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.029$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.069$ | H-atom parameters constrained |
| $S = 1.09$ | $w = 1/[\sigma^2(F_o^2) + (0.0298P)^2 + 2.1769P]$ where $P = (F_o^2 + 2F_c^2)/3$ |

| | |
|---|---|
| 6565 reflections | $(\Delta/\sigma)_{max} = 0.002$ |
| 461 parameters | $\Delta\rho_{max} = 0.91$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.46$ e Å$^{-3}$ |

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Nd1 | 0.754510 (13) | 0.201262 (9) | 0.532547 (11) | 0.02286 (6) |
| O1 | 0.65947 (18) | −0.20624 (13) | 0.48248 (16) | 0.0353 (6) |
| O2 | 0.66289 (17) | 0.31699 (12) | 0.56350 (14) | 0.0284 (5) |
| O3 | 0.87760 (16) | 0.30266 (12) | 0.59043 (15) | 0.0297 (5) |
| O4 | 0.7676 (2) | 0.26540 (18) | 0.28068 (18) | 0.0557 (8) |
| O5 | 0.8192 (2) | 0.18627 (14) | 0.39321 (17) | 0.0406 (6) |
| O6 | 0.73546 (19) | 0.29852 (13) | 0.40375 (16) | 0.0359 (6) |
| O7 | 0.6621 (2) | 0.11468 (16) | 0.75275 (16) | 0.0447 (7) |
| O8 | 0.78009 (18) | 0.16492 (16) | 0.69217 (15) | 0.0381 (6) |
| O9 | 0.62830 (17) | 0.14135 (14) | 0.61564 (15) | 0.0343 (6) |
| N1 | 0.91391 (19) | 0.10513 (15) | 0.57890 (17) | 0.0253 (6) |
| N2 | 0.73078 (19) | 0.04405 (15) | 0.49459 (17) | 0.0226 (6) |
| N3 | 0.5878 (2) | 0.15850 (15) | 0.42526 (17) | 0.0272 (6) |
| N4 | 0.7744 (2) | 0.25116 (18) | 0.3572 (2) | 0.0365 (7) |
| N5 | 0.6896 (2) | 0.13977 (17) | 0.68938 (19) | 0.0307 (6) |
| C1 | 1.0065 (2) | 0.1370 (2) | 0.6148 (2) | 0.0303 (8) |
| H1A | 1.0126 | 0.1945 | 0.6190 | 0.036* |
| C2 | 1.0924 (3) | 0.0903 (2) | 0.6457 (2) | 0.0316 (8) |
| H2A | 1.1550 | 0.1154 | 0.6694 | 0.038* |
| C3 | 1.0836 (3) | 0.0049 (2) | 0.6407 (2) | 0.0307 (8) |
| H3A | 1.1403 | −0.0289 | 0.6610 | 0.037* |
| C4 | 0.9891 (2) | −0.02924 (19) | 0.6049 (2) | 0.0292 (7) |
| H4A | 0.9817 | −0.0867 | 0.6015 | 0.035* |
| C5 | 0.9050 (2) | 0.02128 (18) | 0.57400 (19) | 0.0217 (7) |
| C6 | 0.8018 (2) | −0.01195 (18) | 0.53183 (19) | 0.0221 (7) |
| C7 | 0.7835 (2) | −0.09649 (19) | 0.5309 (2) | 0.0266 (7) |
| H7A | 0.8338 | −0.1331 | 0.5590 | 0.032* |
| C8 | 0.6886 (3) | −0.12537 (18) | 0.4872 (2) | 0.0273 (7) |
| C9 | 0.6162 (2) | −0.06896 (19) | 0.4457 (2) | 0.0268 (7) |

| | | | | |
|---|---|---|---|---|
| H9A | 0.5529 | −0.0873 | 0.4143 | 0.032* |
| C10 | 0.6386 (2) | 0.01495 (18) | 0.45141 (19) | 0.0221 (7) |
| C11 | 0.5613 (2) | 0.07775 (19) | 0.4104 (2) | 0.0241 (7) |
| C12 | 0.4668 (2) | 0.0560 (2) | 0.3595 (2) | 0.0306 (8) |
| H12A | 0.4500 | 0.0003 | 0.3488 | 0.037* |
| C13 | 0.3977 (3) | 0.1170 (2) | 0.3246 (2) | 0.0345 (8) |
| H13A | 0.3332 | 0.1029 | 0.2918 | 0.041* |
| C14 | 0.4251 (3) | 0.1991 (2) | 0.3389 (2) | 0.0344 (8) |
| H14A | 0.3804 | 0.2414 | 0.3148 | 0.041* |
| C15 | 0.5201 (2) | 0.2169 (2) | 0.3894 (2) | 0.0312 (8) |
| H15A | 0.5385 | 0.2724 | 0.3994 | 0.037* |
| C16 | 0.7296 (3) | −0.2675 (2) | 0.5289 (2) | 0.0360 (9) |
| H16A | 0.6917 | −0.3175 | 0.5357 | 0.043* |
| H16B | 0.7602 | −0.2464 | 0.5859 | 0.043* |
| C17 | 0.8127 (3) | −0.2887 (2) | 0.4840 (3) | 0.0404 (9) |
| H17A | 0.7947 | −0.2985 | 0.4251 | 0.048* |
| C18 | 0.9096 (3) | −0.2942 (2) | 0.5230 (3) | 0.0482 (10) |
| H18A | 0.9297 | −0.2846 | 0.5819 | 0.058* |
| H18B | 0.9583 | −0.3076 | 0.4919 | 0.058* |
| C19 | 0.4968 (2) | 0.4175 (2) | 0.5694 (2) | 0.0303 (8) |
| H19A | 0.4850 | 0.3694 | 0.5364 | 0.036* |
| C20 | 0.4149 (3) | 0.4633 (2) | 0.5825 (2) | 0.0348 (8) |
| H20A | 0.3482 | 0.4463 | 0.5579 | 0.042* |
| C21 | 0.4313 (3) | 0.5348 (2) | 0.6323 (2) | 0.0354 (8) |
| H21A | 0.3761 | 0.5662 | 0.6407 | 0.042* |
| C22 | 0.5302 (3) | 0.5587 (2) | 0.6692 (2) | 0.0330 (8) |
| H22A | 0.5415 | 0.6058 | 0.7038 | 0.040* |
| C23 | 0.6124 (3) | 0.5138 (2) | 0.6556 (2) | 0.0308 (8) |
| H23A | 0.6787 | 0.5312 | 0.6806 | 0.037* |
| C24 | 0.5976 (2) | 0.44244 (19) | 0.6050 (2) | 0.0251 (7) |
| C25 | 0.6845 (2) | 0.39060 (19) | 0.5897 (2) | 0.0253 (7) |
| C26 | 0.7840 (2) | 0.4243 (2) | 0.6058 (2) | 0.0285 (7) |
| H26 | 0.7904 | 0.4809 | 0.6174 | 0.034* |
| C27 | 0.8732 (2) | 0.38068 (19) | 0.6059 (2) | 0.0256 (7) |
| C28 | 0.9738 (2) | 0.4246 (2) | 0.6312 (2) | 0.0281 (7) |
| C29 | 0.9844 (3) | 0.5074 (2) | 0.6094 (3) | 0.0413 (9) |
| H29A | 0.9280 | 0.5365 | 0.5785 | 0.050* |
| C30 | 1.0788 (3) | 0.5464 (2) | 0.6338 (3) | 0.0544 (12) |
| H30A | 1.0857 | 0.6012 | 0.6176 | 0.065* |
| C31 | 1.1621 (3) | 0.5051 (2) | 0.6814 (3) | 0.0474 (10) |
| H31A | 1.2248 | 0.5323 | 0.6985 | 0.057* |
| C32 | 1.1530 (3) | 0.4234 (2) | 0.7041 (2) | 0.0378 (9) |
| H32A | 1.2093 | 0.3953 | 0.7368 | 0.045* |
| C33 | 1.0595 (2) | 0.3832 (2) | 0.6780 (2) | 0.0304 (8) |
| H33A | 1.0540 | 0.3276 | 0.6919 | 0.036* |
| N6 | 0.6450 (3) | 0.3229 (2) | 0.7792 (2) | 0.0617 (10) |
| C34 | 0.5672 (3) | 0.2950 (2) | 0.7485 (2) | 0.0437 (9) |
| C35 | 0.4712 (3) | 0.2565 (3) | 0.7093 (3) | 0.0672 (14) |
| H35A | 0.4633 | 0.2553 | 0.6480 | 0.101* |

| | | | | |
|---|---|---|---|---|
| H35B | 0.4159 | 0.2876 | 0.7233 | 0.101* |
| H35C | 0.4701 | 0.2007 | 0.7305 | 0.101* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Nd1 | 0.01860 (9) | 0.01540 (8) | 0.03276 (10) | −0.00015 (7) | 0.00199 (7) | −0.00221 (8) |
| O1 | 0.0337 (13) | 0.0161 (11) | 0.0516 (15) | −0.0058 (10) | 0.0004 (11) | −0.0030 (11) |
| O2 | 0.0249 (12) | 0.0218 (11) | 0.0377 (13) | 0.0013 (9) | 0.0056 (10) | −0.0055 (10) |
| O3 | 0.0175 (11) | 0.0207 (11) | 0.0493 (14) | −0.0011 (9) | 0.0042 (10) | −0.0045 (11) |
| O4 | 0.077 (2) | 0.0503 (17) | 0.0436 (17) | 0.0050 (16) | 0.0222 (16) | 0.0098 (14) |
| O5 | 0.0416 (15) | 0.0335 (14) | 0.0478 (15) | 0.0110 (11) | 0.0128 (12) | 0.0039 (12) |
| O6 | 0.0406 (14) | 0.0231 (11) | 0.0472 (14) | 0.0069 (11) | 0.0168 (12) | 0.0005 (11) |
| O7 | 0.0451 (16) | 0.0499 (16) | 0.0405 (15) | 0.0039 (13) | 0.0128 (13) | 0.0123 (13) |
| O8 | 0.0231 (13) | 0.0509 (15) | 0.0372 (14) | −0.0033 (12) | −0.0001 (11) | 0.0041 (12) |
| O9 | 0.0273 (13) | 0.0358 (13) | 0.0363 (14) | −0.0086 (11) | 0.0000 (11) | −0.0002 (11) |
| N1 | 0.0224 (14) | 0.0195 (13) | 0.0330 (15) | −0.0005 (11) | 0.0038 (12) | −0.0016 (12) |
| N2 | 0.0212 (14) | 0.0163 (12) | 0.0287 (14) | −0.0015 (11) | 0.0022 (11) | −0.0001 (11) |
| N3 | 0.0249 (15) | 0.0216 (14) | 0.0329 (16) | 0.0029 (12) | 0.0022 (12) | 0.0002 (12) |
| N4 | 0.0354 (18) | 0.0287 (17) | 0.046 (2) | −0.0041 (14) | 0.0112 (15) | 0.0031 (14) |
| N5 | 0.0266 (16) | 0.0260 (14) | 0.0378 (18) | 0.0053 (12) | 0.0035 (14) | 0.0025 (13) |
| C1 | 0.0252 (18) | 0.0207 (16) | 0.043 (2) | −0.0014 (14) | 0.0024 (16) | −0.0021 (15) |
| C2 | 0.0236 (18) | 0.0329 (18) | 0.0362 (19) | −0.0023 (15) | 0.0023 (15) | −0.0035 (16) |
| C3 | 0.0244 (18) | 0.0315 (18) | 0.0323 (19) | 0.0083 (15) | −0.0019 (15) | 0.0017 (15) |
| C4 | 0.0295 (19) | 0.0203 (16) | 0.0364 (19) | 0.0010 (14) | 0.0045 (15) | 0.0007 (14) |
| C5 | 0.0232 (17) | 0.0187 (15) | 0.0232 (16) | −0.0002 (13) | 0.0051 (13) | −0.0002 (13) |
| C6 | 0.0171 (16) | 0.0218 (15) | 0.0276 (17) | 0.0012 (13) | 0.0052 (13) | −0.0031 (13) |
| C7 | 0.0253 (17) | 0.0203 (15) | 0.0325 (18) | 0.0027 (13) | 0.0030 (15) | −0.0014 (14) |
| C8 | 0.0304 (18) | 0.0180 (15) | 0.0339 (19) | −0.0020 (14) | 0.0081 (15) | −0.0037 (14) |
| C9 | 0.0204 (17) | 0.0250 (16) | 0.0330 (18) | −0.0030 (13) | 0.0016 (14) | −0.0031 (14) |
| C10 | 0.0201 (16) | 0.0207 (15) | 0.0248 (16) | −0.0021 (13) | 0.0035 (13) | −0.0019 (13) |
| C11 | 0.0224 (17) | 0.0255 (16) | 0.0238 (16) | −0.0017 (13) | 0.0043 (13) | −0.0025 (13) |
| C12 | 0.0250 (18) | 0.0301 (17) | 0.0347 (19) | −0.0038 (15) | 0.0026 (15) | 0.0000 (15) |
| C13 | 0.0221 (18) | 0.046 (2) | 0.0308 (19) | 0.0003 (16) | −0.0043 (15) | 0.0022 (16) |
| C14 | 0.0306 (19) | 0.0372 (19) | 0.0336 (19) | 0.0076 (17) | 0.0037 (15) | 0.0069 (17) |
| C15 | 0.0269 (18) | 0.0276 (18) | 0.0360 (19) | 0.0026 (14) | 0.0009 (15) | 0.0003 (14) |
| C16 | 0.038 (2) | 0.0177 (15) | 0.050 (2) | −0.0010 (15) | 0.0051 (19) | 0.0008 (16) |
| C17 | 0.050 (2) | 0.0289 (19) | 0.039 (2) | 0.0042 (17) | 0.0052 (18) | −0.0038 (16) |
| C18 | 0.055 (3) | 0.040 (2) | 0.053 (2) | 0.016 (2) | 0.017 (2) | 0.001 (2) |
| C19 | 0.0275 (18) | 0.0242 (17) | 0.039 (2) | −0.0009 (14) | 0.0061 (15) | −0.0052 (15) |
| C20 | 0.0235 (18) | 0.0361 (19) | 0.045 (2) | 0.0012 (15) | 0.0073 (16) | −0.0022 (17) |
| C21 | 0.035 (2) | 0.0285 (18) | 0.046 (2) | 0.0088 (16) | 0.0145 (17) | 0.0014 (16) |
| C22 | 0.037 (2) | 0.0238 (17) | 0.038 (2) | 0.0009 (15) | 0.0098 (17) | −0.0066 (15) |
| C23 | 0.0261 (18) | 0.0256 (17) | 0.039 (2) | 0.0000 (14) | 0.0037 (15) | −0.0037 (15) |
| C24 | 0.0260 (17) | 0.0242 (16) | 0.0257 (17) | 0.0034 (14) | 0.0072 (14) | 0.0007 (13) |
| C25 | 0.0266 (17) | 0.0226 (16) | 0.0252 (17) | −0.0001 (14) | 0.0024 (14) | 0.0010 (13) |
| C26 | 0.0213 (17) | 0.0234 (16) | 0.038 (2) | −0.0002 (14) | 0.0012 (15) | 0.0002 (14) |
| C27 | 0.0235 (17) | 0.0231 (16) | 0.0272 (17) | −0.0022 (13) | −0.0003 (14) | −0.0014 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C28 | 0.0228 (17) | 0.0262 (17) | 0.0346 (19) | −0.0028 (14) | 0.0050 (15) | −0.0073 (14) |
| C29 | 0.027 (2) | 0.0290 (18) | 0.062 (3) | −0.0025 (16) | −0.0009 (18) | 0.0064 (18) |
| C30 | 0.040 (2) | 0.033 (2) | 0.085 (3) | −0.0126 (18) | 0.003 (2) | 0.007 (2) |
| C31 | 0.026 (2) | 0.045 (2) | 0.068 (3) | −0.0131 (18) | 0.0032 (19) | −0.003 (2) |
| C32 | 0.0223 (18) | 0.041 (2) | 0.046 (2) | 0.0005 (16) | 0.0007 (16) | −0.0059 (18) |
| C33 | 0.0257 (18) | 0.0282 (17) | 0.0362 (19) | −0.0008 (14) | 0.0048 (15) | −0.0040 (15) |
| N6 | 0.067 (3) | 0.061 (2) | 0.047 (2) | −0.009 (2) | −0.007 (2) | 0.0015 (18) |
| C34 | 0.050 (3) | 0.047 (2) | 0.033 (2) | 0.006 (2) | 0.0069 (19) | 0.0003 (19) |
| C35 | 0.044 (3) | 0.080 (4) | 0.074 (3) | −0.006 (3) | 0.006 (3) | 0.007 (3) |

*Geometric parameters (Å, °)*

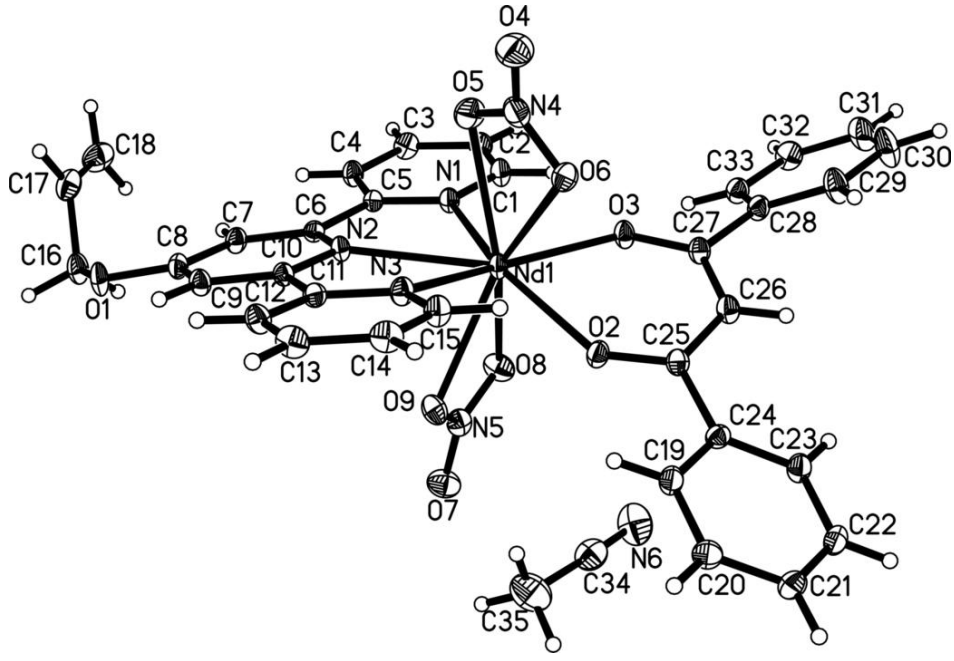
| | | | |
|---|---|---|---|
| Nd1—O2 | 2.343 (2) | C12—H12A | 0.9300 |
| Nd1—O3 | 2.354 (2) | C13—C14 | 1.377 (5) |
| Nd1—O6 | 2.550 (2) | C13—H13A | 0.9300 |
| Nd1—O9 | 2.558 (2) | C14—C15 | 1.373 (5) |
| Nd1—O8 | 2.559 (2) | C14—H14A | 0.9300 |
| Nd1—O5 | 2.571 (3) | C15—H15A | 0.9300 |
| Nd1—N3 | 2.578 (3) | C16—C17 | 1.491 (5) |
| Nd1—N1 | 2.603 (2) | C16—H16A | 0.9700 |
| Nd1—N2 | 2.605 (2) | C16—H16B | 0.9700 |
| Nd1—N4 | 2.979 (3) | C17—C18 | 1.307 (5) |
| Nd1—N5 | 2.995 (3) | C17—H17A | 0.9300 |
| O1—C8 | 1.356 (3) | C18—H18A | 0.9300 |
| O1—C16 | 1.445 (4) | C18—H18B | 0.9300 |
| O2—C25 | 1.268 (4) | C19—C20 | 1.374 (5) |
| O3—C27 | 1.284 (4) | C19—C24 | 1.398 (4) |
| O4—N4 | 1.224 (4) | C19—H19A | 0.9300 |
| O5—N4 | 1.275 (4) | C20—C21 | 1.388 (5) |
| O6—N4 | 1.257 (4) | C20—H20A | 0.9300 |
| O7—N5 | 1.220 (3) | C21—C22 | 1.375 (5) |
| O8—N5 | 1.267 (3) | C21—H21A | 0.9300 |
| O9—N5 | 1.273 (3) | C22—C23 | 1.373 (5) |
| N1—C1 | 1.343 (4) | C22—H22A | 0.9300 |
| N1—C5 | 1.356 (4) | C23—C24 | 1.392 (4) |
| N2—C6 | 1.347 (4) | C23—H23A | 0.9300 |
| N2—C10 | 1.353 (4) | C24—C25 | 1.495 (4) |
| N3—C15 | 1.341 (4) | C25—C26 | 1.405 (4) |
| N3—C11 | 1.355 (4) | C26—C27 | 1.384 (4) |
| C1—C2 | 1.368 (4) | C26—H26 | 0.9300 |
| C1—H1A | 0.9300 | C27—C28 | 1.493 (4) |
| C2—C3 | 1.382 (5) | C28—C33 | 1.388 (5) |
| C2—H2A | 0.9300 | C28—C29 | 1.392 (5) |
| C3—C4 | 1.377 (4) | C29—C30 | 1.384 (5) |
| C3—H3A | 0.9300 | C29—H29A | 0.9300 |
| C4—C5 | 1.386 (4) | C30—C31 | 1.371 (5) |
| C4—H4A | 0.9300 | C30—H30A | 0.9300 |
| C5—C6 | 1.491 (4) | C31—C32 | 1.377 (5) |
| C6—C7 | 1.383 (4) | C31—H31A | 0.9300 |

| | | | |
|---|---|---|---|
| C7—C8 | 1.383 (4) | C32—C33 | 1.386 (5) |
| C7—H7A | 0.9300 | C32—H32A | 0.9300 |
| C8—C9 | 1.382 (4) | C33—H33A | 0.9300 |
| C9—C10 | 1.382 (4) | N6—C34 | 1.138 (5) |
| C9—H9A | 0.9300 | C34—C35 | 1.436 (6) |
| C10—C11 | 1.488 (4) | C35—H35A | 0.9600 |
| C11—C12 | 1.384 (4) | C35—H35B | 0.9600 |
| C12—C13 | 1.377 (5) | C35—H35C | 0.9600 |
| O2—Nd1—O3 | 73.64 (7) | N1—C5—C6 | 116.3 (3) |
| O2—Nd1—O6 | 73.70 (7) | C4—C5—C6 | 123.0 (3) |
| O3—Nd1—O6 | 79.86 (8) | N2—C6—C7 | 123.3 (3) |
| O2—Nd1—O9 | 75.72 (7) | N2—C6—C5 | 116.6 (3) |
| O3—Nd1—O9 | 122.89 (8) | C7—C6—C5 | 120.1 (3) |
| O6—Nd1—O9 | 133.74 (8) | C6—C7—C8 | 118.5 (3) |
| O2—Nd1—O8 | 86.05 (8) | C6—C7—H7A | 120.8 |
| O3—Nd1—O8 | 81.01 (8) | C8—C7—H7A | 120.8 |
| O6—Nd1—O8 | 155.32 (8) | O1—C8—C9 | 116.3 (3) |
| O9—Nd1—O8 | 49.77 (7) | O1—C8—C7 | 124.7 (3) |
| O2—Nd1—O5 | 123.40 (8) | C9—C8—C7 | 119.0 (3) |
| O3—Nd1—O5 | 93.58 (8) | C10—C9—C8 | 119.5 (3) |
| O6—Nd1—O5 | 49.70 (7) | C10—C9—H9A | 120.2 |
| O9—Nd1—O5 | 143.33 (8) | C8—C9—H9A | 120.2 |
| O8—Nd1—O5 | 147.45 (8) | N2—C10—C9 | 122.1 (3) |
| O2—Nd1—N3 | 86.42 (8) | N2—C10—C11 | 116.8 (3) |
| O3—Nd1—N3 | 150.31 (8) | C9—C10—C11 | 121.1 (3) |
| O6—Nd1—N3 | 73.44 (8) | N3—C11—C12 | 121.0 (3) |
| O9—Nd1—N3 | 70.77 (8) | N3—C11—C10 | 116.5 (3) |
| O8—Nd1—N3 | 120.05 (8) | C12—C11—C10 | 122.5 (3) |
| O5—Nd1—N3 | 79.05 (8) | C13—C12—C11 | 119.8 (3) |
| O2—Nd1—N1 | 147.86 (8) | C13—C12—H12A | 120.1 |
| O3—Nd1—N1 | 81.13 (8) | C11—C12—H12A | 120.1 |
| O6—Nd1—N1 | 121.37 (8) | C14—C13—C12 | 119.3 (3) |
| O9—Nd1—N1 | 102.84 (8) | C14—C13—H13A | 120.4 |
| O8—Nd1—N1 | 70.39 (8) | C12—C13—H13A | 120.4 |
| O5—Nd1—N1 | 77.07 (8) | C15—C14—C13 | 118.3 (3) |
| N3—Nd1—N1 | 124.02 (8) | C15—C14—H14A | 120.8 |
| O2—Nd1—N2 | 141.22 (8) | C13—C14—H14A | 120.8 |
| O3—Nd1—N2 | 143.39 (7) | N3—C15—C14 | 123.4 (3) |
| O6—Nd1—N2 | 115.13 (8) | N3—C15—H15A | 118.3 |
| O9—Nd1—N2 | 72.18 (8) | C14—C15—H15A | 118.3 |
| O8—Nd1—N2 | 89.48 (8) | O1—C16—C17 | 112.2 (3) |
| O5—Nd1—N2 | 75.82 (8) | O1—C16—H16A | 109.2 |
| N3—Nd1—N2 | 62.91 (8) | C17—C16—H16A | 109.2 |
| N1—Nd1—N2 | 62.43 (8) | O1—C16—H16B | 109.2 |
| O2—Nd1—N4 | 98.34 (8) | C17—C16—H16B | 109.2 |
| O3—Nd1—N4 | 88.77 (8) | H16A—C16—H16B | 107.9 |
| O6—Nd1—N4 | 24.74 (7) | C18—C17—C16 | 123.5 (4) |
| O9—Nd1—N4 | 142.86 (8) | C18—C17—H17A | 118.2 |
| O8—Nd1—N4 | 167.30 (8) | C16—C17—H17A | 118.2 |

| | | | |
|---|---|---|---|
| O5—Nd1—N4 | 25.20 (7) | C17—C18—H18A | 120.0 |
| N3—Nd1—N4 | 72.29 (8) | C17—C18—H18B | 120.0 |
| N1—Nd1—N4 | 100.72 (8) | H18A—C18—H18B | 120.0 |
| N2—Nd1—N4 | 94.35 (8) | C20—C19—C24 | 120.9 (3) |
| O2—Nd1—N5 | 79.81 (7) | C20—C19—H19A | 119.6 |
| O3—Nd1—N5 | 102.15 (8) | C24—C19—H19A | 119.6 |
| O6—Nd1—N5 | 151.74 (7) | C19—C20—C21 | 120.2 (3) |
| O9—Nd1—N5 | 24.95 (7) | C19—C20—H20A | 119.9 |
| O8—Nd1—N5 | 24.82 (7) | C21—C20—H20A | 119.9 |
| O5—Nd1—N5 | 155.25 (7) | C22—C21—C20 | 119.3 (3) |
| N3—Nd1—N5 | 95.51 (8) | C22—C21—H21A | 120.3 |
| N1—Nd1—N5 | 86.52 (8) | C20—C21—H21A | 120.3 |
| N2—Nd1—N5 | 80.20 (8) | C23—C22—C21 | 120.8 (3) |
| N4—Nd1—N5 | 167.79 (8) | C23—C22—H22A | 119.6 |
| C8—O1—C16 | 118.8 (3) | C21—C22—H22A | 119.6 |
| C25—O2—Nd1 | 136.2 (2) | C22—C23—C24 | 120.8 (3) |
| C27—O3—Nd1 | 134.1 (2) | C22—C23—H23A | 119.6 |
| N4—O5—Nd1 | 95.62 (19) | C24—C23—H23A | 119.6 |
| N4—O6—Nd1 | 97.14 (18) | C23—C24—C19 | 118.0 (3) |
| N5—O8—Nd1 | 97.23 (18) | C23—C24—C25 | 122.8 (3) |
| N5—O9—Nd1 | 97.11 (18) | C19—C24—C25 | 119.2 (3) |
| C1—N1—C5 | 117.8 (3) | O2—C25—C26 | 123.8 (3) |
| C1—N1—Nd1 | 120.7 (2) | O2—C25—C24 | 116.6 (3) |
| C5—N1—Nd1 | 121.33 (19) | C26—C25—C24 | 119.6 (3) |
| C6—N2—C10 | 117.6 (3) | C27—C26—C25 | 125.8 (3) |
| C6—N2—Nd1 | 120.74 (19) | C27—C26—H26 | 117.1 |
| C10—N2—Nd1 | 120.26 (19) | C25—C26—H26 | 117.1 |
| C15—N3—C11 | 118.3 (3) | O3—C27—C26 | 125.0 (3) |
| C15—N3—Nd1 | 119.7 (2) | O3—C27—C28 | 116.0 (3) |
| C11—N3—Nd1 | 121.7 (2) | C26—C27—C28 | 118.9 (3) |
| O4—N4—O6 | 121.9 (3) | C33—C28—C29 | 118.4 (3) |
| O4—N4—O5 | 121.6 (3) | C33—C28—C27 | 120.1 (3) |
| O6—N4—O5 | 116.5 (3) | C29—C28—C27 | 121.5 (3) |
| O4—N4—Nd1 | 169.6 (2) | C30—C29—C28 | 120.2 (3) |
| O6—N4—Nd1 | 58.12 (16) | C30—C29—H29A | 119.9 |
| O5—N4—Nd1 | 59.18 (17) | C28—C29—H29A | 119.9 |
| O7—N5—O8 | 122.7 (3) | C31—C30—C29 | 120.7 (4) |
| O7—N5—O9 | 121.4 (3) | C31—C30—H30A | 119.7 |
| O8—N5—O9 | 115.9 (3) | C29—C30—H30A | 119.7 |
| O7—N5—Nd1 | 179.3 (2) | C30—C31—C32 | 120.0 (3) |
| O8—N5—Nd1 | 57.95 (16) | C30—C31—H31A | 120.0 |
| O9—N5—Nd1 | 57.94 (15) | C32—C31—H31A | 120.0 |
| N1—C1—C2 | 124.2 (3) | C31—C32—C33 | 119.6 (3) |
| N1—C1—H1A | 117.9 | C31—C32—H32A | 120.2 |
| C2—C1—H1A | 117.9 | C33—C32—H32A | 120.2 |
| C1—C2—C3 | 118.2 (3) | C32—C33—C28 | 121.1 (3) |
| C1—C2—H2A | 120.9 | C32—C33—H33A | 119.4 |
| C3—C2—H2A | 120.9 | C28—C33—H33A | 119.4 |
| C4—C3—C2 | 118.6 (3) | N6—C34—C35 | 177.6 (5) |

| | | | |
|---|---|---|---|
| C4—C3—H3A | 120.7 | C34—C35—H35A | 109.5 |
| C2—C3—H3A | 120.7 | C34—C35—H35B | 109.5 |
| C3—C4—C5 | 120.6 (3) | H35A—C35—H35B | 109.5 |
| C3—C4—H4A | 119.7 | C34—C35—H35C | 109.5 |
| C5—C4—H4A | 119.7 | H35A—C35—H35C | 109.5 |
| N1—C5—C4 | 120.7 (3) | H35B—C35—H35C | 109.5 |

**Fig. 1**


O4
O5
N4
C3
C4
C2
C18
C17
C5
N1
O6
C31
C32
C33
C30
C29
C6
C1
O3
C27
C28
C7
C8
C10
N2
C16
C11
N3
Nd1
C26
O1
C9
C12
C15
O2
C25
C13
C14
O8
O9
C24
N5
C23
C19
O7
C22
N6
C34
C20
C21
C35