# metal-organic compounds

## catena-Poly[[[(1,10-phenanthroline-κ²N,N′)praseodymium(III)]-di-μ-4-hydroxybenzoato-κ⁴O¹:O¹′-μ-nitrato-κ³O,O′:O] bis(1,10-phenanthroline)]

### Panfeng Wang, Dingding Xu and Xinqing Wang*

College of Materials Science and Engineering, China Jiliang University, Hangzhou 310018, People's Republic of China

Correspondence e-mail: wxqnano@cjlu.edu.cn

The title complex, $[Pr(C_7H_5O_3)_2(NO_3)(C_{12}H_8N_2)]\cdot2C_{12}H_8N_2$, has a polymeric chain structure, with two uncoordinated 1,10-phenanthroline molecules in the lattice. The $Pr^{III}$ centre has a monocapped square-antiprismatic coordination geometry, comprised of two N atoms from one chelating 1,10-phenanthroline ligand, four carboxylate O atoms from four 4-hydroxybenzoate anions and three O atoms from two nitrate anions. The 4-hydroxybenzoate and nitrate anions function as $\mu_2$-bridging ligands and link the $Pr^{III}$ ions into a one-dimensional chain structure along the $c$ axis. Intermolecular O—H···N hydrogen bonds are observed between the 4-hydroxybenzoate anions and the uncoordinated 1,10-phenanthroline molecules.

## Related literature

For related structures, see: Zhou *et al.* (2008); Zhu *et al.* (2010)
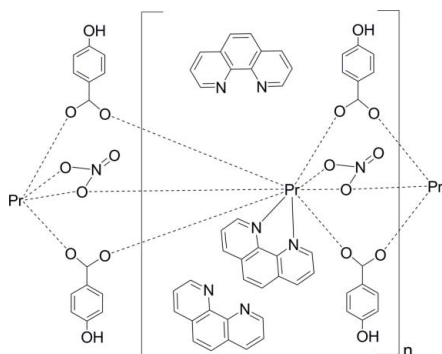


## Experimental

### Crystal data

| | |
|---|---|
| $[Pr(C_7H_5O_3)_2(NO_3)$ $(C_{12}H_8N_2)]\cdot2C_{12}H_8N_2$ | $\beta = 98.899$ (1)° |
| $M_r = 1017.75$ | $V = 4299.88$ (7) Å³ |
| Monoclinic, $P2_1/c$ | $Z = 4$ |
| $a = 21.5625$ (2) Å | Cu $K\alpha$ radiation |
| $b = 23.4621$ (2) Å | $\mu = 9.27$ mm⁻¹ |
| $c = 8.6030$ (1) Å | $T = 291$ K |
| | $0.40 \times 0.33 \times 0.30$ mm |

### Data collection

| | |
|---|---|
| Oxford Diffraction Gemini S Ultra diffractometer | 13264 measured reflections |
| Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2006) | 7308 independent reflections |
| | 6794 reflections with $I > 2\sigma(I)$ |
| | $R_{int} = 0.029$ |
| $T_{min} = 0.119$, $T_{max} = 0.167$ | |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.035$ | 606 parameters |
| $wR(F^2) = 0.092$ | H-atom parameters constrained |
| $S = 1.06$ | $\Delta\rho_{max} = 0.74$ e Å⁻³ |
| 7308 reflections | $\Delta\rho_{min} = -1.31$ e Å⁻³ |

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O6—H6···N4ⁱ | 0.82 | 2.07 | 2.851 (4) | 158 |
| O3—H3···N6ⁱⁱ | 0.82 | 2.04 | 2.782 (5) | 150 |

Symmetry codes: (i) $x + 1, -y + \frac{3}{2}, z - \frac{1}{2}$; (ii) $-x + 1, -y + 1, -z + 1$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

## References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Oxford Diffraction (2006). *CrysAlis PRO, CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhou, Y. X., Shen, X. Q., Zhang, H. Y., Du, C. X., Wu, B. L. & Hou, H. W. (2008). *J. Coord. Chem.* E**61**, 3981–3992.
Zhu, Y.-M., Feng, P.-P., Yang, Y.-Y. & Ng, S. W. (2010). *Acta Cryst.* E**66**, m54–m55.

# supporting information

# *catena*-Poly[[[(1,10-phenanthroline-*κ²N,N′*)praseodymium(III)]-di-*μ*-4-hydroxy-benzoato-*κ⁴O¹:O¹′*-*μ*-nitrato-*κ³O,O′:O*] bis(1,10-phenanthroline)]

**Panfeng Wang, Dingding Xu and Xinqing Wang**

### S1. Experimental

Each reagent was commercially available and of analytical grade. $Pr(NO_3)_3 \cdot 6H_2O$ (0.217 g, 0.5 mmol), *p*-Hydroxybenzoic acid (0.069 g 0.5 mmol), 1, 10-phenanthroline (0.090 g, 0.5 mmol) and $NaHCO_3$ (0.042 g, 0.5 mmol) were dissolved in water-ethanol solution (10 ml, 5:5). The solution was refluxed for 4 h, and filtered after cooling to room temperature. White single crystals were obtained from the filtrate after 7 days.

### S2. Refinement

H atoms were positioned geometrically (C—H = 0.93 Å and O—H = 0.82 Å) and refined as riding, with $U_{iso}$ (H) = 1.2Ueq (C) and $U_{iso}$(H) = 1.5Ueq (O).
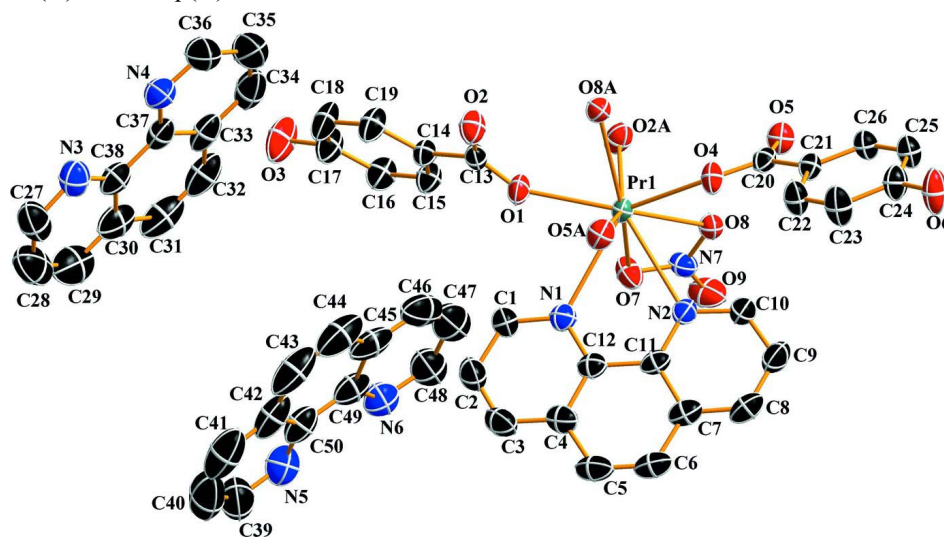


**Figure 1**

The molecular structure of title compound. Displacement ellipsoids are drawn at the 30% probablility level and H atoms are omitted for clarity.
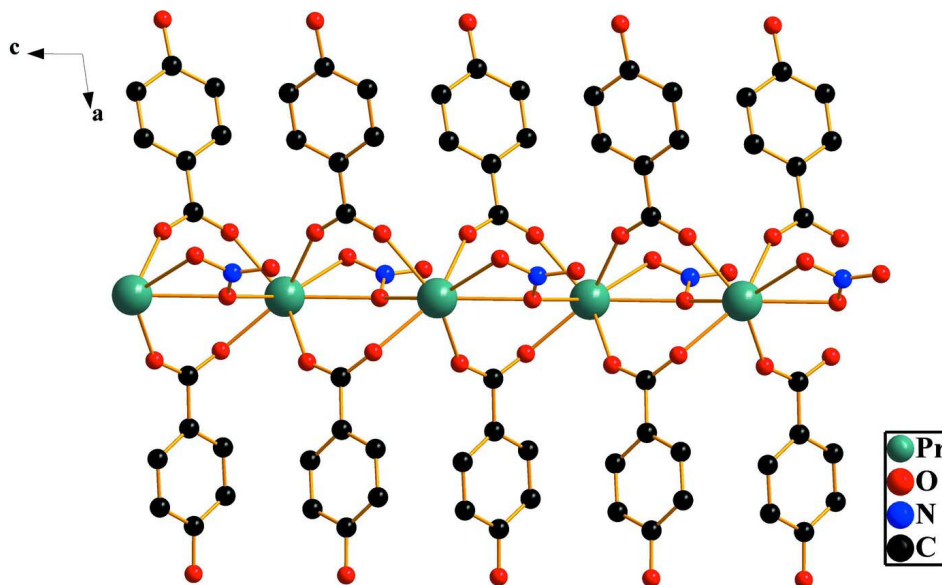
**Figure 2**

One-dimensional network structure view along b direction.

## *catena*-Poly[[[(1,10-phenanthroline- $\kappa^2N,N'$)praseodymium(III)]-di-$\mu$-4-hydroxybenzoato- $\kappa^4O^1$:$O^{1'}$-$\mu$-nitrato-$\kappa^3O,O'$:$O$] bis(1,10-phenanthroline)]

*Crystal data*

| | |
|---|---|
| [Pr(C₇H₅O₃)₂(NO₃)(C₁₂H₈N₂)]·2C₁₂H₈N₂ | $F(000) = 2056$ |
| $M_r = 1017.75$ | $D_x = 1.572$ Mg m⁻³ |
| Monoclinic, $P2_1/c$ | Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 9626 reflections |
| $a = 21.5625$ (2) Å | $\theta = 1.9$–67.4° |
| $b = 23.4621$ (2) Å | $\mu = 9.27$ mm⁻¹ |
| $c = 8.6030$ (1) Å | $T = 291$ K |
| $\beta = 98.899$ (1)° | Needle, white |
| $V = 4299.88$ (7) Å³ | $0.40 \times 0.33 \times 0.30$ mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Gemini S Ultra diffractometer | $T_{min} = 0.119$, $T_{max} = 0.167$ |
| | 13264 measured reflections |
| Radiation source: Enhance Ultra (Cu) X-ray Source | 7308 independent reflections |
| | 6794 reflections with $I > 2\sigma(I)$ |
| Mirror monochromator | $R_{int} = 0.029$ |
| Detector resolution: 15.9149 pixels mm⁻¹ | $\theta_{max} = 65.1°$, $\theta_{min} = 2.1°$ |
| $\omega$ scans | $h = -25 \rightarrow 25$ |
| Absorption correction: multi-scan | $k = -27 \rightarrow 16$ |
| (*CrysAlis PRO*; Oxford Diffraction, 2006) | $l = -9 \rightarrow 10$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | 7308 reflections |
| Least-squares matrix: full | 606 parameters |
| $R[F^2 > 2\sigma(F^2)] = 0.035$ | 0 restraints |
| $wR(F^2) = 0.092$ | Primary atom site location: structure-invariant |
| $S = 1.06$ | direct methods |

| | |
|---|---|
| Secondary atom site location: difference Fourier map | $w = 1/[\sigma^2(F_o^2) + (0.060P)^2]$ |
| | where $P = (F_o^2 + 2F_c^2)/3$ |
| Hydrogen site location: inferred from neighbouring sites | $(\Delta/\sigma)_{max} = 0.001$ |
| | $\Delta\rho_{max} = 0.74$ e Å$^{-3}$ |
| H-atom parameters constrained | $\Delta\rho_{min} = -1.31$ e Å$^{-3}$ |

*Special details*

**Experimental**. CrysAlisPro, Oxford Diffraction Ltd., Version 1.171.34.36 Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

**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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Pr1 | 0.911380 (7) | 0.703539 (6) | 0.660845 (17) | 0.02673 (8) |
| O1 | 0.82724 (10) | 0.69075 (10) | 0.8105 (3) | 0.0402 (5) |
| O2 | 0.82646 (10) | 0.74065 (11) | 1.0300 (3) | 0.0446 (5) |
| O3 | 0.54691 (13) | 0.65243 (17) | 0.9284 (4) | 0.0741 (10) |
| H3 | 0.5307 | 0.6376 | 0.8457 | 0.111* |
| O4 | 0.99741 (10) | 0.76381 (10) | 0.6186 (3) | 0.0388 (5) |
| O5 | 0.98379 (10) | 0.81352 (10) | 0.3967 (3) | 0.0393 (5) |
| O6 | 1.27882 (11) | 0.83426 (15) | 0.5929 (3) | 0.0609 (8) |
| H6 | 1.2891 | 0.8501 | 0.5159 | 0.091* |
| O7 | 0.85863 (12) | 0.63832 (10) | 0.4358 (3) | 0.0473 (6) |
| O8 | 0.91180 (11) | 0.70593 (8) | 0.3492 (3) | 0.0344 (5) |
| O9 | 0.87386 (16) | 0.63694 (11) | 0.1925 (3) | 0.0620 (8) |
| N1 | 0.91051 (12) | 0.58977 (11) | 0.7443 (3) | 0.0372 (6) |
| N2 | 0.99832 (12) | 0.63129 (11) | 0.5726 (3) | 0.0360 (6) |
| N3 | 0.29434 (16) | 0.53994 (16) | 0.9226 (4) | 0.0588 (8) |
| N4 | 0.32464 (19) | 0.64182 (15) | 0.8063 (4) | 0.0628 (9) |
| N5 | 0.50294 (18) | 0.33752 (18) | 0.4667 (5) | 0.0684 (10) |
| N6 | 0.52702 (16) | 0.42317 (16) | 0.2691 (4) | 0.0608 (9) |
| N7 | 0.88073 (13) | 0.65978 (11) | 0.3208 (3) | 0.0382 (6) |
| C1 | 0.86749 (17) | 0.56790 (15) | 0.8203 (4) | 0.0452 (8) |
| H1 | 0.8333 | 0.5905 | 0.8339 | 0.054* |
| C2 | 0.8705 (2) | 0.51245 (17) | 0.8815 (5) | 0.0570 (10) |
| H2 | 0.8385 | 0.4987 | 0.9324 | 0.068* |
| C3 | 0.9202 (2) | 0.47938 (16) | 0.8658 (4) | 0.0560 (10) |
| H3A | 0.9230 | 0.4426 | 0.9064 | 0.067* |
| C4 | 0.96762 (18) | 0.50076 (15) | 0.7881 (4) | 0.0455 (8) |
| C5 | 1.0222 (2) | 0.46801 (16) | 0.7694 (4) | 0.0542 (9) |
| H5 | 1.0271 | 0.4316 | 0.8125 | 0.065* |

| C6 | 1.06627 (19) | 0.48895 (16) | 0.6909 (5) | 0.0532 (9) |
| H6A | 1.1014 | 0.4670 | 0.6810 | 0.064* |
| C7 | 1.05998 (16) | 0.54452 (15) | 0.6224 (4) | 0.0450 (8) |
| C8 | 1.10422 (18) | 0.56691 (18) | 0.5375 (5) | 0.0554 (10) |
| H8 | 1.1401 | 0.5461 | 0.5269 | 0.066* |
| C9 | 1.09484 (17) | 0.61956 (18) | 0.4694 (5) | 0.0541 (9) |
| H9 | 1.1240 | 0.6349 | 0.4119 | 0.065* |
| C10 | 1.04075 (16) | 0.64978 (15) | 0.4880 (4) | 0.0440 (8) |
| H10 | 1.0340 | 0.6849 | 0.4382 | 0.053* |
| C11 | 1.00721 (15) | 0.57883 (13) | 0.6386 (4) | 0.0360 (7) |
| C12 | 0.96066 (15) | 0.55657 (13) | 0.7261 (4) | 0.0368 (7) |
| C13 | 0.80099 (15) | 0.70958 (12) | 0.9199 (4) | 0.0322 (7) |
| C14 | 0.73337 (15) | 0.69387 (13) | 0.9191 (4) | 0.0334 (6) |
| C15 | 0.69901 (15) | 0.66640 (15) | 0.7909 (4) | 0.0393 (7) |
| H15 | 0.7182 | 0.6573 | 0.7044 | 0.047* |
| C16 | 0.63630 (16) | 0.65238 (16) | 0.7902 (4) | 0.0470 (8) |
| H16 | 0.6135 | 0.6347 | 0.7028 | 0.056* |
| C17 | 0.60788 (16) | 0.66489 (18) | 0.9204 (5) | 0.0517 (9) |
| C18 | 0.64241 (19) | 0.6915 (2) | 1.0494 (5) | 0.0602 (11) |
| H18 | 0.6239 | 0.6994 | 1.1377 | 0.072* |
| C19 | 0.70412 (18) | 0.70630 (15) | 1.0472 (5) | 0.0475 (9) |
| H19 | 0.7265 | 0.7250 | 1.1335 | 0.057* |
| C20 | 1.01715 (15) | 0.79388 (12) | 0.5157 (4) | 0.0317 (7) |
| C21 | 1.08667 (14) | 0.80619 (13) | 0.5374 (4) | 0.0312 (6) |
| C22 | 1.12756 (16) | 0.77961 (17) | 0.6560 (4) | 0.0457 (8) |
| H22 | 1.1119 | 0.7551 | 0.7255 | 0.055* |
| C23 | 1.19154 (18) | 0.78935 (18) | 0.6716 (5) | 0.0543 (10) |
| H23 | 1.2185 | 0.7713 | 0.7513 | 0.065* |
| C24 | 1.21567 (15) | 0.82586 (16) | 0.5690 (4) | 0.0432 (8) |
| C25 | 1.17529 (15) | 0.85264 (15) | 0.4508 (4) | 0.0409 (7) |
| H25 | 1.1908 | 0.8776 | 0.3822 | 0.049* |
| C26 | 1.11146 (15) | 0.84181 (14) | 0.4357 (4) | 0.0371 (7) |
| H26 | 1.0846 | 0.8591 | 0.3545 | 0.045* |
| C27 | 0.2817 (2) | 0.4893 (2) | 0.9770 (7) | 0.0762 (14) |
| H27 | 0.2878 | 0.4838 | 1.0853 | 0.091* |
| C28 | 0.2599 (3) | 0.4442 (3) | 0.8801 (10) | 0.097 (2) |
| H28 | 0.2521 | 0.4092 | 0.9237 | 0.116* |
| C29 | 0.2501 (2) | 0.4509 (3) | 0.7224 (9) | 0.0909 (18) |
| H29 | 0.2343 | 0.4209 | 0.6573 | 0.109* |
| C30 | 0.26354 (17) | 0.5030 (2) | 0.6578 (6) | 0.0656 (12) |
| C31 | 0.2559 (2) | 0.5159 (3) | 0.4895 (6) | 0.0795 (17) |
| H31 | 0.2396 | 0.4880 | 0.4178 | 0.095* |
| C32 | 0.2714 (2) | 0.5660 (3) | 0.4363 (6) | 0.0729 (14) |
| H32 | 0.2657 | 0.5724 | 0.3283 | 0.087* |
| C33 | 0.29633 (18) | 0.6099 (2) | 0.5385 (5) | 0.0578 (11) |
| C34 | 0.3163 (2) | 0.6624 (2) | 0.4868 (6) | 0.0741 (14) |
| H34 | 0.3126 | 0.6700 | 0.3796 | 0.089* |
| C35 | 0.3411 (4) | 0.7024 (2) | 0.5929 (8) | 0.093 (2) |

| | | | |
|---|---|---|---|
| H35 | 0.3564 | 0.7368 | 0.5604 | 0.112* |
| C36 | 0.3430 (3) | 0.6902 (2) | 0.7513 (7) | 0.0863 (17) |
| H36 | 0.3583 | 0.7182 | 0.8237 | 0.104* |
| C37 | 0.30263 (17) | 0.60086 (18) | 0.7031 (4) | 0.0505 (9) |
| C38 | 0.28600 (16) | 0.54654 (18) | 0.7640 (5) | 0.0508 (9) |
| C39 | 0.4948 (3) | 0.2955 (2) | 0.5625 (8) | 0.0887 (18) |
| H39 | 0.4729 | 0.2635 | 0.5204 | 0.106* |
| C40 | 0.5173 (4) | 0.2960 (3) | 0.7245 (9) | 0.108 (3) |
| H40 | 0.5115 | 0.2648 | 0.7873 | 0.130* |
| C41 | 0.5475 (3) | 0.3430 (4) | 0.7867 (7) | 0.103 (2) |
| H41 | 0.5621 | 0.3446 | 0.8942 | 0.124* |
| C42 | 0.5571 (2) | 0.3895 (3) | 0.6909 (6) | 0.0754 (15) |
| C43 | 0.5878 (2) | 0.4410 (4) | 0.7490 (7) | 0.095 (2) |
| H43 | 0.6026 | 0.4443 | 0.8560 | 0.113* |
| C44 | 0.5958 (2) | 0.4845 (3) | 0.6533 (8) | 0.092 (2) |
| H44 | 0.6146 | 0.5179 | 0.6955 | 0.110* |
| C45 | 0.57586 (18) | 0.4804 (2) | 0.4878 (7) | 0.0728 (14) |
| C46 | 0.5861 (2) | 0.5236 (2) | 0.3827 (9) | 0.0855 (17) |
| H46 | 0.6047 | 0.5577 | 0.4203 | 0.103* |
| C47 | 0.5686 (2) | 0.5157 (3) | 0.2249 (10) | 0.0897 (18) |
| H47 | 0.5763 | 0.5434 | 0.1529 | 0.108* |
| C48 | 0.5387 (2) | 0.4646 (2) | 0.1750 (7) | 0.0743 (13) |
| H48 | 0.5262 | 0.4595 | 0.0676 | 0.089* |
| C49 | 0.54567 (17) | 0.42982 (19) | 0.4263 (5) | 0.0579 (10) |
| C50 | 0.53442 (17) | 0.3839 (2) | 0.5292 (5) | 0.0589 (10) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Pr1 | 0.02430 (11) | 0.03072 (12) | 0.02603 (11) | 0.00020 (5) | 0.00666 (7) | −0.00008 (5) |
| O1 | 0.0344 (11) | 0.0491 (12) | 0.0408 (13) | −0.0055 (10) | 0.0173 (10) | −0.0017 (10) |
| O2 | 0.0381 (12) | 0.0556 (14) | 0.0408 (13) | −0.0136 (11) | 0.0080 (10) | −0.0071 (11) |
| O3 | 0.0370 (14) | 0.111 (3) | 0.078 (2) | −0.0256 (15) | 0.0191 (14) | −0.0280 (19) |
| O4 | 0.0333 (10) | 0.0483 (13) | 0.0367 (12) | −0.0096 (9) | 0.0113 (9) | 0.0016 (10) |
| O5 | 0.0331 (11) | 0.0512 (13) | 0.0323 (11) | −0.0029 (10) | 0.0008 (9) | 0.0005 (10) |
| O6 | 0.0308 (12) | 0.102 (2) | 0.0493 (15) | −0.0079 (13) | 0.0055 (11) | 0.0225 (15) |
| O7 | 0.0578 (14) | 0.0437 (13) | 0.0404 (13) | −0.0166 (11) | 0.0074 (11) | 0.0008 (10) |
| O8 | 0.0381 (12) | 0.0333 (12) | 0.0330 (12) | −0.0010 (8) | 0.0090 (10) | 0.0008 (8) |
| O9 | 0.100 (2) | 0.0472 (14) | 0.0361 (13) | 0.0003 (15) | 0.0019 (14) | −0.0124 (11) |
| N1 | 0.0403 (14) | 0.0380 (14) | 0.0334 (13) | 0.0007 (11) | 0.0057 (11) | −0.0008 (11) |
| N2 | 0.0361 (13) | 0.0383 (14) | 0.0349 (13) | 0.0030 (11) | 0.0101 (11) | −0.0013 (11) |
| N3 | 0.0498 (18) | 0.071 (2) | 0.057 (2) | 0.0027 (16) | 0.0108 (15) | 0.0065 (17) |
| N4 | 0.085 (3) | 0.055 (2) | 0.0530 (19) | 0.0041 (18) | 0.0268 (19) | −0.0061 (16) |
| N5 | 0.059 (2) | 0.086 (3) | 0.060 (2) | −0.004 (2) | 0.0087 (18) | −0.003 (2) |
| N6 | 0.0463 (17) | 0.068 (2) | 0.066 (2) | 0.0057 (16) | 0.0029 (16) | −0.0012 (18) |
| N7 | 0.0494 (15) | 0.0292 (13) | 0.0352 (15) | −0.0003 (12) | 0.0043 (12) | −0.0014 (11) |
| C1 | 0.0495 (19) | 0.0416 (18) | 0.0469 (19) | −0.0023 (15) | 0.0156 (16) | 0.0044 (15) |
| C2 | 0.071 (3) | 0.052 (2) | 0.052 (2) | −0.0089 (19) | 0.023 (2) | 0.0068 (17) |

| | | | | | |
|------|-----------|-------------|-------------|-------------|-------------|-------------|
| C3 | 0.083 (3) | 0.0395 (18) | 0.046 (2) | 0.0005 (19) | 0.012 (2) | 0.0078 (16) |
| C4 | 0.062 (2) | 0.0403 (17) | 0.0318 (16) | 0.0057 (16) | 0.0014 (15) | 0.0013 (14) |
| C5 | 0.077 (3) | 0.0399 (18) | 0.0433 (19) | 0.0168 (19) | 0.0006 (19) | 0.0007 (15) |
| C6 | 0.059 (2) | 0.047 (2) | 0.051 (2) | 0.0202 (17) | 0.0000 (18) | −0.0073 (17) |
| C7 | 0.0457 (18) | 0.0481 (19) | 0.0394 (17) | 0.0121 (15) | 0.0011 (15) | −0.0086 (15) |
| C8 | 0.0423 (18) | 0.063 (2) | 0.061 (2) | 0.0181 (17) | 0.0112 (17) | −0.0090 (19) |
| C9 | 0.0437 (19) | 0.062 (2) | 0.062 (2) | 0.0063 (17) | 0.0236 (18) | −0.0072 (19) |
| C10 | 0.0434 (18) | 0.0438 (18) | 0.0481 (19) | 0.0003 (14) | 0.0171 (15) | −0.0040 (15) |
| C11 | 0.0368 (15) | 0.0385 (17) | 0.0315 (15) | 0.0068 (13) | 0.0013 (12) | −0.0072 (13) |
| C12 | 0.0434 (16) | 0.0364 (16) | 0.0294 (15) | 0.0030 (13) | 0.0026 (13) | −0.0046 (12) |
| C13 | 0.0292 (15) | 0.0345 (15) | 0.0343 (17) | −0.0015 (11) | 0.0088 (13) | 0.0078 (12) |
| C14 | 0.0297 (15) | 0.0376 (15) | 0.0339 (16) | −0.0031 (12) | 0.0080 (13) | −0.0012 (12) |
| C15 | 0.0346 (15) | 0.0486 (18) | 0.0353 (16) | −0.0042 (14) | 0.0071 (13) | −0.0068 (14) |
| C16 | 0.0372 (17) | 0.057 (2) | 0.0459 (19) | −0.0091 (15) | 0.0035 (15) | −0.0128 (16) |
| C17 | 0.0328 (16) | 0.066 (2) | 0.057 (2) | −0.0124 (16) | 0.0119 (16) | −0.0113 (18) |
| C18 | 0.043 (2) | 0.087 (3) | 0.056 (2) | −0.013 (2) | 0.0251 (19) | −0.024 (2) |
| C19 | 0.0377 (19) | 0.065 (2) | 0.041 (2) | −0.0108 (15) | 0.0098 (16) | −0.0185 (15) |
| C20 | 0.0310 (16) | 0.0336 (16) | 0.0319 (16) | −0.0030 (11) | 0.0090 (13) | −0.0083 (12) |
| C21 | 0.0299 (15) | 0.0368 (15) | 0.0277 (15) | −0.0026 (12) | 0.0064 (12) | −0.0029 (12) |
| C22 | 0.0383 (17) | 0.058 (2) | 0.0409 (18) | −0.0041 (16) | 0.0072 (15) | 0.0152 (17) |
| C23 | 0.0362 (19) | 0.079 (3) | 0.047 (2) | −0.0011 (17) | 0.0010 (16) | 0.0241 (18) |
| C24 | 0.0317 (15) | 0.059 (2) | 0.0392 (17) | −0.0079 (15) | 0.0059 (13) | 0.0031 (15) |
| C25 | 0.0370 (16) | 0.0492 (19) | 0.0370 (17) | −0.0066 (14) | 0.0071 (14) | 0.0091 (14) |
| C26 | 0.0331 (15) | 0.0425 (17) | 0.0355 (16) | −0.0029 (13) | 0.0047 (13) | 0.0047 (13) |
| C27 | 0.061 (3) | 0.077 (3) | 0.092 (4) | −0.006 (2) | 0.016 (3) | 0.024 (3) |
| C28 | 0.065 (3) | 0.074 (4) | 0.154 (6) | −0.010 (3) | 0.026 (4) | 0.021 (4) |
| C29 | 0.055 (3) | 0.084 (4) | 0.134 (5) | −0.019 (3) | 0.014 (3) | −0.034 (4) |
| C30 | 0.0308 (17) | 0.077 (3) | 0.089 (3) | −0.0004 (19) | 0.0083 (19) | −0.024 (2) |
| C31 | 0.040 (2) | 0.117 (5) | 0.078 (3) | 0.006 (2) | −0.002 (2) | −0.049 (3) |
| C32 | 0.045 (2) | 0.118 (4) | 0.055 (3) | 0.015 (3) | 0.0059 (19) | −0.018 (3) |
| C33 | 0.0412 (19) | 0.088 (3) | 0.046 (2) | 0.021 (2) | 0.0110 (16) | −0.002 (2) |
| C34 | 0.072 (3) | 0.099 (4) | 0.056 (3) | 0.028 (3) | 0.026 (2) | 0.023 (3) |
| C35 | 0.133 (6) | 0.070 (4) | 0.086 (4) | 0.017 (3) | 0.047 (4) | 0.018 (3) |
| C36 | 0.130 (5) | 0.056 (3) | 0.082 (4) | 0.001 (3) | 0.047 (4) | −0.002 (3) |
| C37 | 0.0444 (18) | 0.067 (2) | 0.0424 (19) | 0.0175 (17) | 0.0140 (15) | 0.0004 (17) |
| C38 | 0.0319 (16) | 0.066 (2) | 0.056 (2) | 0.0061 (16) | 0.0088 (15) | −0.0082 (18) |
| C39 | 0.088 (4) | 0.094 (4) | 0.089 (4) | −0.003 (3) | 0.029 (4) | 0.014 (3) |
| C40 | 0.112 (6) | 0.137 (7) | 0.083 (5) | 0.021 (4) | 0.039 (4) | 0.035 (4) |
| C41 | 0.084 (4) | 0.169 (7) | 0.060 (3) | 0.034 (4) | 0.019 (3) | −0.001 (4) |
| C42 | 0.047 (2) | 0.124 (5) | 0.056 (3) | 0.020 (3) | 0.011 (2) | −0.017 (3) |
| C43 | 0.053 (3) | 0.157 (6) | 0.073 (4) | 0.010 (3) | 0.006 (2) | −0.056 (4) |
| C44 | 0.050 (3) | 0.122 (5) | 0.105 (4) | 0.000 (3) | 0.011 (3) | −0.061 (4) |
| C45 | 0.0330 (19) | 0.081 (3) | 0.103 (4) | 0.012 (2) | 0.008 (2) | −0.037 (3) |
| C46 | 0.048 (3) | 0.061 (3) | 0.150 (6) | 0.005 (2) | 0.024 (3) | −0.013 (4) |
| C47 | 0.050 (3) | 0.082 (4) | 0.140 (6) | 0.013 (2) | 0.023 (3) | 0.022 (4) |
| C48 | 0.054 (2) | 0.077 (3) | 0.092 (4) | 0.007 (2) | 0.009 (2) | 0.015 (3) |
| C49 | 0.0313 (16) | 0.071 (3) | 0.070 (3) | 0.0110 (17) | 0.0049 (17) | −0.016 (2) |
| C50 | 0.0372 (18) | 0.087 (3) | 0.053 (2) | 0.0113 (19) | 0.0060 (16) | −0.011 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Pr1—O2ⁱ | 2.387 (2) | C15—H15 | 0.9300 |
| Pr1—O5ⁱⁱ | 2.395 (2) | C16—C17 | 1.389 (5) |
| Pr1—O1 | 2.400 (2) | C16—H16 | 0.9300 |
| Pr1—O4 | 2.404 (2) | C17—C18 | 1.385 (6) |
| Pr1—O7 | 2.589 (2) | C18—C19 | 1.378 (5) |
| Pr1—O8ⁱⁱ | 2.671 (2) | C18—H18 | 0.9300 |
| Pr1—O8 | 2.683 (2) | C19—H19 | 0.9300 |
| Pr1—N2 | 2.721 (3) | C20—C21 | 1.509 (4) |
| Pr1—N1 | 2.765 (3) | C21—C26 | 1.376 (5) |
| O1—C13 | 1.251 (4) | C21—C22 | 1.389 (5) |
| O2—C13 | 1.253 (4) | C22—C23 | 1.384 (5) |
| O2—Pr1ⁱⁱ | 2.387 (2) | C22—H22 | 0.9300 |
| O3—C17 | 1.359 (4) | C23—C24 | 1.388 (5) |
| O3—H3 | 0.8200 | C23—H23 | 0.9300 |
| O4—C20 | 1.257 (4) | C24—C25 | 1.383 (5) |
| O5—C20 | 1.245 (4) | C25—C26 | 1.386 (4) |
| O5—Pr1ⁱ | 2.395 (2) | C25—H25 | 0.9300 |
| O6—C24 | 1.360 (4) | C26—H26 | 0.9300 |
| O6—H6 | 0.8200 | C27—C28 | 1.385 (9) |
| O7—N7 | 1.267 (4) | C27—H27 | 0.9300 |
| O8—N7 | 1.277 (3) | C28—C29 | 1.349 (9) |
| O8—Pr1ⁱ | 2.671 (2) | C28—H28 | 0.9300 |
| O9—N7 | 1.215 (4) | C29—C30 | 1.392 (8) |
| N1—C1 | 1.318 (4) | C29—H29 | 0.9300 |
| N1—C12 | 1.361 (4) | C30—C38 | 1.407 (6) |
| N2—C10 | 1.327 (4) | C30—C31 | 1.463 (7) |
| N2—C11 | 1.357 (4) | C31—C32 | 1.325 (8) |
| N3—C27 | 1.320 (6) | C31—H31 | 0.9300 |
| N3—C38 | 1.357 (5) | C32—C33 | 1.407 (7) |
| N4—C36 | 1.314 (6) | C32—H32 | 0.9300 |
| N4—C37 | 1.344 (5) | C33—C34 | 1.399 (7) |
| N5—C39 | 1.314 (7) | C33—C37 | 1.418 (5) |
| N5—C50 | 1.350 (6) | C34—C35 | 1.360 (9) |
| N6—C48 | 1.314 (6) | C34—H34 | 0.9300 |
| N6—C49 | 1.359 (6) | C35—C36 | 1.387 (8) |
| C1—C2 | 1.401 (5) | C35—H35 | 0.9300 |
| C1—H1 | 0.9300 | C36—H36 | 0.9300 |
| C2—C3 | 1.347 (6) | C37—C38 | 1.444 (6) |
| C2—H2 | 0.9300 | C39—C40 | 1.403 (10) |
| C3—C4 | 1.399 (6) | C39—H39 | 0.9300 |
| C3—H3A | 0.9300 | C40—C41 | 1.350 (10) |
| C4—C12 | 1.413 (5) | C40—H40 | 0.9300 |
| C4—C5 | 1.436 (5) | C41—C42 | 1.402 (10) |
| C5—C6 | 1.341 (6) | C41—H41 | 0.9300 |
| C5—H5 | 0.9300 | C42—C50 | 1.407 (6) |
| C6—C7 | 1.429 (5) | C42—C43 | 1.429 (9) |

| | | | |
|---|---|---|---|
| C6—H6A | 0.9300 | C43—C44 | 1.340 (10) |
| C7—C8 | 1.391 (6) | C43—H43 | 0.9300 |
| C7—C11 | 1.418 (4) | C44—C45 | 1.425 (8) |
| C8—C9 | 1.368 (6) | C44—H44 | 0.9300 |
| C8—H8 | 0.9300 | C45—C46 | 1.399 (8) |
| C9—C10 | 1.395 (5) | C45—C49 | 1.416 (6) |
| C9—H9 | 0.9300 | C46—C47 | 1.364 (9) |
| C10—H10 | 0.9300 | C46—H46 | 0.9300 |
| C11—C12 | 1.442 (5) | C47—C48 | 1.397 (8) |
| C13—C14 | 1.503 (4) | C47—H47 | 0.9300 |
| C14—C19 | 1.383 (5) | C48—H48 | 0.9300 |
| C14—C15 | 1.388 (5) | C49—C50 | 1.438 (7) |
| C15—C16 | 1.391 (5) | | |
| | | | |
| O2$^i$—Pr1—O5$^{ii}$ | 147.50 (8) | C17—C16—H16 | 120.1 |
| O2$^i$—Pr1—O1 | 74.53 (8) | C15—C16—H16 | 120.1 |
| O5$^{ii}$—Pr1—O1 | 88.43 (8) | O3—C17—C18 | 117.4 (3) |
| O2$^i$—Pr1—O4 | 99.18 (8) | O3—C17—C16 | 123.1 (3) |
| O5$^{ii}$—Pr1—O4 | 79.01 (8) | C18—C17—C16 | 119.4 (3) |
| O1—Pr1—O4 | 145.03 (8) | C19—C18—C17 | 120.2 (3) |
| O2$^i$—Pr1—O7 | 75.83 (9) | C19—C18—H18 | 119.9 |
| O5$^{ii}$—Pr1—O7 | 133.49 (8) | C17—C18—H18 | 119.9 |
| O1—Pr1—O7 | 92.65 (8) | C18—C19—C14 | 121.2 (3) |
| O4—Pr1—O7 | 119.63 (7) | C18—C19—H19 | 119.4 |
| O2$^i$—Pr1—O8$^{ii}$ | 77.31 (8) | C14—C19—H19 | 119.4 |
| O5$^{ii}$—Pr1—O8$^{ii}$ | 71.23 (8) | O5—C20—O4 | 124.8 (3) |
| O1—Pr1—O8$^{ii}$ | 72.90 (7) | O5—C20—C21 | 117.9 (3) |
| O4—Pr1—O8$^{ii}$ | 72.17 (7) | O4—C20—C21 | 117.3 (3) |
| O7—Pr1—O8$^{ii}$ | 152.09 (8) | C26—C21—C22 | 118.3 (3) |
| O2$^i$—Pr1—O8 | 68.78 (7) | C26—C21—C20 | 120.9 (3) |
| O5$^{ii}$—Pr1—O8 | 138.38 (7) | C22—C21—C20 | 120.7 (3) |
| O1—Pr1—O8 | 131.16 (8) | C23—C22—C21 | 120.4 (3) |
| O4—Pr1—O8 | 73.42 (7) | C23—C22—H22 | 119.8 |
| O7—Pr1—O8 | 48.24 (7) | C21—C22—H22 | 119.8 |
| O8$^{ii}$—Pr1—O8 | 126.12 (4) | C22—C23—C24 | 120.4 (3) |
| O2$^i$—Pr1—N2 | 136.17 (8) | C22—C23—H23 | 119.8 |
| O5$^{ii}$—Pr1—N2 | 75.24 (8) | C24—C23—H23 | 119.8 |
| O1—Pr1—N2 | 133.02 (8) | O6—C24—C25 | 123.2 (3) |
| O4—Pr1—N2 | 75.13 (8) | O6—C24—C23 | 117.3 (3) |
| O7—Pr1—N2 | 70.43 (8) | C25—C24—C23 | 119.5 (3) |
| O8$^{ii}$—Pr1—N2 | 136.62 (8) | C24—C25—C26 | 119.3 (3) |
| O8—Pr1—N2 | 67.99 (7) | C24—C25—H25 | 120.4 |
| O2$^i$—Pr1—N1 | 128.07 (8) | C26—C25—H25 | 120.4 |
| O5$^{ii}$—Pr1—N1 | 69.41 (8) | C21—C26—C25 | 122.0 (3) |
| O1—Pr1—N1 | 72.78 (8) | C21—C26—H26 | 119.0 |
| O4—Pr1—N1 | 130.05 (8) | C25—C26—H26 | 119.0 |
| O7—Pr1—N1 | 66.66 (8) | N3—C27—C28 | 123.0 (5) |
| O8$^{ii}$—Pr1—N1 | 127.56 (7) | N3—C27—H27 | 118.5 |

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|---|---|---|---|
| O8—Pr1—N1 | 106.31 (7) | C28—C27—H27 | 118.5 |
| N2—Pr1—N1 | 60.24 (8) | C29—C28—C27 | 120.1 (6) |
| C13—O1—Pr1 | 145.7 (2) | C29—C28—H28 | 119.9 |
| C13—O2—Pr1ii | 152.9 (2) | C27—C28—H28 | 119.9 |
| C17—O3—H3 | 109.5 | C28—C29—C30 | 119.6 (5) |
| C20—O4—Pr1 | 142.2 (2) | C28—C29—H29 | 120.2 |
| C20—O5—Pr1i | 148.5 (2) | C30—C29—H29 | 120.2 |
| C24—O6—H6 | 109.5 | C29—C30—C38 | 116.8 (5) |
| N7—O7—Pr1 | 100.04 (17) | C29—C30—C31 | 125.3 (5) |
| N7—O8—Pr1i | 127.27 (19) | C38—C30—C31 | 117.9 (5) |
| N7—O8—Pr1 | 95.22 (16) | C32—C31—C30 | 122.0 (4) |
| Pr1i—O8—Pr1 | 128.52 (8) | C32—C31—H31 | 119.0 |
| C1—N1—C12 | 117.8 (3) | C30—C31—H31 | 119.0 |
| C1—N1—Pr1 | 122.5 (2) | C31—C32—C33 | 121.8 (5) |
| C12—N1—Pr1 | 119.0 (2) | C31—C32—H32 | 119.1 |
| C10—N2—C11 | 117.5 (3) | C33—C32—H32 | 119.1 |
| C10—N2—Pr1 | 120.8 (2) | C34—C33—C32 | 123.5 (4) |
| C11—N2—Pr1 | 120.47 (19) | C34—C33—C37 | 117.6 (4) |
| C27—N3—C38 | 117.2 (4) | C32—C33—C37 | 118.9 (5) |
| C36—N4—C37 | 118.4 (4) | C35—C34—C33 | 120.1 (4) |
| C39—N5—C50 | 117.6 (5) | C35—C34—H34 | 119.9 |
| C48—N6—C49 | 118.2 (4) | C33—C34—H34 | 119.9 |
| O9—N7—O7 | 121.7 (3) | C34—C35—C36 | 117.8 (5) |
| O9—N7—O8 | 122.3 (3) | C34—C35—H35 | 121.1 |
| O7—N7—O8 | 115.9 (3) | C36—C35—H35 | 121.1 |
| N1—C1—C2 | 123.5 (3) | N4—C36—C35 | 124.5 (6) |
| N1—C1—H1 | 118.2 | N4—C36—H36 | 117.7 |
| C2—C1—H1 | 118.2 | C35—C36—H36 | 117.7 |
| C3—C2—C1 | 119.2 (4) | N4—C37—C33 | 121.4 (4) |
| C3—C2—H2 | 120.4 | N4—C37—C38 | 118.3 (3) |
| C1—C2—H2 | 120.4 | C33—C37—C38 | 120.3 (4) |
| C2—C3—C4 | 119.6 (3) | N3—C38—C30 | 123.3 (4) |
| C2—C3—H3A | 120.2 | N3—C38—C37 | 117.6 (4) |
| C4—C3—H3A | 120.2 | C30—C38—C37 | 119.1 (4) |
| C3—C4—C12 | 118.0 (3) | N5—C39—C40 | 123.9 (6) |
| C3—C4—C5 | 122.3 (3) | N5—C39—H39 | 118.0 |
| C12—C4—C5 | 119.7 (3) | C40—C39—H39 | 118.0 |
| C6—C5—C4 | 121.1 (3) | C41—C40—C39 | 118.2 (6) |
| C6—C5—H5 | 119.4 | C41—C40—H40 | 120.9 |
| C4—C5—H5 | 119.4 | C39—C40—H40 | 120.9 |
| C5—C6—C7 | 120.9 (3) | C40—C41—C42 | 120.6 (6) |
| C5—C6—H6A | 119.6 | C40—C41—H41 | 119.7 |
| C7—C6—H6A | 119.6 | C42—C41—H41 | 119.7 |
| C8—C7—C11 | 117.6 (3) | C41—C42—C50 | 116.6 (6) |
| C8—C7—C6 | 122.2 (3) | C41—C42—C43 | 123.7 (6) |
| C11—C7—C6 | 120.2 (3) | C50—C42—C43 | 119.7 (6) |
| C9—C8—C7 | 119.8 (3) | C44—C43—C42 | 121.7 (5) |
| C9—C8—H8 | 120.1 | C44—C43—H43 | 119.1 |

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|---|---|---|---|
| C7—C8—H8 | 120.1 | C42—C43—H43 | 119.1 |
| C8—C9—C10 | 118.7 (4) | C43—C44—C45 | 121.0 (6) |
| C8—C9—H9 | 120.6 | C43—C44—H44 | 119.5 |
| C10—C9—H9 | 120.6 | C45—C44—H44 | 119.5 |
| N2—C10—C9 | 123.8 (3) | C46—C45—C49 | 118.4 (5) |
| N2—C10—H10 | 118.1 | C46—C45—C44 | 122.9 (6) |
| C9—C10—H10 | 118.1 | C49—C45—C44 | 118.7 (6) |
| N2—C11—C7 | 122.5 (3) | C47—C46—C45 | 119.9 (5) |
| N2—C11—C12 | 118.8 (3) | C47—C46—H46 | 120.1 |
| C7—C11—C12 | 118.7 (3) | C45—C46—H46 | 120.1 |
| N1—C12—C4 | 121.8 (3) | C46—C47—C48 | 117.7 (6) |
| N1—C12—C11 | 118.8 (3) | C46—C47—H47 | 121.1 |
| C4—C12—C11 | 119.4 (3) | C48—C47—H47 | 121.1 |
| O1—C13—O2 | 125.3 (3) | N6—C48—C47 | 124.7 (6) |
| O1—C13—C14 | 117.5 (3) | N6—C48—H48 | 117.6 |
| O2—C13—C14 | 117.2 (3) | C47—C48—H48 | 117.6 |
| C19—C14—C15 | 118.5 (3) | N6—C49—C45 | 121.1 (5) |
| C19—C14—C13 | 120.4 (3) | N6—C49—C50 | 118.3 (4) |
| C15—C14—C13 | 121.0 (3) | C45—C49—C50 | 120.6 (4) |
| C14—C15—C16 | 120.8 (3) | N5—C50—C42 | 123.0 (5) |
| C14—C15—H15 | 119.6 | N5—C50—C49 | 118.7 (4) |
| C16—C15—H15 | 119.6 | C42—C50—C49 | 118.2 (4) |
| C17—C16—C15 | 119.8 (3) | | |
| | | | |
| O2$^i$—Pr1—O1—C13 | −87.7 (4) | C3—C4—C12—N1 | 1.9 (5) |
| O5$^{ii}$—Pr1—O1—C13 | 64.3 (4) | C5—C4—C12—N1 | −178.3 (3) |
| O4—Pr1—O1—C13 | −3.9 (5) | C3—C4—C12—C11 | −177.0 (3) |
| O7—Pr1—O1—C13 | −162.2 (4) | C5—C4—C12—C11 | 2.8 (5) |
| O8$^{ii}$—Pr1—O1—C13 | −6.5 (4) | N2—C11—C12—N1 | −2.4 (4) |
| O8—Pr1—O1—C13 | −129.9 (4) | C7—C11—C12—N1 | 178.8 (3) |
| N2—Pr1—O1—C13 | 132.3 (4) | N2—C11—C12—C4 | 176.5 (3) |
| N1—Pr1—O1—C13 | 133.2 (4) | C7—C11—C12—C4 | −2.2 (5) |
| O2$^i$—Pr1—O4—C20 | −42.3 (3) | Pr1—O1—C13—O2 | −22.6 (6) |
| O5$^{ii}$—Pr1—O4—C20 | 170.6 (3) | Pr1—O1—C13—C14 | 157.1 (3) |
| O1—Pr1—O4—C20 | −118.4 (3) | Pr1$^{ii}$—O2—C13—O1 | 6.1 (7) |
| O7—Pr1—O4—C20 | 36.5 (4) | Pr1$^{ii}$—O2—C13—C14 | −173.6 (4) |
| O8$^{ii}$—Pr1—O4—C20 | −115.7 (3) | O1—C13—C14—C19 | 170.8 (3) |
| O8—Pr1—O4—C20 | 22.2 (3) | O2—C13—C14—C19 | −9.4 (5) |
| N2—Pr1—O4—C20 | 93.2 (3) | O1—C13—C14—C15 | −8.8 (5) |
| N1—Pr1—O4—C20 | 119.8 (3) | O2—C13—C14—C15 | 171.0 (3) |
| O2$^i$—Pr1—O7—N7 | 78.52 (19) | C19—C14—C15—C16 | 0.9 (5) |
| O5$^{ii}$—Pr1—O7—N7 | −117.83 (18) | C13—C14—C15—C16 | −179.5 (3) |
| O1—Pr1—O7—N7 | 151.84 (19) | C14—C15—C16—C17 | −1.3 (6) |
| O4—Pr1—O7—N7 | −14.1 (2) | C15—C16—C17—O3 | −179.9 (4) |
| O8$^{ii}$—Pr1—O7—N7 | 94.6 (2) | C15—C16—C17—C18 | 0.3 (7) |
| O8—Pr1—O7—N7 | 4.48 (16) | O3—C17—C18—C19 | −178.7 (4) |
| N2—Pr1—O7—N7 | −73.06 (19) | C16—C17—C18—C19 | 1.1 (7) |
| N1—Pr1—O7—N7 | −138.2 (2) | C17—C18—C19—C14 | −1.6 (7) |

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| O2[i]—Pr1—O8—N7 | −94.08 (18) | C15—C14—C19—C18 | 0.5 (6) |
| O5[ii]—Pr1—O8—N7 | 108.21 (19) | C13—C14—C19—C18 | −179.1 (4) |
| O1—Pr1—O8—N7 | −50.1 (2) | Pr1[i]—O5—C20—O4 | −57.3 (5) |
| O4—Pr1—O8—N7 | 158.81 (18) | Pr1[i]—O5—C20—C21 | 121.8 (3) |
| O7—Pr1—O8—N7 | −4.39 (16) | Pr1—O4—C20—O5 | 20.8 (5) |
| O8[ii]—Pr1—O8—N7 | −148.99 (13) | Pr1—O4—C20—C21 | −158.3 (2) |
| N2—Pr1—O8—N7 | 78.51 (17) | O5—C20—C21—C26 | 5.2 (4) |
| N1—Pr1—O8—N7 | 31.05 (18) | O4—C20—C21—C26 | −175.7 (3) |
| O2[i]—Pr1—O8—Pr1[i] | 54.12 (11) | O5—C20—C21—C22 | −171.6 (3) |
| O5[ii]—Pr1—O8—Pr1[i] | −103.59 (13) | O4—C20—C21—C22 | 7.5 (4) |
| O1—Pr1—O8—Pr1[i] | 98.11 (13) | C26—C21—C22—C23 | 0.6 (6) |
| O4—Pr1—O8—Pr1[i] | −52.99 (11) | C20—C21—C22—C23 | 177.4 (4) |
| O7—Pr1—O8—Pr1[i] | 143.81 (16) | C21—C22—C23—C24 | 0.1 (7) |
| O8[ii]—Pr1—O8—Pr1[i] | −0.8 (2) | C22—C23—C24—O6 | 178.8 (4) |
| N2—Pr1—O8—Pr1[i] | −133.28 (13) | C22—C23—C24—C25 | 0.1 (6) |
| N1—Pr1—O8—Pr1[i] | 179.25 (10) | O6—C24—C25—C26 | −179.6 (4) |
| O2[i]—Pr1—N1—C1 | −49.4 (3) | C23—C24—C25—C26 | −1.0 (6) |
| O5[ii]—Pr1—N1—C1 | 98.8 (3) | C22—C21—C26—C25 | −1.5 (5) |
| O1—Pr1—N1—C1 | 3.9 (3) | C20—C21—C26—C25 | −178.3 (3) |
| O4—Pr1—N1—C1 | 153.2 (2) | C24—C25—C26—C21 | 1.7 (5) |
| O7—Pr1—N1—C1 | −96.9 (3) | C38—N3—C27—C28 | −1.0 (7) |
| O8[ii]—Pr1—N1—C1 | 55.1 (3) | N3—C27—C28—C29 | −0.6 (9) |
| O8—Pr1—N1—C1 | −125.0 (3) | C27—C28—C29—C30 | 1.7 (9) |
| N2—Pr1—N1—C1 | −176.9 (3) | C28—C29—C30—C38 | −1.2 (7) |
| O2[i]—Pr1—N1—C12 | 139.7 (2) | C28—C29—C30—C31 | 179.2 (5) |
| O5[ii]—Pr1—N1—C12 | −72.0 (2) | C29—C30—C31—C32 | −178.0 (5) |
| O1—Pr1—N1—C12 | −166.9 (2) | C38—C30—C31—C32 | 2.3 (6) |
| O4—Pr1—N1—C12 | −17.6 (3) | C30—C31—C32—C33 | 0.1 (7) |
| O7—Pr1—N1—C12 | 92.3 (2) | C31—C32—C33—C34 | 176.6 (4) |
| O8[ii]—Pr1—N1—C12 | −115.8 (2) | C31—C32—C33—C37 | −2.5 (6) |
| O8—Pr1—N1—C12 | 64.2 (2) | C32—C33—C34—C35 | −178.6 (5) |
| N2—Pr1—N1—C12 | 12.3 (2) | C37—C33—C34—C35 | 0.5 (7) |
| O2[i]—Pr1—N2—C10 | 63.6 (3) | C33—C34—C35—C36 | −2.9 (9) |
| O5[ii]—Pr1—N2—C10 | −106.5 (3) | C37—N4—C36—C35 | 0.3 (9) |
| O1—Pr1—N2—C10 | −179.9 (2) | C34—C35—C36—N4 | 2.7 (11) |
| O4—Pr1—N2—C10 | −24.2 (3) | C36—N4—C37—C33 | −2.9 (6) |
| O7—Pr1—N2—C10 | 105.4 (3) | C36—N4—C37—C38 | 176.4 (4) |
| O8[ii]—Pr1—N2—C10 | −66.2 (3) | C34—C33—C37—N4 | 2.6 (6) |
| O8—Pr1—N2—C10 | 53.6 (3) | C32—C33—C37—N4 | −178.3 (4) |
| N1—Pr1—N2—C10 | 179.1 (3) | C34—C33—C37—C38 | −176.7 (3) |
| O2[i]—Pr1—N2—C11 | −129.3 (2) | C32—C33—C37—C38 | 2.4 (5) |
| O5[ii]—Pr1—N2—C11 | 60.6 (2) | C27—N3—C38—C30 | 1.5 (6) |
| O1—Pr1—N2—C11 | −12.8 (3) | C27—N3—C38—C37 | −177.0 (4) |
| O4—Pr1—N2—C11 | 142.9 (2) | C29—C30—C38—N3 | −0.5 (6) |
| O7—Pr1—N2—C11 | −87.5 (2) | C31—C30—C38—N3 | 179.2 (3) |
| O8[ii]—Pr1—N2—C11 | 100.9 (2) | C29—C30—C38—C37 | 178.0 (4) |
| O8—Pr1—N2—C11 | −139.3 (2) | C31—C30—C38—C37 | −2.3 (5) |
| N1—Pr1—N2—C11 | −13.8 (2) | N4—C37—C38—N3 | −0.7 (5) |

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| Pr1—O7—N7—O9 | 170.5 (3) | C33—C37—C38—N3 | 178.6 (3) |
| Pr1—O7—N7—O8 | −7.8 (3) | N4—C37—C38—C30 | −179.3 (3) |
| Pr1ⁱ—O8—N7—O9 | 40.3 (4) | C33—C37—C38—C30 | 0.0 (5) |
| Pr1—O8—N7—O9 | −170.9 (3) | C50—N5—C39—C40 | −0.5 (9) |
| Pr1ⁱ—O8—N7—O7 | −141.3 (2) | N5—C39—C40—C41 | 1.9 (11) |
| Pr1—O8—N7—O7 | 7.5 (3) | C39—C40—C41—C42 | −1.2 (10) |
| C12—N1—C1—C2 | −0.6 (5) | C40—C41—C42—C50 | −0.7 (8) |
| Pr1—N1—C1—C2 | −171.5 (3) | C40—C41—C42—C43 | 179.0 (6) |
| N1—C1—C2—C3 | 1.3 (6) | C41—C42—C43—C44 | −179.7 (5) |
| C1—C2—C3—C4 | −0.4 (6) | C50—C42—C43—C44 | −0.1 (7) |
| C2—C3—C4—C12 | −1.1 (6) | C42—C43—C44—C45 | −2.3 (8) |
| C2—C3—C4—C5 | 179.1 (4) | C43—C44—C45—C46 | −176.7 (5) |
| C3—C4—C5—C6 | 178.3 (4) | C43—C44—C45—C49 | 1.8 (7) |
| C12—C4—C5—C6 | −1.5 (6) | C49—C45—C46—C47 | −1.8 (6) |
| C4—C5—C6—C7 | −0.4 (6) | C44—C45—C46—C47 | 176.7 (4) |
| C5—C6—C7—C8 | −178.6 (4) | C45—C46—C47—C48 | 2.2 (7) |
| C5—C6—C7—C11 | 1.0 (6) | C49—N6—C48—C47 | −0.7 (7) |
| C11—C7—C8—C9 | −1.9 (6) | C46—C47—C48—N6 | −1.0 (7) |
| C6—C7—C8—C9 | 177.7 (4) | C48—N6—C49—C45 | 1.1 (6) |
| C7—C8—C9—C10 | 0.3 (6) | C48—N6—C49—C50 | −178.4 (4) |
| C11—N2—C10—C9 | −3.0 (5) | C46—C45—C49—N6 | 0.1 (6) |
| Pr1—N2—C10—C9 | 164.5 (3) | C44—C45—C49—N6 | −178.5 (4) |
| C8—C9—C10—N2 | 2.3 (6) | C46—C45—C49—C50 | 179.6 (4) |
| C10—N2—C11—C7 | 1.2 (5) | C44—C45—C49—C50 | 1.0 (6) |
| Pr1—N2—C11—C7 | −166.4 (2) | C39—N5—C50—C42 | −1.6 (7) |
| C10—N2—C11—C12 | −177.6 (3) | C39—N5—C50—C49 | 178.1 (4) |
| Pr1—N2—C11—C12 | 14.9 (4) | C41—C42—C50—N5 | 2.2 (6) |
| C8—C7—C11—N2 | 1.2 (5) | C43—C42—C50—N5 | −177.4 (4) |
| C6—C7—C11—N2 | −178.4 (3) | C41—C42—C50—C49 | −177.5 (4) |
| C8—C7—C11—C12 | 179.9 (3) | C43—C42—C50—C49 | 2.8 (6) |
| C6—C7—C11—C12 | 0.4 (5) | N6—C49—C50—N5 | −3.5 (5) |
| C1—N1—C12—C4 | −1.1 (5) | C45—C49—C50—N5 | 177.0 (3) |
| Pr1—N1—C12—C4 | 170.2 (2) | N6—C49—C50—C42 | 176.3 (3) |
| C1—N1—C12—C11 | 177.9 (3) | C45—C49—C50—C42 | −3.3 (5) |
| Pr1—N1—C12—C11 | −10.9 (4) | | |

Symmetry codes: (i) *x*, −*y*+3/2, *z*−1/2; (ii) *x*, −*y*+3/2, *z*+1/2.

*Hydrogen-bond geometry (Å, º)*

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| O6—H6···N4ⁱⁱⁱ | 0.82 | 2.07 | 2.851 (4) | 158 |
| O3—H3···N6ⁱᵛ | 0.82 | 2.04 | 2.782 (5) | 150 |

Symmetry codes: (iii) *x*+1, −*y*+3/2, *z*−1/2; (iv) −*x*+1, −*y*+1, −*z*+1.