Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Retraction of articles

This article reports the retraction of 39 articles published in *Acta Crystallographica Section E* between 2004 and 2009.

After thorough investigation (see Harrison *et al.*, 2010), 39 additional articles are retracted as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	Retracted by	DOI	Refcode
trans-Bis{1-[3-(cyclohexylamino)propyliminomethyl]-2-naphtholato}copper(II) dichloride dihydrate	Zhang (2004)	Journal	10.1107/S1600536804028296	BIPDUA
Bis(4-bromo-2-formylphenolato-κ^2O,O')copper(II)	Sun & Gao (2005)	Author	10.1107/S160053680500187X	FEYSUY
Bis(salicylaldehydo)zinc(II)	Xiong & Liu (2005)	Journal	10.1107/S1600536805010913	GAMDUU
Bis(4-bromo-2-formylphenolato-κ^2O,O')zinc(II)	Chen (2006)	Journal	10.1107/S1600536805040432	SAZCUS
Bis(2-formylphenolato-κ^2O,O')nickel(II)	Li & Chen (2006)	Journal	10.1107/S1600536806012931	IDAZAP
Bis(2-formylphenolato)cobalt(II)	Qiu (2006)	Journal	10.1107/S1600536806015704	GEJDUV
Bis(2-formylphenolato-κ^2O,O')manganese(II)	Wang & Fang (2006)	Journal	10.1107/S1600536806021039	IDOVED
Tetraaqua(1,10-phenanthroline-κ^2N,N')copper(II) naphthalene-1,5-disulfonate dihydrate	Liu *et al.* (2006)	Author	10.1107/S1600536806030637	GENYOO
Tetraaqua(1,10-phenanthroline-κ^2N,N')nickel(II) naphthalene-1,5-disulfonate dihydrate	Liu & Fan (2006)	Author	10.1107/S1600536806035410	KERBEP
{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratolutetium(III)copper(II)	Sui *et al.* (2006)	Journal	10.1107/S160053680604565X	HESPEP
Bis(2-formylphenolato-κ^2O,O')iron(II)	Yang *et al.* (2007)	Author	10.1107/S1600536807021721	PIFCAJ
2,6-Dimethoxybenzohydrazide	Qadeer *et al.* (2007*a*)	Journal	10.1107/S1600536807022593	PIFHES
2-(2,4-Dichlorophenylsulfanyl)acetohydrazide	Qadeer *et al.* (2007*b*)	Journal	10.1107/S1600536807022891	YIFSOW
{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoeuropium(III)zinc(II)	Hu *et al.* (2007)	Author	10.1107/S1600536807031121	WIHKEE
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratocerium(III)zinc(II)	Sui, Zhang, Hu & Yin (2007)	Author	10.1107/S1600536807032564	WIHREL
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)zinc(II)	Chen *et al.* (2007)	Author	10.1107/S1600536807032540	WIHRIP
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)nickel(II)	Sui, Li *et al.* (2007)	Author	10.1107/S1600536807032618	UFACUA
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-$1\kappa^4O^1,O^{1'},O^6,O^{6'}:2\kappa^4O^1,N,N',O^{1'}$}(methanol-$1\kappa O$)-$\mu$-nitrato-$1:2\kappa^2O:O'$-dinitrato-$1\kappa^4O,O'$-cerium(III)zinc(II)	Sui, Fang, Hu & Lin (2007)	Author	10.1107/S1600536807033314	UDUYIC
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratosamarium(III)nickel(II)	Sui, Zhang, Hu & Jiang (2007)	Author	10.1107/S1600536807037130	AFECEU
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratopraseodymium(III)zinc(II)	Sui, Fang & Yuan (2007)	Author	10.1107/S1600536807037488	AFICEY
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol-μ-nitrato-dinitratolutetium(III)zinc(II)	Sui, Sui *et al.* (2007)	Author	10.1107/S1600536807037737	AFEFOH
catena-Poly[[chloridonickel(II)]-di-μ-chlorido-[chloridonickel(II)]-μ-4,4′-methylenebis(3,5-dimethylpyrazole)-$\kappa^2N^2:N^{2'}$]	Huang & Chen (2007)	Author	10.1107/S1600536807039384	VIJYOD
{2,2′-[*o*-Phenylenebis(nitrilomethylidyne)]diphenolato}zinc(II)	Liu *et al.* (2007*a*)	Author	10.1107/S1600536807040640	DIKYUS
trans-Bis(ethylenediamine-κ^2N,N')bis(nitrato-κO)zinc(II)	Liu, Zeng & Chen (2007)	Author	10.1107/S1600536807042390	XIKYEW
[N,N'-(*o*-Phenylene)bis(picolinamido)-κ^4N,N',N'',N''']cobalt(II)	Liu & Zeng (2007*a*)	Author	10.1107/S1600536807044571	XILFII
[N,N'-(*o*-Phenylene)dipicolinamide-κ^4N]nickel(II)	Liu & Zeng (2007*b*)	Author	10.1107/S1600536807048386	WINWEW
{2,2′-[*o*-Phenylenebis(nitrilomethylidyne)]diphenolato}manganese(II)	Liu *et al.* (2007*b*)	Author	10.1107/S1600536807052993	VIQPIV
N-(2-Amino-3-pyridyl)urea monohydrate	Li *et al.* (2007)	Author	10.1107/S1600536807047526	SIMFEA
N-(2-Fluorophenyl)carbamic acid monohydrate	Yang (2007)	Author	10.1107/S1600536807052464	WINMOW
Aqua(dimethylglyoxime-κ^2N,N')(3,5-dinitro-2-oxidobenzoato-κ^2O^1,O^2)-copper(II)	Liu & Wen (2007)	Author	10.1107/S1600536807054244	HIQCAM
μ-Acetato-tri-μ-ferrocenecarboxylatobis[(*N*,*N*-dimethylformamide)-copper(II)]	Liu, Lin *et al.* (2007)	Journal	10.1107/S1600536807059041	HIQQEE

Table 1 (continued)

Title	Reference	Retracted by	DOI	Refcode
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoeuropium(III)zinc(II)	Hu *et al.* (2008)	Author	10.1107/S160053680706151X	MIRPAF
Bis(4-chloro-2-formylphenolato)nickel(II)	Li *et al.* (2008)	Author	10.1107/S1600536807056309	RISTET
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoterbium(III)zinc(II)	Chen *et al.* (2008)	Author	10.1107/S1600536808006958	QIXHIP
Bis(2-ethoxy-6-formylphenolato-κ^2O^1,O^6)nickel(II)	Han (2008)	Journal	10.1107/S160053680800809X	QIXLIT
{μ-6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-μ-nitrato-dinitratoholmium(III)zinc(II)	Xiao, Sui *et al.* (2008)	Author	10.1107/S1600536808013743	BIZTUA
{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoholmium(III)nickel(II)	Xiao, Fu *et al.* (2008)	Author	10.1107/S1600536808013755	BIZVAI
Hydrogen-bonding patterns in the cocrystal terephthalic acid–4,4′-bipyridine (2/1)	Wang *et al.* (2009)	Journal	10.1107/S160053680903236X	DUCZEH
{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-$1\kappa^4O^1,O^{1'},O^6,O^{6'}:2\kappa^4O^1,N,N',O^{1'}$}(ethanol-1κO)-μ-nitrato-$1:2\kappa^2O:O'$-dinitrato-$1\kappa^4O,O'$-samarium(III)zinc(II)	Huang *et al.* (2009)	Journal	10.1107/S1600536809033558	YUCWAV

References

Chen, Q. (2006). *Acta Cryst.* E**62**, m56–m57.
Chen, J.-R., Sui, Y., Luo, Q.-Y. & Jiang, R.-Q. (2007). *Acta Cryst.* E**63**, m2091–m2092.
Chen, J.-R., Sui, Y., Wen, J.-W. & Yin, L.-Y. (2008). *Acta Cryst.* E**64**, m562–m563.
Han, Z.-Q. (2008). *Acta Cryst.* E**64**, m592.
Harrison, W. T. A., Simpson, J. & Weil, M. (2010). *Acta Cryst.* E**66**, e1–e2.
Hu, R.-H., Sui, Y., Chen, L. & He, C.-M. (2008). *Acta Cryst.* E**64**, m8–m9.
Hu, R.-H., Sui, Y., Fang, X.-N. & Chen, H.-M. (2007). *Acta Cryst.* E**63**, m2039–m2040.
Huang, C.-F. & Chen, H.-L. (2007). *Acta Cryst.* E**63**, m2356–m2357.
Huang, Q., Sui, Y.-H. & Zhang, G.-X. (2009). *Acta Cryst.* E**65**, m1161–m1162.
Li, Y.-G. & Chen, H.-J. (2006). *Acta Cryst.* E**62**, m1038–m1039.
Li, N.-G., Tao, R.-M. & Fu, B.-F (2007). *Acta Cryst.* E**63**, o4228.
Li, Z., Zhang, X. & Pu, X. (2008). *Acta Cryst.* E**64**, m215.
Liu, J.-T. & Fan, S.-D. (2006). *Acta Cryst.* E**62**, m2507–m2508.
Liu, J.-T., Fan, S.-D. & Li, D.-Q. (2006). *Acta Cryst.* E**62**, m2165–m2166.
Liu, D., Lin, J., Xu, Y., Huang, C. & Li, X. (2007). *Acta Cryst.* E**63**, m3094.
Liu, Y.-Q. & Wen, H.-R. (2007). *Acta Cryst.* E**63**, m2928.
Liu, Y.-Q. & Zeng, X.-R. (2007*a*). *Acta Cryst.* E**63**, m2547.
Liu, Y.-Q. & Zeng, X.-R. (2007*b*). *Acta Cryst.* E**63**, m2684.
Liu, Y.-Q., Zeng, X.-R. & Chen, W.-T. (2007). *Acta Cryst.* E**63**, m2462.
Liu, Y.-Q., Zeng, X.-R., Luo, Q.-Y. & Xu, Y.-P. (2007*a*). *Acta Cryst.* E**63**, m2396.
Liu, Y.-Q., Zeng, X.-R., Luo, Q.-Y. & Xu, Y.-P. (2007*b*). *Acta Cryst.* E**63**, m2854.
Qadeer, G., Rama, N. H. & Chen, W.-T. (2007*a*). *Acta Cryst.* E**63**, o2892.
Qadeer, G., Rama, N. H. & Chen, W.-T. (2007*b*). *Acta Cryst.* E**63**, o2932.
Qiu, X.-Y. (2006). *Acta Cryst.* E**62**, m1190–m1191.
Sui, Y., Fang, X.-N., Hu, P. & Lin, J. (2007). *Acta Cryst.* E**63**, m2135–m2136.
Sui, Y., Fang, X.-N. & Yuan, M.-W. (2007). *Acta Cryst.* E**63**, m2275–m2276.
Sui, Y., Li, X.-F., Huang, G.-S. & Wang, G.-J. (2007). *Acta Cryst.* E**63**, m2093–m2094.
Sui, Y., Sui, Y.-H., Luo, Q.-Y. & Wang, Y.-D. (2007). *Acta Cryst.* E**63**, m2277–m2278.
Sui, Y., Xiao, Y.-A., Fang, X.-N., Zeng, X.-R. & Li, M.-H. (2006). *Acta Cryst.* E**62**, m3205–m3207.
Sui, Y., Zhang, J.-H., Hu, R.-H. & Jiang, R.-Q. (2007). *Acta Cryst.* E**63**, m2256–m2257.
Sui, Y., Zhang, J.-H., Hu, R.-H. & Yin, L.-Y. (2007). *Acta Cryst.* E**63**, m2089–m2090.
Sun, Y.-X. & Gao, G.-Z. (2005). *Acta Cryst.* E**61**, m354–m355.
Wang, Q. & Fang, Z.-N. (2006). *Acta Cryst.* E**62**, m1492–m1493.
Wang, S., Yang, T., Li, Z. & Yu, X. (2009). *Acta Cryst.* E**65**, o2198.
Xiao, Y.-A., Fu, X.-K., Sui, Y., Wu, Q. & Xiong, S.-H. (2008). *Acta Cryst.* E**64**, m806–m807.
Xiao, Y.-A., Sui, Y., Yi, X.-G., Wu, J.-H. & Zhang, L.-P. (2008). *Acta Cryst.* E**64**, m804–m805.
Xiong, Z.-Y. & Liu, L.-J. (2005). *Acta Cryst.* E**61**, m863–m864.
Yang, X.-M. (2007). *Acta Cryst.* E**63**, o4453.
Yang, Y.-M., Lu, P.-C., Zhu, T.-T. & Liu, C.-H. (2007). *Acta Cryst.* E**63**, m1613.
Zhang, P. (2004). *Acta Cryst.* E**60**, m1808–m1810.

Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}trinitratopraseodymium(III)nickel(II)

Yan Sui,* Xin-Fa Li, Gan-Sheng Huang and Gui-Juan Wang

JiangXi Province Key Laboratory of Coordination Chemistry, College of Chemistry & Chemical Engineering, JingGangShan University, 343009 Ji'an, JiangXi, People's Republic of China
Correspondence e-mail: ysui@163.com

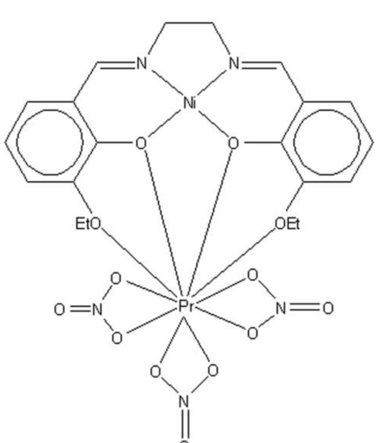
Received 1 July 2007; accepted 4 July 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.028; wR factor = 0.064; data-to-parameter ratio = 16.7.

In the title heteronuclear Ni^{II}–Pr^{III} complex (systematic name: {6,6′-diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}trinitrato-1$\kappa^6O,O'$-praseodymium(III)nickel(II)), $[NiPr(C_{20}H_{22}N_2O_4)(NO_3)_3]$, with the hexadentate Schiff base compartmental ligand N,N'-bis(3-ethoxysalicylidene)ethylenediamine (H_2L), the Ni and Pr atoms are doubly bridged by two phenolate O atoms provided by the Schiff base ligand. The coordination of Ni is square planar with the donor centers of two imine N atoms and two phenolate O atoms. The praseodymium(III) center has a decacoordination environment of O atoms, involving the phenolate O atoms, two ethoxy O atoms and two O atoms each from the three nitrates. Some weak C—H···O and O···Ni [3.146 (4) Å] interactions generate a two-dimensional zigzag sheet.

Related literature

For related literature, see: Baggio *et al.* (2000); Caravan *et al.* (1999); Edder *et al.* (2000); Knoer *et al.* (2005); Sui *et al.* (2006).



Experimental

Crystal data

$[NiPr(C_{20}H_{22}N_2O_4)(NO_3)_3]$
M_r = 740.05
Orthorhombic, $P2_12_12_1$
a = 8.6317 (7) Å
b = 13.8782 (11) Å
c = 21.1267 (16) Å
V = 2530.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.72 mm^{-1}
T = 293 (2) K
0.22 × 0.14 × 0.13 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.586, T_{max} = 0.718
19198 measured reflections
6058 independent reflections
4803 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.064
S = 1.00
6058 reflections
363 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.95 e Å^{-3}
Absolute structure: Flack (1983), with 2527 Friedel pairs
Flack parameter: −0.029 (13)

Table 1
Selected bond lengths (Å).

O1—Ni1	1.900 (3)	Pr1—O8	2.595 (3)
O1—Pr1	2.452 (2)	Pr1—O9	2.541 (3)
Pr1—O2	2.415 (2)	Pr1—O11	2.512 (3)
Pr1—O3	2.675 (3)	Pr1—O12	2.562 (3)
Pr1—O4	2.644 (2)	Ni1—O2	1.902 (3)
Pr1—O5	2.551 (3)	Ni1—N1	1.910 (3)
Pr1—O6	2.582 (3)	Ni1—N2	1.911 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C20—H20A···O9	0.96	2.44	3.154 (5)	131
C17—H17A···O8^{i}	0.97	2.60	3.535 (5)	163
C9—H9A···O7^{ii}	0.97	2.41	3.278 (5)	148
C7—H7···O7^{iii}	0.93	2.36	3.275 (5)	167

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{5}{2}, -z$; (ii) $x-1, y, z$; (iii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *APEX2*; software used to prepare material for publication: *APEX2* and *publCIF* (Westrip, 2007).

The authors gratefully acknowledge financial support from the Department of Education, JiangXi Province (grant Nos. 2007317 and 05YB195) and the Natural Science Foundation of JiangXi Province (grant No. 0620029).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2333).

References

Baggio, R., Garland, M. T., Moreno, Y., Pena, O., Perec, M. & Spodine, E. (2000). *J. Chem. Soc. Dalton Trans.* pp. 2061–2066.
Bruker (2004). *APEX2* (Version 1.22) and *SADABS* (Version 1.22). Bruker AXS Inc., Madison, Wisconsin, USA.
Caravan, P., Ellison, J. J., McMurry, T. J. & Lauffer, R. B. (1999). *Chem. Rev.* **99**, 2293–2352.
Edder, C., Piguet, C., Bernardinelli, G., Mareda, J., Bochet, C. G., Bunzli, J.-C.G. & Hopfgartner, G. (2000). *Inorg. Chem.* **39**, 5059–5073.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Knoer, R., Lin, H.-H., Wei, H.-H. & Mohanta, S. (2005). *Inorg. Chem.* **44**, 3524–3536.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sui, Y., Fang, X.-N., Xiao, Y.-A., Luo, Q.-Y. & Li, M.-H. (2006). *Acta Cryst.* E**62**, m2230–m2232.
Westrip, S. P. (2007). *publCIF*. In preparation.

supplementary materials

Acta Cryst. (2007). E**63**, m2093-m2094 [**doi:10.1107/S1600536807032618**]

{μ-6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}trinitratopraseodymium(III)nickel(II)

Y. Sui, X.-F. Li, G.-S. Huang and G.-J. Wang

Comment

The potential applications of trivalent lanthanide complexes as contrast agent for magnetic resonance imaging and stains for fluorescence imaging have prompted considerable interest in the preparation, magnetic and optical properties of 3 d-4f hetorometallic dinuclear complexes (Baggio *et al.*, 2000; Caravan *et al.*, 1999; Edder *et al.*, 2000; Knoer *et al.*, 2005). As part of our investigations into the structure and applications of 3 d-4f hetorometallic Schiff base complexes(Sui *et al.* 2006), we report here the synthesis and X-ray crystal structure analysis of the title complex, (I), a new Ni^{II}—Pr^{III} complex with salen-type Schiff base *N*,*N*'-bis(3-ethoxysalicylidene) ethylenediamine (H_2L).

Complex (I) crystallizes in the space group $P2_12_12_1$, with nickel and praseodymium doubly bridged by two phenolate O atoms provided by a salen-type Schiff base ligand. The inner salen-type cavity is occupied by nickel(II), while praseodymium(III) is present in the open and larger portion of the dinucleating compartmental Schiff base ligand. The dihedral angles between the mean planes of Ni1/O1/O2 and Pr1/O1/O2 is 3.43 (16)° suggesting that the bridging moiety is almost planar; the deviation of atoms from the least squares Ni1/O1/O2/Pr1 plane being 0.0292 (2)Å for Ni, 0.0197 (3)Å for Pr, −0.0242 (2)Å for O1 and −0.0247 (2)Å for O2.

The praseodymium(III) center in (I) has a decacoordination environment of O atoms. In addition to the phenolate ligands, two ethoxy O atoms coordinate to this metal center, two O atoms from each of the three nitrates chelate to praseodymium to complete the decacoordination. The three kinds of Pr—O bond distances are significantly different, the shortest being the Pr—O(phenolate) and longest being the Pr—*O*(ethoxy) separations.

The coordination of nickel(II) is approximately square planar. The donor centers are alternatively above and below the mean N_2O_2 plane with an average deviation from the plane of 0.0897 (2) Å, while Ni1 is −0.0434 (2)Å below this square plane.

Adjacent molecules are held together by weak interactions (O10···Ni1 = 3.146 (4) Å, C7—H7···O7^{i} = 3.275 (5), C9—H9A···O7^{ii} = 3.278 (5) and C17—H17A···O8^{iii} = 3.535 (5)°; symmetry codes: (i) 1 − *x*, *y* − 1/2, 1/2 − *z*; (ii) *x* − 1, *y*, *z*; (iii) *x* − 1/2, 5/2 − *y*, *z*.) these link the molecules into a two-dimensional zigzag sheet (Fig 2).

Experimental

H_2L was prepared by the 2:1 condensation of 3-ethoxysalicylaldehyde and ethylenediamine in methanol. Complex (I) was obtained by the treatment of nickel(II) acetate tetrahydrate (0.217 g, 1 mmol) with H_2L (0.356 g, 1 mmol) in methanol solution (80 ml) under reflux for 3 h and then for another 3 h after the addition of praseodymium(III) nitrate hexahydrate (0.435 g, 1 mmol). The reaction mixture was cooled and the resulting precipitate was filtered off, washed with diethyl ether and dried *in vacuo*. Single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation at room temperature of a methanol solution. Analysis calculated for $C_{20}H_{22}N_5NiO_{13}Pr$: C 32.46, H 3.00, N 9.46, Ni 7.93, Pr 19.04%; found: C 32.30, H 2.95, N 9.10, Ni 7.80, Pr 19.20%. IR (KBr, cm^{-1}): 1642 (C=N), 1386,1490 (nitrate).

Refinement

The H atoms were positioned geometrically and treated as riding on their parent atoms, with C—H distances of 0.97 (methylene) and 0.96 Å (methyl), and with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms and $1.2U_{eq}(C)$ for other H atoms.

Figures

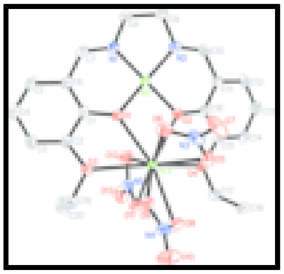


Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids. All the H atoms on carbon have been omitted for clarity.

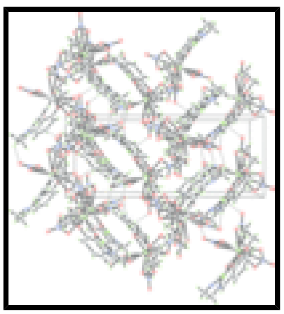


Fig. 2. The packing diagram of (I), viewed along the *b* axis; hydrogen bonds are shown as dashed lines.

{6,6'-diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-\ 1κ^4*O*^{1},*O*$^{1'}$,*O*^{6},*O*$^{6'}$:2κ^4*O*^{1},\ *N*,*N*',*O*$^{1'}$}trinitrato-1κ^6*O*,*O*'-\ praseodymium(III)nickel(II))

Crystal data

$[NiPr(C_{20}H_{22}N_2O_4)(NO_3)_3]$	$F_{000} = 1472$
$M_r = 740.05$	$D_x = 1.942$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 19198 reflections
a = 8.6317 (7) Å	θ = 1.9–28.2°
b = 13.8782 (11) Å	μ = 2.72 mm^{-1}
c = 21.1267 (16) Å	*T* = 293 (2) K
V = 2530.8 (3) Å^3	Block, red
Z = 4	0.22 × 0.14 × 0.13 mm

Data collection

Bruker APEXII area-detector diffractometer	6058 independent reflections
Radiation source: fine-focus sealed tube	4803 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.031$
Detector resolution: 0 pixels mm^{-1}	$\theta_{max} = 28.2°$
$T = 293(2)$ K	$\theta_{min} = 1.9°$
φ and ω scans	$h = -11 \rightarrow 11$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$k = -18 \rightarrow 17$
$T_{min} = 0.586$, $T_{max} = 0.718$	$l = -27 \rightarrow 28$
19198 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.028$	$w = 1/[\sigma^2(F_o^2) + (0.0308P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.064$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.00$	$\Delta\rho_{max} = 0.49$ e Å^{-3}
6058 reflections	$\Delta\rho_{min} = -0.94$ e Å^{-3}
363 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 2527 Freidel pairs
Secondary atom site location: difference Fourier map	Flack parameter: −0.029 (13)

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}
O7	0.9049 (4)	1.0768 (3)	0.27827 (16)	0.0824 (12)
O10	1.2400 (4)	1.0390 (4)	0.0732 (2)	0.0940 (13)
O13	0.5733 (5)	1.0011 (3)	−0.08811 (14)	0.0778 (9)

O1	0.5857 (3)	0.87476 (17)	0.13660 (13)	0.0400 (6)
Pr1	0.75873 (2)	0.999679 (15)	0.094894 (9)	0.03254 (6)
Ni1	0.43318 (5)	0.94379 (3)	0.18298 (2)	0.03345 (11)
O2	0.5375 (3)	1.05625 (18)	0.15415 (12)	0.0370 (6)
C16	0.4776 (4)	1.1446 (2)	0.15618 (18)	0.0335 (8)
N2	0.3003 (4)	1.0132 (3)	0.23914 (15)	0.0413 (8)
C2	0.7085 (4)	0.7431 (3)	0.08984 (18)	0.0346 (8)
N1	0.3205 (4)	0.8321 (2)	0.20893 (16)	0.0386 (8)
O3	0.8107 (3)	0.81360 (18)	0.06952 (13)	0.0390 (6)
C1	0.5858 (5)	0.7798 (3)	0.12641 (19)	0.0350 (9)
C15	0.5384 (4)	1.2127 (3)	0.11356 (19)	0.0357 (9)
O4	0.6541 (3)	1.17618 (17)	0.07522 (13)	0.0379 (6)
C10	0.2788 (4)	1.1051 (3)	0.23934 (19)	0.0409 (9)
H10	0.2096	1.1305	0.2687	0.049*
C11	0.3559 (5)	1.1717 (3)	0.1965 (2)	0.0397 (10)
C6	0.4755 (5)	0.7163 (3)	0.15066 (19)	0.0385 (9)
C8	0.1866 (5)	0.8550 (3)	0.2490 (2)	0.0469 (11)
H8A	0.1683	0.8033	0.2790	0.056*
H8B	0.0946	0.8629	0.2232	0.056*
C7	0.3494 (5)	0.7458 (3)	0.1916 (2)	0.0418 (10)
H7	0.2839	0.6978	0.2066	0.050*
C9	0.2229 (5)	0.9480 (3)	0.28394 (19)	0.0455 (9)
H9A	0.1281	0.9771	0.2995	0.055*
H9B	0.2900	0.9350	0.3198	0.055*
O11	0.7686 (3)	1.0124 (2)	−0.02366 (14)	0.0567 (8)
N5	0.6275 (4)	0.9943 (3)	−0.03484 (17)	0.0509 (8)
O6	0.8208 (4)	0.9677 (2)	0.21260 (15)	0.0558 (9)
O5	0.8644 (3)	1.1119 (2)	0.18023 (16)	0.0535 (7)
O8	1.0055 (4)	1.0815 (3)	0.04986 (17)	0.0672 (10)
O9	1.0438 (3)	0.9620 (2)	0.11169 (16)	0.0580 (8)
O12	0.5474 (4)	0.9686 (2)	0.01221 (14)	0.0615 (9)
N3	0.8635 (4)	1.0513 (3)	0.22533 (19)	0.0508 (9)
N4	1.1002 (4)	1.0287 (3)	0.07769 (19)	0.0554 (11)
C3	0.7179 (5)	0.6468 (3)	0.0751 (2)	0.0452 (10)
H3	0.7996	0.6234	0.0509	0.054*
C17	0.7260 (5)	1.2411 (3)	0.02947 (19)	0.0445 (10)
H17A	0.6465	1.2804	0.0099	0.053*
H17B	0.7751	1.2033	−0.0035	0.053*
C19	0.9471 (5)	0.7816 (3)	0.0349 (2)	0.0462 (10)
H19A	0.9904	0.8356	0.0117	0.055*
H19B	0.9170	0.7327	0.0045	0.055*
C4	0.6025 (5)	0.5846 (3)	0.0972 (2)	0.0524 (11)
H4	0.6063	0.5197	0.0865	0.063*
C5	0.4853 (5)	0.6174 (3)	0.1340 (2)	0.0462 (10)
H5	0.4103	0.5747	0.1485	0.055*
C20	1.0682 (5)	0.7411 (3)	0.0783 (2)	0.0605 (13)
H20A	1.0980	0.7892	0.1086	0.091*
H20B	1.1571	0.7220	0.0540	0.091*
H20C	1.0271	0.6860	0.1001	0.091*

C14	0.4812 (5)	1.3050 (3)	0.1115 (2)	0.0434 (10)
H14	0.5215	1.3495	0.0829	0.052*
C12	0.3023 (5)	1.2675 (3)	0.1951 (2)	0.0494 (12)
H12	0.2260	1.2872	0.2234	0.059*
C13	0.3612 (5)	1.3314 (3)	0.1529 (2)	0.0521 (12)
H13	0.3215	1.3937	0.1514	0.063*
C18	0.8450 (5)	1.3056 (3)	0.0597 (2)	0.0584 (13)
H18A	0.7959	1.3454	0.0910	0.088*
H18B	0.8914	1.3457	0.0279	0.088*
H18C	0.9235	1.2670	0.0794	0.088*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O7	0.090 (3)	0.111 (3)	0.0456 (18)	0.047 (2)	−0.020 (2)	−0.024 (2)
O10	0.0355 (18)	0.136 (4)	0.111 (3)	−0.019 (2)	0.003 (2)	0.005 (3)
O13	0.107 (3)	0.076 (2)	0.0507 (19)	−0.006 (2)	−0.0241 (19)	0.000 (2)
O1	0.0453 (16)	0.0226 (13)	0.0522 (17)	−0.0030 (11)	0.0151 (14)	0.0004 (12)
Pr1	0.03262 (9)	0.02703 (9)	0.03797 (10)	−0.00125 (11)	0.00380 (9)	0.00237 (10)
Ni1	0.0331 (2)	0.0257 (2)	0.0415 (2)	−0.00120 (19)	0.0100 (2)	0.0037 (2)
O2	0.0360 (14)	0.0270 (13)	0.0481 (15)	0.0025 (11)	0.0063 (12)	0.0024 (13)
C16	0.035 (2)	0.0254 (18)	0.040 (2)	−0.0005 (14)	−0.0053 (17)	0.0018 (16)
N2	0.0403 (15)	0.047 (2)	0.0362 (17)	−0.0028 (15)	0.0060 (13)	0.0048 (16)
C2	0.039 (2)	0.0304 (19)	0.034 (2)	−0.0007 (14)	−0.0049 (18)	0.0029 (16)
N1	0.0376 (18)	0.0369 (19)	0.041 (2)	−0.0055 (14)	0.0047 (16)	0.0091 (16)
O3	0.0381 (14)	0.0321 (15)	0.0470 (17)	0.0025 (11)	0.0101 (13)	−0.0006 (12)
C1	0.039 (2)	0.0278 (19)	0.038 (2)	−0.0009 (16)	−0.0064 (19)	0.0002 (17)
C15	0.034 (2)	0.032 (2)	0.041 (2)	−0.0006 (15)	−0.0024 (18)	−0.0022 (17)
O4	0.0446 (15)	0.0262 (14)	0.0430 (16)	−0.0018 (11)	0.0062 (13)	0.0079 (12)
C10	0.039 (2)	0.044 (2)	0.040 (2)	0.0068 (18)	0.0054 (18)	0.0026 (18)
C11	0.038 (2)	0.038 (2)	0.044 (3)	0.0036 (16)	0.0011 (19)	0.0022 (19)
C6	0.046 (2)	0.030 (2)	0.040 (2)	−0.0042 (16)	−0.0066 (19)	0.0039 (18)
C8	0.038 (2)	0.053 (3)	0.049 (3)	−0.0039 (18)	0.014 (2)	0.012 (2)
C7	0.040 (2)	0.039 (2)	0.046 (3)	−0.0090 (17)	0.000 (2)	0.013 (2)
C9	0.043 (2)	0.048 (2)	0.046 (2)	−0.0003 (19)	0.0116 (19)	0.012 (2)
O11	0.0582 (19)	0.064 (2)	0.0482 (16)	−0.0133 (18)	0.0061 (14)	0.0024 (14)
N5	0.066 (2)	0.0401 (19)	0.046 (2)	0.002 (2)	−0.0013 (18)	−0.009 (2)
O6	0.062 (2)	0.059 (2)	0.0460 (18)	0.0054 (16)	0.0048 (16)	0.0144 (15)
O5	0.0565 (18)	0.0494 (17)	0.0546 (19)	0.0014 (14)	−0.0069 (17)	−0.0058 (17)
O8	0.0465 (19)	0.081 (3)	0.074 (2)	−0.0140 (16)	−0.0007 (17)	0.031 (2)
O9	0.0447 (17)	0.0463 (17)	0.083 (2)	0.0006 (14)	0.0058 (17)	0.0058 (16)
O12	0.0528 (18)	0.080 (3)	0.0517 (18)	−0.0097 (16)	0.0012 (16)	−0.0041 (16)
N3	0.041 (2)	0.067 (3)	0.045 (2)	0.023 (2)	−0.0022 (18)	−0.006 (2)
N4	0.041 (2)	0.068 (3)	0.057 (2)	−0.0100 (18)	0.0071 (19)	−0.013 (2)
C3	0.059 (3)	0.032 (2)	0.045 (2)	0.0056 (18)	0.000 (2)	−0.0027 (17)
C17	0.057 (3)	0.036 (2)	0.041 (2)	−0.0040 (18)	0.009 (2)	0.0077 (17)
C19	0.042 (2)	0.043 (2)	0.053 (3)	0.0039 (18)	0.007 (2)	−0.006 (2)
C4	0.069 (3)	0.027 (2)	0.061 (3)	−0.0009 (18)	−0.007 (3)	0.000 (2)

C5	0.058 (3)	0.026 (2)	0.055 (3)	−0.0094 (17)	−0.001 (2)	0.0054 (19)
C20	0.049 (3)	0.051 (3)	0.081 (4)	0.010 (2)	−0.004 (3)	−0.009 (2)
C14	0.047 (2)	0.033 (2)	0.050 (3)	0.0005 (16)	−0.005 (2)	0.0065 (19)
C12	0.051 (3)	0.037 (2)	0.060 (3)	0.0114 (18)	0.007 (2)	−0.007 (2)
C13	0.061 (3)	0.027 (2)	0.068 (3)	0.0093 (19)	0.001 (2)	0.002 (2)
C18	0.059 (3)	0.041 (3)	0.075 (3)	−0.010 (2)	0.021 (3)	−0.003 (2)

Geometric parameters (Å, °)

O7—N3	1.226 (5)	C6—C5	1.419 (5)
O10—N4	1.218 (4)	C6—C7	1.450 (6)
O13—N5	1.222 (4)	C8—C9	1.519 (6)
O1—C1	1.335 (4)	C8—H8A	0.9700
O1—Ni1	1.900 (3)	C8—H8B	0.9700
O1—Pr1	2.452 (2)	C7—H7	0.9300
Pr1—O2	2.415 (2)	C9—H9A	0.9700
Pr1—O3	2.675 (3)	C9—H9B	0.9700
Pr1—O4	2.644 (2)	O11—N5	1.266 (4)
Pr1—O5	2.551 (3)	N5—O12	1.262 (4)
Pr1—O6	2.582 (3)	O6—N3	1.248 (5)
Pr1—O8	2.595 (3)	O5—N3	1.271 (5)
Pr1—O9	2.541 (3)	O8—N4	1.245 (5)
Pr1—O11	2.512 (3)	O9—N4	1.268 (5)
Pr1—O12	2.562 (3)	C3—C4	1.398 (6)
Ni1—O2	1.902 (3)	C3—H3	0.9300
Ni1—N1	1.910 (3)	C17—C18	1.505 (6)
Ni1—N2	1.911 (3)	C17—H17A	0.9700
O2—C16	1.332 (4)	C17—H17B	0.9700
C16—C11	1.404 (5)	C19—C20	1.500 (6)
C16—C15	1.407 (5)	C19—H19A	0.9700
N2—C10	1.289 (5)	C19—H19B	0.9700
N2—C9	1.471 (5)	C4—C5	1.354 (6)
C2—C3	1.374 (5)	C4—H4	0.9300
C2—O3	1.386 (4)	C5—H5	0.9300
C2—C1	1.406 (5)	C20—H20A	0.9600
N1—C7	1.276 (5)	C20—H20B	0.9600
N1—C8	1.468 (5)	C20—H20C	0.9600
O3—C19	1.456 (5)	C14—C13	1.405 (6)
C1—C6	1.396 (5)	C14—H14	0.9300
C15—C14	1.374 (5)	C12—C13	1.357 (6)
C15—O4	1.382 (4)	C12—H12	0.9300
O4—C17	1.460 (4)	C13—H13	0.9300
C10—C11	1.454 (5)	C18—H18A	0.9600
C10—H10	0.9300	C18—H18B	0.9600
C11—C12	1.409 (6)	C18—H18C	0.9600
C1—O1—Ni1	125.5 (2)	N2—C10—C11	124.1 (4)
C1—O1—Pr1	129.8 (2)	N2—C10—H10	118.0
Ni1—O1—Pr1	104.52 (10)	C11—C10—H10	118.0
O2—Pr1—O1	64.02 (8)	C16—C11—C12	119.0 (4)

O2—Pr1—O11	121.39 (9)	C16—C11—C10	123.4 (3)
O1—Pr1—O11	115.38 (10)	C12—C11—C10	117.6 (4)
O2—Pr1—O9	139.51 (9)	C1—C6—C5	118.6 (4)
O1—Pr1—O9	113.22 (10)	C1—C6—C7	123.5 (3)
O11—Pr1—O9	96.94 (10)	C5—C6—C7	117.8 (4)
O2—Pr1—O5	73.61 (9)	N1—C8—C9	107.6 (3)
O1—Pr1—O5	113.30 (9)	N1—C8—H8A	110.2
O11—Pr1—O5	130.50 (10)	C9—C8—H8A	110.2
O9—Pr1—O5	71.38 (10)	N1—C8—H8B	110.2
O2—Pr1—O12	81.09 (10)	C9—C8—H8B	110.2
O1—Pr1—O12	72.09 (10)	H8A—C8—H8B	108.5
O11—Pr1—O12	49.93 (9)	N1—C7—C6	125.6 (4)
O9—Pr1—O12	138.61 (10)	N1—C7—H7	117.2
O5—Pr1—O12	147.03 (10)	C6—C7—H7	117.2
O2—Pr1—O6	73.78 (9)	N2—C9—C8	107.7 (3)
O1—Pr1—O6	70.04 (10)	N2—C9—H9A	110.2
O11—Pr1—O6	164.82 (10)	C8—C9—H9A	110.2
O9—Pr1—O6	68.24 (10)	N2—C9—H9B	110.2
O5—Pr1—O6	49.49 (10)	C8—C9—H9B	110.2
O12—Pr1—O6	140.83 (10)	H9A—C9—H9B	108.5
O2—Pr1—O8	134.21 (11)	N5—O11—Pr1	98.0 (2)
O1—Pr1—O8	160.24 (10)	O13—N5—O12	122.5 (4)
O11—Pr1—O8	64.90 (10)	O13—N5—O11	121.6 (4)
O9—Pr1—O8	49.15 (10)	O12—N5—O11	115.8 (3)
O5—Pr1—O8	72.45 (11)	N3—O6—Pr1	96.2 (3)
O12—Pr1—O8	114.09 (10)	N3—O5—Pr1	97.1 (3)
O6—Pr1—O8	104.95 (11)	N4—O8—Pr1	96.2 (2)
O2—Pr1—O4	60.66 (8)	N4—O9—Pr1	98.2 (2)
O1—Pr1—O4	120.23 (8)	N5—O12—Pr1	95.7 (2)
O11—Pr1—O4	77.87 (9)	O7—N3—O6	123.4 (5)
O9—Pr1—O4	122.93 (9)	O7—N3—O5	119.4 (5)
O5—Pr1—O4	70.57 (9)	O6—N3—O5	117.1 (4)
O12—Pr1—O4	78.77 (10)	O10—N4—O8	123.0 (4)
O6—Pr1—O4	112.44 (9)	O10—N4—O9	120.6 (5)
O8—Pr1—O4	79.49 (10)	O8—N4—O9	116.4 (3)
O2—Pr1—O3	123.39 (8)	C2—C3—C4	118.9 (4)
O1—Pr1—O3	59.45 (8)	C2—C3—H3	120.6
O11—Pr1—O3	82.09 (9)	C4—C3—H3	120.6
O9—Pr1—O3	70.55 (9)	O4—C17—C18	112.1 (3)
O5—Pr1—O3	132.15 (9)	O4—C17—H17A	109.2
O12—Pr1—O3	79.66 (10)	C18—C17—H17A	109.2
O6—Pr1—O3	89.55 (10)	O4—C17—H17B	109.2
O8—Pr1—O3	102.19 (10)	C18—C17—H17B	109.2
O4—Pr1—O3	156.95 (10)	H17A—C17—H17B	107.9
O1—Ni1—O2	85.44 (11)	O3—C19—C20	111.8 (4)
O1—Ni1—N1	95.25 (13)	O3—C19—H19A	109.3
O2—Ni1—N1	177.17 (13)	C20—C19—H19A	109.3
O1—Ni1—N2	171.95 (13)	O3—C19—H19B	109.3
O2—Ni1—N2	93.96 (12)	C20—C19—H19B	109.3

N1—Ni1—N2	85.74 (15)	H19A—C19—H19B	107.9
C16—O2—Ni1	124.2 (2)	C5—C4—C3	121.1 (4)
C16—O2—Pr1	128.6 (2)	C5—C4—H4	119.5
Ni1—O2—Pr1	105.88 (11)	C3—C4—H4	119.5
O2—C16—C11	123.8 (3)	C4—C5—C6	120.8 (4)
O2—C16—C15	116.9 (3)	C4—C5—H5	119.6
C11—C16—C15	119.2 (3)	C6—C5—H5	119.6
C10—N2—C9	122.8 (3)	C19—C20—H20A	109.5
C10—N2—Ni1	126.0 (3)	C19—C20—H20B	109.5
C9—N2—Ni1	111.2 (3)	H20A—C20—H20B	109.5
C3—C2—O3	125.4 (4)	C19—C20—H20C	109.5
C3—C2—C1	121.4 (4)	H20A—C20—H20C	109.5
O3—C2—C1	113.2 (3)	H20B—C20—H20C	109.5
C7—N1—C8	121.5 (4)	C15—C14—C13	119.2 (4)
C7—N1—Ni1	125.4 (3)	C15—C14—H14	120.4
C8—N1—Ni1	113.0 (3)	C13—C14—H14	120.4
C2—O3—C19	117.1 (3)	C13—C12—C11	120.5 (4)
C2—O3—Pr1	120.8 (2)	C13—C12—H12	119.7
C19—O3—Pr1	122.1 (2)	C11—C12—H12	119.7
O1—C1—C6	124.3 (4)	C12—C13—C14	121.0 (4)
O1—C1—C2	116.5 (3)	C12—C13—H13	119.5
C6—C1—C2	119.1 (3)	C14—C13—H13	119.5
C14—C15—O4	125.7 (4)	C17—C18—H18A	109.5
C14—C15—C16	120.9 (4)	C17—C18—H18B	109.5
O4—C15—C16	113.5 (3)	H18A—C18—H18B	109.5
C15—O4—C17	118.0 (3)	C17—C18—H18C	109.5
C15—O4—Pr1	119.6 (2)	H18A—C18—H18C	109.5
C17—O4—Pr1	122.0 (2)	H18B—C18—H18C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C20—H20A···O9	0.96	2.44	3.154 (5)	131
C17—H17A···O8^{i}	0.97	2.60	3.535 (5)	163
C9—H9A···O7^{ii}	0.97	2.41	3.278 (5)	148
C7—H7···O7^{iii}	0.93	2.36	3.275 (5)	167

Symmetry codes: (i) *x*−1/2, −*y*+5/2, −*z*; (ii) *x*−1, *y*, *z*; (iii) −*x*+1, *y*−1/2, −*z*+1/2.

Fig. 1

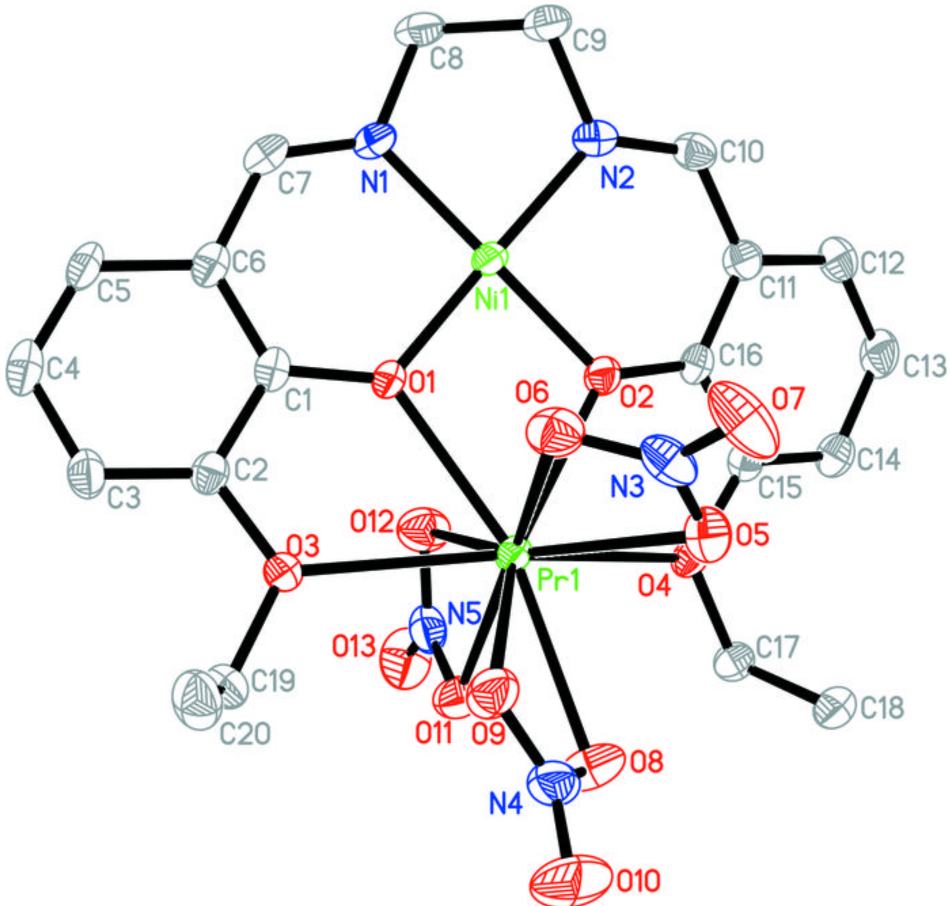

C8
C9
C7
N1
N2
C10
C5
C6
Ni1
C11
C12
C4
C1
O1
O2
C16
C13
O6
O7
C3
C2
N3
C15
C14
O12
O3
Pr1
O5
O4
N5
O13
C19
C17
C20
O11
O9
C18
O8
N4
O10

Fig. 2