atoms were placed in calculated positions and were assigned common isotropic displacement parameters, $U = 0.08$ Å^2. The H atoms of two of the tetrahydrofuran ligands and also of the tetrahydrofuran solvate molecule were not located.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AL1056). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Isomorphous Compounds $[Nd(TDTD)_{1.5}(pic)_3]$ and $[Er(TDTD)_{1.5}(pic)_3]$ (pic = Picrate, TDTD = *trans*-1,4-Dithiane *S,S'*-Dioxide)

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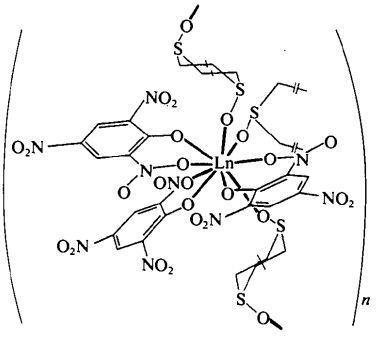
Abstract

The structures of two isomorphous and isostructural lanthanide derivatives, poly[tri(picrato-O^1,O^2)neodymium-μ-(*trans*-1,4-dithione *S,S'*-dioxide-*S*:*S'*)$_{1.5}$], $[Nd(C_6H_2N_3O_7)_3(C_4H_8O_2S_2)_{1.5}]$, and poly[tri(picrato-$O^1,O^2$)erbium-$\mu$-(*trans*-1,4-dithiane *S,S'*-dioxide-*S*:*S'*)$_{1.5}$], $[Er(C_6H_2N_3O_7)_3(C_4H_8O_2S_2)_{1.5}]$, consist of nine-coordinate metal ions, linked to three bidentate picrate ligands, bound *via* the phenoxo O atom and one O atom of an adjacent nitro group, and to three O atoms of three TDTD ligands. The TDTD ligands act as bridges that join three neighbouring lanthanide ions, to give three-dimensional polymers. The coordination polyhedra of the Nd^{III} and Er^{III} ions may best be described as tricapped trigonal prisms.

Comment

We are currently studying the crystal structures and some spectroscopic properties of a series of lanthanide picrates with TDTD as a neutral ligand (Ayala, Zinner, Vicentini, Del Pra & Bombieri, 1993). The title compounds, (I) and (II), have polymeric structures in which the conformations of the picrate (Herbstein & Kaftory, 1976) and TDTD (Shearer, 1959) ligands are unchanged with respect to those of the free ligands. The only feature of note is the shortening of the C—O phenoxo bond [average distance 1.24 (1) Å] with respect to the corresponding distance in picric acid [1.327 (3) Å (Herbstein & Kaftory, 1976)] as has been found in a series of dipicrate derivatives (Nardelli, Pelizzi, Vitali, Bordi, Plazzi & Vitali, 1987) which present a comparable average value of 1.247 (3) Å. This shortening suggests a tendency of the picrate ligand to assume a quinone-like structure.



(I) Ln = Nd
(II) Ln = Er

The structures of the Nd and Er complexes (Figs. 1 and 2) are characterized by similar trends in the Ln—O distances, which can be classified into three types, depending on the nature of the O atom. The shortest distance is Ln—$O_{phenoxo}$ [average Nd—O = 2.348 (5); average Er—O = 2.247 (5) Å], the intermediate distance is Ln—O_{TDTD} [average Nd—O = 2.403 (5); average Er—O = 2.304 (6) Å] and the largest distance is Ln—O_{nitro} [average Nd—O = 2.690 (6); average Er—O = 2.662 (6) Å]. The same trend was observed in the analogous derivatives of the lighter lanthanides, $[Ce(TDTD)_{1.5}(pic)_3].H_2O$ and $[Eu(TDTD)_{1.5}(pic)_3]$ (Ayala *et al.*, 1993).

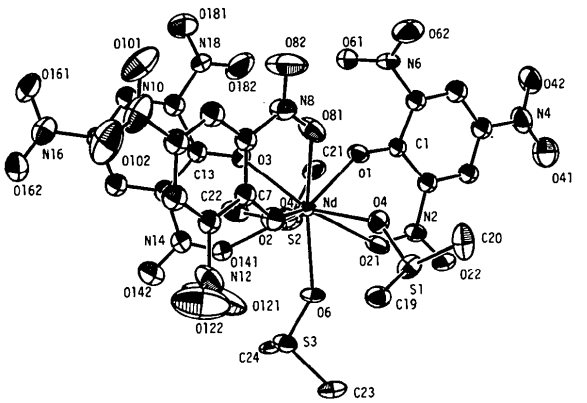


Fig. 1. *ORTEP*II (Johnson, 1976) view of the $[Nd(TDTD)_{1.5}(pic)_3]$ unit showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. (Only the asymmetric part of the TDTD molecules is shown.)

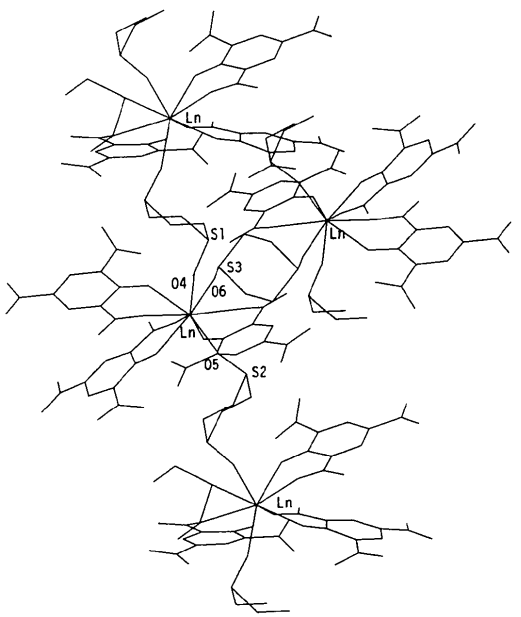


Fig. 2. A schematic perspective view of the polymeric structures. (Only the O and S atoms of the TDTD ligand are numbered for clarity.)

Experimental

Compound (I)

Crystal data

$[Nd(C_6H_2N_3O_7)_3(C_4H_8O_2S_2)_{1.5}]$
$M_r = 1056.89$
Monoclinic
$P2_1/c$
$a = 12.793$ (4) Å
$b = 17.292$ (2) Å
$c = 17.244$ (4) Å
$\beta = 110.36$ (2)°
$V = 3576$ (2) Å^3
$Z = 4$
$D_x = 1.96$ Mg m^{-3}
Mo $K\alpha$ radiation
$\lambda = 0.7107$ Å
Cell parameters from 25 reflections
$\theta = 8$–12°
$\mu = 1.730$ mm^{-1}
$T = 298$ K
Irregular prism
0.30 × 0.15 × 0.05 mm
Yellow

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: empirical (ψ scan)
$T_{min} = 0.825$, $T_{max} = 0.995$
7726 measured reflections
5604 independent reflections
4102 observed reflections $[I \geq 2.5\sigma(I)]$
$R_{int} = 0.020$
$\theta_{max} = 25°$
$h = -15 \rightarrow 14$
$k = -1 \rightarrow 20$
$l = -1 \rightarrow 20$
3 standard reflections
frequency: 60 min
intensity variation: none

Refinement

Refinement on F
$R = 0.039$
$wR = 0.040$
$S = 1.22$
4102 reflections
497 parameters
$w = 1/[\sigma^2(F_o) + 0.001045(F_o)^2]$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.89$ e Å^{-3}
$\Delta\rho_{min} = -0.92$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Compound (II)

Crystal data

$[Er(C_6H_2N_3O_7)_3(C_4H_8O_2S_2)_{1.5}]$
$M_r = 1079.91$
Monoclinic
$P2_1/c$
$a = 12.735$ (5) Å
$b = 16.967$ (4) Å
$c = 17.354$ (2) Å
$\beta = 111.11$ (2)°
$V = 3498$ (2) Å^3
$Z = 4$
$D_x = 2.05$ Mg m^{-3}
Mo $K\alpha$ radiation
$\lambda = 0.7107$ Å
Cell parameters from 25 reflections
$\theta = 8$–12°
$\mu = 2.560$ mm^{-1}
$T = 298$ K
Irregular prism
0.20 × 0.20 × 0.13 mm
Yellow

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: empirical (ψ scan)
$T_{min} = 0.770$, $T_{max} = 0.999$
5153 measured reflections
4694 independent reflections
4235 observed reflections $[I \geq 2.5\sigma(I)]$
$R_{int} = 0.036$
$\theta_{max} = 25°$
$h = 0 \rightarrow 15$
$k = 0 \rightarrow 20$
$l = -18 \rightarrow 18$
3 standard reflections
frequency: 60 min
intensity variation: none

Refinement

Refinement on F
$R = 0.040$
$wR = 0.048$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.04$ e Å^{-3}
$\Delta\rho_{min} = -1.02$ e Å^{-3}

$S = 1.84$
4235 reflections
550 parameters
$w = 1/[\sigma^2(F_o) + 0.001468(F_o)^2]$

Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters* (Å²) *for complex* (I)

U_{iso} for C1–C18; $U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$ for others.

	x	y	z	U_{iso}/U_{eq}
Nd	0.06491 (3)	0.06168 (2)	0.26910 (2)	0.0204 (1)
S(1)	−0.0917 (2)	−0.1196 (1)	0.2362 (1)	0.0355 (7)
S(2)	−0.0080 (2)	0.2434 (1)	0.3698 (1)	0.0391 (8)
S(3)	0.1176 (2)	−0.0259 (1)	0.4769 (1)	0.0352 (7)
O(1)	−0.0790 (4)	0.1191 (3)	0.1621 (3)	0.033 (2)
O(2)	0.2012 (4)	−0.0312 (3)	0.2727 (3)	0.038 (2)
O(3)	0.1998 (4)	0.1477 (3)	0.2537 (3)	0.037 (2)
O(4)	−0.0431 (4)	−0.0517 (3)	0.2061 (3)	0.033 (2)
O(5)	0.0463 (4)	0.1763 (3)	0.3421 (3)	0.039 (2)
O(6)	0.0590 (4)	−0.0102 (3)	0.3850 (3)	0.031 (2)
O(21)	−0.1359 (4)	0.0659 (3)	0.2877 (3)	0.040 (2)
O(22)	−0.3090 (4)	0.0531 (4)	0.2703 (3)	0.045 (2)
O(41)	−0.5972 (5)	0.1490 (5)	0.0404 (5)	0.073 (3)
O(42)	−0.5614 (5)	0.2084 (4)	−0.0581 (4)	0.062 (3)
O(61)	−0.0742 (5)	0.2218 (4)	0.0408 (4)	0.061 (3)
O(62)	−0.1702 (6)	0.1534 (4)	−0.0636 (4)	0.070 (3)
O(81)	0.1029 (4)	0.0344 (4)	0.1269 (3)	0.047 (2)
O(82)	0.1886 (7)	0.0355 (5)	0.0403 (5)	0.092 (4)
O(101)	0.5622 (6)	−0.0431 (4)	0.1061 (5)	0.069 (4)
O(102)	0.6427 (5)	−0.1102 (5)	0.2172 (6)	0.081 (4)
O(121)	0.344 (1)	−0.0863 (9)	0.4141 (6)	0.178 (8)
O(122)	0.426 (1)	−0.1814 (5)	0.3869 (6)	0.121 (6)
O(141)	0.2459 (4)	0.0867 (3)	0.4026 (3)	0.042 (2)
O(142)	0.4114 (6)	0.0860 (8)	0.4836 (5)	0.140 (6)
O(161)	0.6894 (5)	0.2268 (4)	0.2967 (4)	0.062 (3)
O(162)	0.7177 (5)	0.1686 (4)	0.4131 (4)	0.059 (3)
O(181)	0.3199 (6)	0.2842 (5)	0.1161 (5)	0.088 (4)
O(182)	0.1881 (7)	0.237 (1)	0.1308 (8)	0.240 (9)
N(2)	−0.2341 (5)	0.0738 (3)	0.2452 (4)	0.029 (2)
N(4)	−0.5328 (5)	0.1722 (4)	0.0077 (5)	0.051 (3)
N(6)	−0.1521 (5)	0.1800 (4)	0.0052 (4)	0.039 (3)
N(8)	0.1875 (6)	0.0228 (4)	0.1086 (4)	0.043 (3)
N(10)	0.5648 (6)	−0.0712 (5)	0.1717 (6)	0.057 (4)
N(12)	0.3816 (6)	−0.1205 (5)	0.3699 (5)	0.056 (3)
N(14)	0.3446 (5)	0.0978 (5)	0.4158 (4)	0.051 (3)
N(16)	0.6557 (6)	0.1922 (4)	0.3456 (5)	0.045 (3)
N(18)	0.2824 (5)	0.2432 (5)	0.1529 (4)	0.050 (3)
C(1)	−0.1822 (5)	0.1289 (4)	0.1296 (4)	0.024 (1)
C(2)	−0.2649 (6)	0.1087 (4)	0.1638 (5)	0.031 (2)
C(3)	−0.3784 (6)	0.1226 (4)	0.1239 (5)	0.032 (2)
C(4)	−0.4143 (6)	0.1548 (5)	0.0467 (5)	0.037 (2)
C(5)	−0.3404 (6)	0.1727 (5)	0.0069 (5)	0.037 (2)
C(6)	−0.2297 (6)	0.1603 (4)	0.0469 (5)	0.032 (2)
C(7)	0.2820 (6)	−0.0401 (4)	0.2470 (5)	0.031 (2)
C(8)	0.2861 (6)	−0.0124 (4)	0.1691 (5)	0.032 (2)
C(9)	0.3770 (7)	−0.0223 (5)	0.1463 (6)	0.040 (2)
C(10)	0.4686 (6)	−0.0600 (5)	0.1972 (5)	0.041 (2)
C(11)	0.4722 (6)	−0.0919 (5)	0.2722 (5)	0.040 (2)
C(12)	0.3787 (6)	−0.0821 (4)	0.2951 (5)	0.034 (2)
C(13)	0.3045 (6)	0.1601 (4)	0.2775 (5)	0.030 (2)
C(14)	0.3823 (6)	0.1319 (4)	0.3537 (5)	0.032 (2)
C(15)	0.4972 (6)	0.1418 (5)	0.3755 (5)	0.036 (2)
C(16)	0.5365 (6)	0.1811 (4)	0.3224 (5)	0.032 (2)
C(17)	0.4662 (6)	0.2119 (5)	0.2489 (5)	0.034 (2)
C(18)	0.3538 (6)	0.2036 (4)	0.2283 (5)	0.034 (2)
C(19)	0.0200 (7)	−0.1879 (5)	0.2778 (5)	0.037 (3)
C(20)	−0.1705 (6)	−0.1709 (5)	0.1446 (6)	0.053 (4)
C(21)	−0.0851 (6)	0.2957 (5)	0.2792 (5)	0.042 (3)
C(22)	0.0993 (8)	0.3124 (5)	0.4125 (5)	0.050 (4)
C(23)	0.0220 (7)	−0.0883 (4)	0.5017 (5)	0.042 (3)
C(24)	0.0973 (7)	0.0588 (5)	0.5306 (5)	0.041 (3)

Table 2. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å²) *for complex* (II)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
Er	0.06789 (2)	−0.06382 (2)	−0.22425 (2)	0.0185 (2)
S(1)	−0.0914 (1)	0.1132 (1)	−0.2584 (1)	0.0267 (6)
S(2)	0.0060 (2)	−0.2464 (1)	−0.1274 (1)	0.0330 (7)
S(3)	0.1177 (2)	0.0244 (1)	−0.0244 (1)	0.0295 (7)
O(1)	0.1959 (4)	0.0291 (3)	−0.2207 (3)	0.031 (2)
O(2)	−0.0634 (4)	−0.1231 (3)	−0.3296 (3)	0.029 (2)
O(3)	0.1985 (4)	−0.1417 (3)	−0.2466 (3)	0.033 (2)
O(4)	−0.0449 (4)	0.0438 (3)	−0.2894 (3)	0.028 (2)
O(5)	0.0609 (5)	−0.1792 (3)	−0.1565 (4)	0.039 (2)
O(6)	0.0577 (4)	0.0041 (3)	−0.1148 (3)	0.028 (2)
O(21)	0.0975 (4)	−0.0313 (4)	−0.3703 (4)	0.049 (2)
O(22)	0.1968 (8)	−0.0509 (8)	−0.4423 (7)	0.117 (5)
O(41)	0.6463 (5)	0.1088 (4)	−0.2632 (5)	0.061 (3)
O(42)	0.5675 (6)	0.0416 (4)	−0.3757 (5)	0.059 (3)
O(61)	0.325 (1)	0.101 (1)	−0.0834 (7)	0.152 (7)
O(62)	0.425 (1)	0.1869 (5)	−0.1055 (6)	0.099 (5)
O(81)	−0.1280 (5)	−0.0775 (4)	−0.2059 (4)	0.040 (2)
O(82)	−0.3017 (5)	−0.0595 (3)	−0.2282 (4)	0.041 (2)
O(101)	−0.5503 (6)	−0.2020 (4)	−0.5660 (5)	0.063 (3)
O(102)	−0.5903 (5)	−0.1402 (5)	−0.4720 (5)	0.066 (3)
O(121)	−0.1508 (7)	−0.1435 (4)	−0.5586 (4)	0.061 (3)
O(122)	−0.0554 (5)	−0.2154 (4)	−0.4566 (4)	0.055 (3)
O(141)	0.2484 (5)	−0.0862 (4)	−0.0948 (4)	0.042 (2)
O(142)	0.4183 (7)	−0.0756 (8)	−0.0179 (6)	0.130 (6)
O(161)	0.6885 (5)	−0.2340 (4)	−0.2021 (5)	0.058 (3)
O(162)	0.7202 (5)	−0.1726 (4)	−0.0862 (4)	0.056 (3)
O(181)	0.1807 (6)	−0.2622 (5)	−0.3494 (5)	0.073 (4)
O(182)	0.3171 (6)	−0.2660 (5)	−0.3940 (5)	0.069 (4)
N(2)	0.1859 (6)	−0.0252 (5)	−0.3820 (4)	0.041 (3)
N(4)	0.5695 (7)	0.0715 (4)	−0.3106 (6)	0.047 (4)
N(6)	0.3737 (6)	0.1275 (5)	−0.1239 (5)	0.045 (3)
N(8)	−0.2273 (5)	−0.0799 (4)	−0.2521 (4)	0.027 (2)
N(10)	−0.5235 (6)	−0.1648 (5)	−0.5014 (5)	0.050 (3)
N(12)	−0.1336 (6)	−0.1729 (4)	−0.4923 (4)	0.039 (3)
N(14)	0.3476 (6)	−0.0964 (5)	−0.0823 (4)	0.040 (3)
N(16)	0.6574 (6)	−0.1969 (4)	−0.1533 (5)	0.042 (3)
N(18)	0.2783 (6)	−0.2416 (4)	−0.3448 (5)	0.042 (3)
C(1)	0.2763 (6)	0.0412 (5)	−0.2453 (5)	0.028 (3)
C(2)	0.2849 (6)	0.0107 (4)	−0.3200 (5)	0.028 (3)
C(3)	0.3776 (7)	0.0207 (4)	−0.3417 (5)	0.033 (3)
C(4)	0.4690 (7)	0.0607 (4)	−0.2893 (6)	0.037 (4)
C(5)	0.4688 (6)	0.0942 (5)	−0.2155 (6)	0.033 (3)
C(6)	0.3744 (6)	0.0849 (5)	−0.1972 (5)	0.028 (3)
C(7)	−0.1694 (6)	−0.1278 (4)	−0.3667 (4)	0.025 (3)
C(8)	−0.2541 (6)	−0.1108 (4)	−0.3347 (5)	0.027 (3)
C(9)	−0.3698 (6)	−0.1224 (4)	−0.3783 (5)	0.033 (3)
C(10)	−0.4016 (6)	−0.1491 (5)	−0.4576 (5)	0.034 (3)
C(11)	−0.3256 (7)	−0.1647 (5)	−0.4948 (5)	0.035 (3)
C(12)	−0.2160 (6)	−0.1562 (4)	−0.4514 (5)	0.030 (3)
C(13)	0.3021 (6)	−0.1567 (4)	−0.2227 (5)	0.026 (3)
C(14)	0.3834 (6)	−0.1315 (4)	−0.1467 (5)	0.029 (3)
C(15)	0.4988 (6)	−0.1421 (5)	−0.1218 (5)	0.034 (3)
C(16)	0.5379 (6)	−0.1809 (4)	−0.1770 (5)	0.032 (3)
C(17)	0.4653 (7)	−0.2125 (5)	−0.2502 (5)	0.033 (3)
C(18)	0.3509 (6)	−0.2015 (4)	−0.2715 (5)	0.027 (3)
C(19)	0.0216 (7)	0.1833 (4)	−0.2217 (5)	0.029 (3)
C(20)	−0.1762 (6)	0.1632 (5)	−0.3510 (6)	0.041 (3)
C(21)	0.1150 (8)	−0.3194 (5)	−0.0897 (5)	0.042 (3)
C(22)	−0.0808 (6)	−0.2988 (4)	−0.2173 (5)	0.031 (3)
C(23)	0.0227 (7)	0.0906 (5)	−0.0027 (5)	0.033 (3)
C(24)	0.0976 (7)	−0.0605 (5)	0.0312 (5)	0.040 (3)

Table 3. *Selected bond lengths* (Å) *and angles* (°) *in the coordination spheres of complexes* (I) *and* (I)

Complex (I)			
Nd—O(1)	2.327 (4)	Nd—O(2)	2.355 (6)
Nd—O(3)	2.362 (5)	Nd—O(4)	2.427 (5)
Nd—O(5)	2.404 (5)	Nd—O(6)	2.377 (5)
Nd—O(21)	2.698 (6)	Nd—O(81)	2.701 (6)
Nd—O(141)	2.672 (5)		

O(4)—Nd—O(5)	139.1 (2)	O(3)—Nd—O(141)	63.1 (2)
O(3)—Nd—O(5)	75.5 (2)	O(3)—Nd—O(4)	141.5 (2)
O(2)—Nd—O(81)	62.6 (2)	O(1)—Nd—O(21)	63.8 (2)
Complex (II)			
Er—O(1)	2.253 (5)	Er—O(2)	2.224 (5)
Er—O(3)	2.264 (6)	Er—O(4)	2.346 (5)
Er—O(5)	2.302 (6)	Er—O(6)	2.265 (6)
Er—O(21)	2.749 (7)	Er—O(81)	2.636 (7)
Er—O(141)	2.600 (5)		
O(4)—Er—O(5)	141.1 (2)	O(3)—Er—O(141)	65.6 (2)
O(3)—Er—O(5)	75.9 (2)	O(3)—Er—O(4)	137.0 (2)
O(2)—Er—O(81)	66.1 (2)	O(1)—Er—O(21)	63.0 (2)

Table 4. *Summary of the structural parameters* (Å, °) *for the picrate and trans*-1,4-*dithiane S,S'-dioxide ligands in complexes* (I) *and* (II)

	(I)	(II)
Picrate		
C_{sp^2}—O	1.266 (8)	1.263 (6)
C_{sp^2}—N	1.46 (1)	1.47 (1)
N—O	1.21 (1)	1.21 (1)
C_{sp^2}—C_{sp^2}	1.395 (9)	1.39 (1)
C—C—C	119.9 (7)	120.0 (8)
O—C—C	123.2 (7)	123.9 (7)
O—N—C	118.9 (8)	118.6 (8)
N—C—C	118.6 (7)	118.0 (7)
O—N—O	122.2 (8)	122.7 (8)
trans-1,4-Dithiane *S,S'*-dioxide		
S—O	1.513 (6)	1.511 (6)
C_{sp^3}—S	1.788 (9)	1.795 (9)
C_{sp^3}—C_{sp^3}	1.54 (1)	1.53 (1)
O—S—C	105.6 (4)	105.0 (4)
C—S—C	98.1 (4)	98.3 (4)

The space groups for the Nd and Er complexes were determined unambiguously, from the systematic absences, to be $P2_1/c$ (No. 14). In both the Nd and Er compounds, the H-atom contributions were introduced in calculated positions (C—H = 0.98 Å, U_{iso} = 0.07 Å^2) For both compounds, Enraf–Nonius CAD-4 software was used for data collection and cell refinement. Data reduction was acheived using *MolEN* (Fair, 1990). Structure solution and refinement were performed using *SHELX*76 (Sheldrick, 1976) and molecular graphics were produced using *ORTEP*II (Johnson, 1976).

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Lists of structure factors for both complexes, anisotropic displacement parameters, H-atom coordinates and complete geometry for complex (I) have been deposited with the IUCr (Reference: NA1059). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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A Novel Inorganic/Organic Macrocycle Involving a Binuclear Zn^{II} Complex of Tetra(2′-pyridyl)pyrazine (TPPZ): Bis[$Zn_2(\mu$-TPPZ)$H_2OCl(\mu$-$ZnCl_4)(\mu$-$ZnCl_2)(\mu$-$ZnCl_3H_2O)$]

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Abstract

The macrocycle, *cyclo*-tetraaqua-1κO,2κO,6κO,7κO-octa-μ-chloro-1:2κ^2Cl;2:3κ^2Cl;3:4κ^2Cl;4:5κ^2Cl;6:7-κ^2Cl;7:8κ^2Cl;8:9κ^2Cl;9:10κ^2Cl-dodecachloro-2κCl,-3κ^2Cl,4κ^2Cl,5κCl,7κCl,8κ^2Cl,9κ^2Cl,10κCl-bis[μ-2,3,5,6-tetra(2-pyridyl)pyrazine]-1$\kappa^3N^{1,2,6}$:10$\kappa^3N^{3,4,5}$;-5$\kappa^3N^{1,2,6}$:6$\kappa^3N^{3,4,5}$-decazinc, $[Zn_5Cl_{10}(C_{24}H_{16}N_6)(H_2O)_2]_2$, is composed of two twisted binuclear Zn^{II} complexes of the ligand tetra(2′-pyridyl)pyrazine connected end to end by two chains of three Cl···Zn···Cl bridging units.

Comment

The ligand tetra(2′-pyridyl)pyrazine (TPPZ) was originally synthesized by Goodwin & Lions (1959). It was thought unlikely that it would act as a bis(tridentate) ligand owing to the steric repulsions between adjacent coplanar pyridine rings. However, binuclear complexes have been prepared with Ru^{II} (Thummel & Chirayil, 1988; Ruminski, Kipling, Cockcroft & Chase, 1989), Cu^{II} (Escuer, Comas, Ribas, Vicente, Solans, Zanchini & Gatteschi, 1989) and Rh^{II} (Ruminski & Letner, 1989). Recently Arana & Abruna (1993) prepared a series of monometallic and homo- and hetero-, bi- and trimetallic complexes of Ru^{II} and Os^{II}. We have shown, crystallographically, that TPPZ forms both mononuclear complexes with Cu^{II} and Zn^{II} (Graf, Greaves & Stoeckli-