Table 1. Crystal data and structure refinement for complex 1.

Identification code	complex **1**
Empirical formula	$C_{22}H_{27}NdOS$
Formula weight	483.74
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal habit	Pale blue prism
Crystal size	0.70 x 0.50 x 0.40 mm
Crystal system	Monoclinic
Space group	$P2_1/n$ (No. 14)
Unit cell dimensions	a = 8.541(2) Å α = 90° b = 18.048(3) Å β = 106.58(2)° c = 14.618(2) Å γ = 90°
Volume	2159.6(7) $Å^3$
Z	4
Density (calculated)	1.488 Mg/m^3
Absorption coefficient	2.507 mm^{-1}
F(000)	972
Diffractometer used	Siemens P4
θ range for data collection	2.26 to 26.00°
Index ranges	$-1 \le h \le 10$, $-1 \le k \le 22$, $-18 \le \ell \le 17$
Reflections collected	5473
Independent reflections	4252 (R_{int} = 0.0335)
Observed reflections	3208(I >2sigma(I))
Absorption correction	Empirical
Max. and min. transmission	0.348 and 0.291
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4252 / 81 / 226
Goodness-of-fit on F^2	1.019
Final R indices [$I>2\sigma(I)$]	R1 = 0.0406, wR2 = 0.0877
R indices (all data)	R1 = 0.0633, wR2 = 0.0969
Largest and mean Δ/σ	0.000, 0.000
Largest diff. peak and hole	1.216 and -0.692 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^5 for Nd, x 10^4 for others] and equivalent isotropic displacement parameters [$Å^2$ x 10^4 for Nd, $Å^2$ x 10^3 for others] for complex **1**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Nd(1)	4840(3)	13288(1)	4690(2)	331(1)
C(1)	3761(6)	906(3)	1245(4)	58(2)
C(2)	3436(6)	1408(3)	1899(4)	52(2)
C(3)	3164(6)	2110(3)	1477(4)	52(2)
C(4)	3325(7)	2056(4)	559(4)	61(2)
C(5)	3682(7)	1321(4)	419(4)	70(2)
C(6)	4209(8)	105(4)	1400(6)	103(3)
C(7)	-677(8)	2732(3)	-271(4)	68(2)
C(8)	-1913(8)	2426(3)	48(4)	65(2)
C(9)	-2560(6)	1819(3)	-509(4)	56(2)
C(10)	-1719(7)	1751(3)	-1188(4)	52(2)
C(11)	-553(7)	2288(3)	-1043(4)	62(2)
C(12)	253(12)	3423(4)	72(7)	129(4)
S(1)	-509(2)	-147(1)	908(1)	43(1)
C(13)	-283(6)	-404(3)	2117(3)	47(1)
C(14)	-1383(9)	-870(4)	2333(4)	82(2)
C(15)	-1210(12)	-1046(5)	3281(5)	123(3)
C(16)	21(11)	-773(5)	3997(5)	122(4)
C(17)	1106(11)	-316(5)	3788(4)	102(3)
C(18)	971(9)	-133(4)	2847(4)	70(2)
O(1)	-492(4)	1540(2)	1936(2)	44(1)
C(19)	-2122(6)	1344(4)	1971(4)	57(2)
C(20)	-2128(9)	1444(6)	2959(5)	113(3)
C(21)	-876(9)	2002(6)	3348(5)	116(3)
C(22)	201(8)	2013(4)	2731(4)	80(2)

Table 3. Bond lengths [Å] and angles [°] for complex 1

Nd(1)-O(1)	2.542(3)	Nd(1)-C(10)	2.718(5)
Nd(1)-C(4)	2.729(5)	Nd(1)-C(9)	2.732(5)
Nd(1)-C(3)	2.733(5)	Nd(1)-C(11)	2.748(5)
Nd(1)-C(5)	2.753(5)	Nd(1)-C(2)	2.782(5)
Nd(1)-C(8)	2.789(6)	Nd(1)-C(1)	2.809(5)
Nd(1)-C(7)	2.821(6)	Nd(1)-S(1)	2.9216(14)
C(1)-C(2)	1.401(7)	C(1)-C(5)	1.405(8)
C(1)-C(6)	1.497(8)	C(2)-C(3)	1.399(7)
C(3)-C(4)	1.391(7)	C(4)-C(5)	1.390(8)
C(7)-C(8)	1.385(8)	C(7)-C(11)	1.412(8)
C(7)-C(12)	1.487(9)	C(8)-C(9)	1.383(7)
C(9)-C(10)	1.387(7)	C(10)-C(11)	1.363(7)
S(1)-C(13)	1.785(5)	S(1)-Nd(1)#1	2.9364(13)
C(13)-C(14)	1.363(8)	C(13)-C(18)	1.368(7)
C(14)-C(15)	1.388(8)	C(15)-C(16)	1.348(10)
C(16)-C(17)	1.340(10)	C(17)-C(18)	1.386(8)
O(1)-C(22)	1.427(6)	O(1)-C(19)	1.451(6)
C(19)-C(20)	1.458(8)	C(20)-C(21)	1.461(10)
C(21)-C(22)	1.460(8)		

O(1)-Nd(1)-C(10)	113.55(14)	O(1)-Nd(1)-C(4)	112.86(14)
C(10)-Nd(1)-C(4)	106.74(18)	O(1)-Nd(1)-C(9)	84.29(15)
C(10)-Nd(1)-C(9)	29.49(16)	C(4)-Nd(1)-C(9)	124.74(18)
O(1)-Nd(1)-C(3)	83.89(14)	C(10)-Nd(1)-C(3)	126.60(17)
C(4)-Nd(1)-C(3)	29.51(15)	C(9)-Nd(1)-C(3)	129.84(17)
O(1)-Nd(1)-C(11)	118.42(15)	C(10)-Nd(1)-C(11)	28.86(15)
C(4)-Nd(1)-C(11)	79.27(18)	C(9)-Nd(1)-C(11)	48.32(17)
C(3)-Nd(1)-C(11)	97.87(18)	O(1)-Nd(1)-C(5)	126.16(14)
C(10)-Nd(1)-C(5)	114.69(18)	C(4)-Nd(1)-C(5)	29.38(16)
C(9)-Nd(1)-C(5)	142.29(19)	C(3)-Nd(1)-C(5)	48.13(17)
C(11)-Nd(1)-C(5)	94.40(19)	O(1)-Nd(1)-C(2)	78.67(14)
C(10)-Nd(1)-C(2)	154.67(17)	C(4)-Nd(1)-C(2)	48.42(16)
C(9)-Nd(1)-C(2)	154.12(17)	C(3)-Nd(1)-C(2)	29.38(15)
C(11)-Nd(1)-C(2)	125.96(17)	C(5)-Nd(1)-C(2)	47.69(17)
O(1)-Nd(1)-C(8)	71.49(15)	C(10)-Nd(1)-C(8)	47.65(16)
C(4)-Nd(1)-C(8)	104.8(2)	C(9)-Nd(1)-C(8)	29.00(15)
C(3)-Nd(1)-C(8)	101.64(18)	C(11)-Nd(1)-C(8)	47.70(18)
C(5)-Nd(1)-C(8)	132.03(19)	C(2)-Nd(1)-C(8)	125.48(17)
O(1)-Nd(1)-C(1)	103.25(14)	C(10)-Nd(1)-C(1)	142.42(17)
C(4)-Nd(1)-C(1)	48.79(18)	C(9)-Nd(1)-C(1)	171.48(17)
C(3)-Nd(1)-C(1)	48.52(16)	C(11)-Nd(1)-C(1)	123.45(18)
C(5)-Nd(1)-C(1)	29.24(16)	C(2)-Nd(1)-C(1)	29.01(15)
C(8)-Nd(1)-C(1)	150.02(18)	O(1)-Nd(1)-C(7)	91.42(16)
C(10)-Nd(1)-C(7)	47.81(17)	C(4)-Nd(1)-C(7)	78.29(19)
C(9)-Nd(1)-C(7)	47.99(17)	C(3)-Nd(1)-C(7)	83.82(17)
C(11)-Nd(1)-C(7)	29.35(16)	C(5)-Nd(1)-C(7)	103.7(2)
C(2)-Nd(1)-C(7)	112.72(17)	C(8)-Nd(1)-C(7)	28.58(16)
C(1)-Nd(1)-C(7)	126.82(17)	O(1)-Nd(1)-S(1)	76.46(8)
C(10)-Nd(1)-S(1)	106.30(13)	C(4)-Nd(1)-S(1)	137.55(14)
C(9)-Nd(1)-S(1)	96.74(13)	C(3)-Nd(1)-S(1)	127.06(12)
C(11)-Nd(1)-S(1)	134.74(13)	C(5)-Nd(1)-S(1)	110.69(15)
C(2)-Nd(1)-S(1)	98.01(12)	C(8)-Nd(1)-S(1)	117.08(14)
C(1)-Nd(1)-S(1)	88.98(12)	C(7)-Nd(1)-S(1)	144.14(14)
C(2)-C(1)-C(5)	105.8(5)	C(2)-C(1)-C(6)	127.7(6)
C(5)-C(1)-C(6)	126.3(6)	C(2)-C(1)-Nd(1)	74.4(3)
C(5)-C(1)-Nd(1)	73.2(3)	C(6)-C(1)-Nd(1)	120.4(4)
C(3)-C(2)-C(1)	108.9(5)	C(3)-C(2)-Nd(1)	73.4(3)

C(4)-C(3)-Nd(1)	75.1(3)	C(2)-C(3)-Nd(1)	77.2(3)
C(5)-C(4)-C(3)	107.1(5)	C(5)-C(4)-Nd(1)	76.3(3)
C(3)-C(4)-Nd(1)	75.4(3)	C(4)-C(5)-C(1)	109.9(5)
C(4)-C(5)-Nd(1)	74.3(3)	C(1)-C(5)-Nd(1)	77.6(3)
C(8)-C(7)-C(11)	106.3(5)	C(8)-C(7)-C(12)	127.3(7)
C(11)-C(7)-C(12)	126.2(7)	C(8)-C(7)-Nd(1)	74.4(3)
C(11)-C(7)-Nd(1)	72.5(3)	C(12)-C(7)-Nd(1)	121.9(5)
C(9)-C(8)-C(7)	109.4(5)	C(9)-C(8)-Nd(1)	73.2(3)
C(7)-C(8)-Nd(1)	77.0(3)	C(8)-C(9)-C(10)	106.9(5)
C(8)-C(9)-Nd(1)	77.8(3)	C(10)-C(9)-Nd(1)	74.7(3)
C(11)-C(10)-C(9)	109.3(5)	C(11)-C(10)-Nd(1)	76.8(3)
C(9)-C(10)-Nd(1)	75.8(3)	C(10)-C(11)-C(7)	108.1(5)
C(10)-C(11)-Nd(1)	74.4(3)	C(7)-C(11)-Nd(1)	78.2(3)
C(13)-S(1)-Nd(1)	119.87(18)	C(13)-S(1)-Nd(1)#1	118.08(18)
Nd(1)-S(1)-Nd(1)#1	116.90(4)	C(14)-C(13)-C(18)	118.6(5)
C(14)-C(13)-S(1)	120.2(4)	C(18)-C(13)-S(1)	121.3(4)
C(13)-C(14)-C(15)	119.2(7)	C(16)-C(15)-C(14)	121.9(8)
C(17)-C(16)-C(15)	119.0(7)	C(16)-C(17)-C(18)	120.4(7)
C(13)-C(18)-C(17)	120.8(7)	C(22)-O(1)-C(19)	107.2(4)
C(22)-O(1)-Nd(1)	128.1(3)	C(19)-O(1)-Nd(1)	122.8(3)
O(1)-C(19)-C(20)	106.3(4)	C(19)-C(20)-C(21)	105.1(6)
C(22)-C(21)-C(20)	106.8(5)	O(1)-C(22)-C(21)	107.9(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^4 for Nd, $Å^2$ x 10^3 for others] for complex 1

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Nd(1)	341(1)	347(1)	319(1)	-11(1)	118(1)	-22(1)
C(1)	28(3)	56(4)	85(4)	-12(3)	10(3)	-4(3)
C(2)	35(3)	70(4)	47(3)	-3(3)	4(2)	-16(3)
C(3)	46(3)	50(3)	62(3)	-9(3)	17(3)	-13(3)
C(4)	52(3)	75(4)	60(4)	2(3)	20(3)	-26(3)
C(5)	43(3)	110(6)	65(4)	-31(4)	29(3)	-24(4)
C(6)	47(4)	81(6)	173(8)	-13(6)	21(5)	9(4)
C(7)	81(5)	37(3)	79(5)	11(3)	14(4)	8(3)
C(8)	77(4)	62(4)	59(4)	9(3)	25(3)	34(4)
C(9)	40(3)	54(4)	69(4)	14(3)	8(3)	11(3)
C(10)	61(4)	47(3)	41(3)	4(3)	3(3)	18(3)
C(11)	66(4)	68(4)	57(4)	26(3)	25(3)	7(3)
C(12)	167(10)	48(4)	154(8)	9(5)	15(7)	2(6)
S(1)	61(1)	39(1)	33(1)	-1(1)	20(1)	-5(1)
C(13)	69(4)	45(3)	36(3)	7(2)	27(3)	14(3)
C(14)	131(6)	66(4)	63(4)	8(3)	47(4)	-19(5)
C(15)	208(9)	109(7)	86(5)	24(5)	95(6)	-23(7)
C(16)	229(11)	98(7)	60(4)	38(4)	74(6)	43(7)
C(17)	145(8)	111(7)	41(4)	11(4)	14(4)	42(6)
C(18)	92(5)	74(4)	42(3)	4(3)	15(3)	7(4)
O(1)	41(2)	55(2)	38(2)	-12(2)	15(2)	-10(2)
C(19)	44(3)	72(4)	61(3)	-18(3)	26(3)	-12(3)
C(20)	70(4)	199(10)	86(5)	-58(5)	48(4)	-49(5)
C(21)	87(5)	186(9)	93(5)	-84(5)	57(4)	-54(5)
C(22)	68(4)	117(6)	65(4)	-50(4)	35(3)	-37(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for complex 1

	x	y	z	U(eq)
H(2)	3406	1293	2514	63
H(3)	2917	2538	1761	63
H(4)	3215	2440	121	73
H(5)	3845	1131	-138	84
H(6A)	4166	-42	2024	154
H(6B)	5294	31	1350	154
H(6C)	3452	-189	927	154
H(8)	-2256	2602	558	78
H(9)	-3397	1514	-440	67
H(10)	-1920	1395	-1668	62
H(11)	194	2352	-1391	74
H(12A)	1037	3503	-275	194
H(12B)	810	3377	740	194
H(12C)	-487	3835	-26	194
H(14)	-2240	-1067	1851	99
H(15)	-1965	-1363	3426	148
H(16)	115	-899	4627	147
H(17)	1955	-121	4276	122
H(18)	1743	178	2710	84
H(19A)	-2368	834	1773	68
H(19B)	-2929	1663	1552	68
H(20A)	-1868	982	3311	135
H(20B)	-3189	1614	2991	135
H(21A)	-1374	2484	3354	139
H(21B)	-264	1875	3996	139
H(22A)	298	2514	2513	96
H(22B)	1281	1839	3079	96

Table 1. Crystal data and structure refinement for complex **2**.

Crystal habit	Pale blue prism
Crystal size	0.30 x 0.40 x 0.80 mm
Empirical formula	C50 H48 N2 Nd2 O2 S2
Formula weight	1061.50
Temperature	294(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
space group	P2(1)/n (No. 14)
Unit cell dimensions	a = 13.589(1)Å alpha = 90 deg.
	b = 17.643(1)Å beta = 95.93(1) deg.
	c = 18.711(1)Å gamma = 90 deg.
Volume	4462.0(5) Å^3
Z, Calculated density	4 , 1.580 Mg/m^3
Absorption coefficient	2.436 mm^-1
F(000)	2120
Theta range for data collection	1.77 to 25.55 deg.
Limiting indices	0<=h<=15, -21<=k<=21, -22<=l<=22
Reflections collected / unique	13007 / 7181 [R(int) = 0.0599]
Completeness to theta = 25.55	85.8 %
Absorption correction	ABSCOR
Max. and min. transmission	1.071 and 0.898
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7181 / 325 / 523
Goodness-of-fit on F^2	1.082
Final R indices [I>2sigma(I)]	R1 = 0.0731 , wR2 = 0.1961
R indices (all data)	R1 = 0.0815 , wR2 = 0.2049
Max. and min. shift	0.005 and 0.000
Largest diff. peak and hole	2.134 and -1.458 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for complex **2**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Nd(1)	11085(1)	3244(1)	3283(1)	57(1)
Nd(2)	8950(1)	4225(1)	1832(1)	55(1)
C(1)	11831(5)	1801(4)	3538(4)	75(2)
C(2)	11236(5)	1741(4)	2880(4)	81(2)
C(3)	10266(6)	1840(5)	3018(5)	85(3)
C(4)	10232(5)	1976(5)	3733(5)	87(3)
C(5)	11197(5)	1941(5)	4065(4)	78(2)
C(6)	12926(6)	1715(6)	3645(5)	109(3)
C(7)	12075(6)	4562(5)	3703(4)	96(3)
C(8)	11233(7)	4570(6)	4071(5)	111(4)
C(9)	11336(8)	3994(6)	4578(5)	125(4)
C(10)	12212(8)	3631(6)	4514(5)	130(5)
C(11)	12678(6)	3966(6)	3982(6)	110(4)
C(12)	12401(11)	5073(8)	3149(7)	210(8)
C(13)	12927(5)	2855(4)	1986(3)	62(2)
C(14)	12804(5)	2281(4)	1486(4)	74(2)
C(15)	13610(6)	1876(5)	1291(5)	94(3)
C(16)	14540(6)	2056(5)	1601(5)	96(3)
C(17)	14669(5)	2608(5)	2116(5)	93(3)
C(18)	13868(5)	3023(4)	2300(4)	71(2)
N(1)	12108(4)	3253(3)	2220(3)	59(2)
C(19)	11437(5)	3591(4)	1790(4)	63(2)
O(1)	10626(3)	3780(3)	2036(3)	67(1)
S(1)	11508(2)	3831(2)	864(1)	87(1)
C(20)	12771(5)	4068(4)	830(4)	65(2)
C(21)	13365(5)	3647(5)	435(4)	81(2)
C(22)	14342(6)	3865(5)	387(4)	94(3)
C(23)	14693(7)	4498(5)	749(5)	97(3)
C(24)	14110(7)	4929(5)	1137(5)	103(3)
C(25)	13143(6)	4713(5)	1172(5)	86(3)
C(26)	8203(5)	5650(5)	1545(4)	83(3)
C(27)	8800(7)	5487(5)	1001(4)	92(3)
C(28)	9776(6)	5470(5)	1285(5)	103(3)
C(29)	9809(6)	5632(5)	1997(5)	94(3)

C(30)	8850(6)	5724(4)	2170(5)	85(3)
C(31)	7120(6)	5752(6)	1484(7)	122(4)
C(32)	7917(5)	2884(4)	1484(4)	76(2)
C(33)	7360(6)	3464(5)	1134(4)	82(2)
C(34)	7876(6)	3771(5)	606(4)	90(3)
C(35)	8759(7)	3388(5)	611(5)	94(3)
C(36)	8803(6)	2841(5)	1154(4)	86(3)
C(37)	7637(8)	2388(5)	2061(6)	111(3)
C(38)	7084(4)	4605(4)	3131(3)	59(2)
C(39)	6163(5)	4435(5)	2799(4)	79(2)
C(40)	5352(6)	4859(5)	2969(4)	95(3)
C(41)	5472(6)	5433(5)	3456(5)	94(3)
C(42)	6383(6)	5606(5)	3785(5)	91(3)
C(43)	7204(6)	5195(4)	3619(4)	75(2)
N(2)	7913(4)	4214(3)	2908(3)	61(2)
C(44)	8580(5)	3868(4)	3339(4)	64(2)
O(2)	9399(3)	3685(3)	3089(2)	68(1)
S(2)	8511(2)	3594(2)	4247(1)	90(1)
C(45)	7249(5)	3435(4)	4339(4)	73(2)
C(46)	6753(6)	3906(5)	4767(4)	89(3)
C(47)	5776(6)	3714(6)	4868(5)	116(4)
C(48)	5320(8)	3073(6)	4569(6)	133(5)
C(49)	5834(7)	2622(6)	4141(6)	121(4)
C(50)	6805(7)	2798(5)	4032(5)	96(3)

Table 3. Bond lengths [A] and angles [deg] for complex **2**.

Nd(1)-O(2)	2.411(4)
Nd(1)-O(1)	2.535(5)
Nd(1)-N(1)	2.543(6)
Nd(1)-C(4)	2.695(8)
Nd(1)-C(10)	2.718(9)
Nd(1)-C(5)	2.721(8)
Nd(1)-C(11)	2.726(9)
Nd(1)-C(3)	2.741(8)
Nd(1)-C(9)	2.749(9)
Nd(1)-C(8)	2.761(9)
Nd(1)-C(1)	2.763(7)
Nd(1)-C(7)	2.759(8)
Nd(2)-O(1)	2.402(4)
Nd(2)-O(2)	2.553(5)
Nd(2)-N(2)	2.573(6)
Nd(2)-C(35)	2.710(8)
Nd(2)-C(27)	2.713(8)
Nd(2)-C(34)	2.709(8)
Nd(2)-C(28)	2.715(8)
Nd(2)-C(30)	2.727(8)
Nd(2)-C(26)	2.744(8)
Nd(2)-C(29)	2.748(9)
Nd(2)-C(36)	2.749(9)
Nd(2)-C(33)	2.756(8)
C(1)-C(5)	1.396(9)
C(1)-C(2)	1.406(9)
C(1)-C(6)	1.488(10)
C(2)-C(3)	1.380(9)
C(3)-C(4)	1.365(10)
C(4)-C(5)	1.393(9)
C(7)-C(8)	1.395(10)
C(7)-C(11)	1.400(10)
C(7)-C(12)	1.476(12)
C(8)-C(9)	1.388(11)
C(9)-C(10)	1.367(12)
C(10)-C(11)	1.369(11)
C(13)-C(14)	1.376(8)
C(13)-C(18)	1.384(8)
C(13)-N(1)	1.423(8)
C(14)-C(15)	1.388(9)

C(15)-C(16)	1.372(10)
C(16)-C(17)	1.369(10)
C(17)-C(18)	1.384(9)
N(1)-C(19)	1.297(8)
C(19)-O(1)	1.281(8)
C(19)-S(1)	1.796(7)
S(1)-C(20)	1.774(7)
C(20)-C(21)	1.368(9)
C(20)-C(25)	1.376(9)
C(21)-C(22)	1.394(9)
C(22)-C(23)	1.366(10)
C(23)-C(24)	1.361(10)
C(24)-C(25)	1.377(10)
C(26)-C(30)	1.394(9)
C(26)-C(27)	1.395(10)
C(26)-C(31)	1.475(10)
C(27)-C(28)	1.377(10)
C(28)-C(29)	1.360(11)
C(29)-C(30)	1.384(10)
C(32)-C(33)	1.396(9)
C(32)-C(36)	1.410(9)
C(32)-C(37)	1.470(10)
C(33)-C(34)	1.379(10)
C(34)-C(35)	1.376(11)
C(35)-C(36)	1.399(10)
C(38)-C(39)	1.371(8)
C(38)-C(43)	1.384(8)
C(38)-N(2)	1.420(8)
C(39)-C(40)	1.395(9)
C(40)-C(41)	1.361(10)
C(41)-C(42)	1.360(10)
C(42)-C(43)	1.392(9)
N(2)-C(44)	1.301(8)
C(44)-O(2)	1.292(8)
C(44)-S(2)	1.777(7)
S(2)-C(45)	1.764(8)
C(45)-C(50)	1.373(10)
C(45)-C(46)	1.377(9)
C(46)-C(47)	1.403(10)
C(47)-C(48)	1.379(11)
C(48)-C(49)	1.370(11)
C(49)-C(50)	1.392(10)

O(2)-Nd(1)-O(1)	66.53(16)

O(2)-Nd(1)-N(1)	117.90(16)
O(1)-Nd(1)-N(1)	51.65(16)
O(2)-Nd(1)-C(4)	83.2(2)
O(1)-Nd(1)-C(4)	121.6(2)
N(1)-Nd(1)-C(4)	122.5(2)
O(2)-Nd(1)-C(10)	119.3(3)
O(1)-Nd(1)-C(10)	138.6(3)
N(1)-Nd(1)-C(10)	110.9(3)
C(4)-Nd(1)-C(10)	99.6(3)
O(2)-Nd(1)-C(5)	110.68(19)
O(1)-Nd(1)-C(5)	143.5(2)
N(1)-Nd(1)-C(5)	114.9(2)
C(4)-Nd(1)-C(5)	29.8(2)
C(10)-Nd(1)-C(5)	76.2(3)
O(2)-Nd(1)-C(11)	128.1(2)
O(1)-Nd(1)-C(11)	112.0(3)
N(1)-Nd(1)-C(11)	84.3(3)
C(4)-Nd(1)-C(11)	125.8(3)
C(10)-Nd(1)-C(11)	29.1(2)
C(5)-Nd(1)-C(11)	98.0(3)
O(2)-Nd(1)-C(3)	84.4(2)
O(1)-Nd(1)-C(3)	96.5(2)
N(1)-Nd(1)-C(3)	96.2(2)
C(4)-Nd(1)-C(3)	29.1(2)
C(10)-Nd(1)-C(3)	124.3(3)
C(5)-Nd(1)-C(3)	48.1(2)
C(11)-Nd(1)-C(3)	142.8(3)
O(2)-Nd(1)-C(9)	90.4(3)
O(1)-Nd(1)-C(9)	128.9(3)
N(1)-Nd(1)-C(9)	131.2(2)
C(4)-Nd(1)-C(9)	98.2(3)
C(10)-Nd(1)-C(9)	29.0(3)
C(5)-Nd(1)-C(9)	86.5(3)
C(11)-Nd(1)-C(9)	48.2(3)
C(3)-Nd(1)-C(9)	127.3(3)
O(2)-Nd(1)-C(8)	79.8(2)
O(1)-Nd(1)-C(8)	100.0(2)
N(1)-Nd(1)-C(8)	113.4(2)
C(4)-Nd(1)-C(8)	123.2(3)
C(10)-Nd(1)-C(8)	48.0(3)
C(5)-Nd(1)-C(8)	115.6(3)
C(11)-Nd(1)-C(8)	48.5(3)
C(3)-Nd(1)-C(8)	150.3(3)
C(9)-Nd(1)-C(8)	29.2(2)

O(2)-Nd(1)-C(1)	130.48(19)
O(1)-Nd(1)-C(1)	123.57(19)
N(1)-Nd(1)-C(1)	85.41(19)
C(4)-Nd(1)-C(1)	48.9(2)
C(10)-Nd(1)-C(1)	85.4(3)
C(5)-Nd(1)-C(1)	29.48(19)
C(11)-Nd(1)-C(1)	95.1(3)
C(3)-Nd(1)-C(1)	48.2(2)
C(9)-Nd(1)-C(1)	106.3(3)
C(8)-Nd(1)-C(1)	133.1(3)
O(2)-Nd(1)-C(7)	101.5(2)
O(1)-Nd(1)-C(7)	90.8(2)
N(1)-Nd(1)-C(7)	85.8(2)
C(4)-Nd(1)-C(7)	145.5(3)
C(10)-Nd(1)-C(7)	48.1(3)
C(5)-Nd(1)-C(7)	124.1(2)
C(11)-Nd(1)-C(7)	29.6(2)
C(3)-Nd(1)-C(7)	172.0(2)
C(9)-Nd(1)-C(7)	48.1(3)
C(8)-Nd(1)-C(7)	29.3(2)
C(1)-Nd(1)-C(7)	124.6(2)
O(1)-Nd(2)-O(2)	66.37(16)
O(1)-Nd(2)-N(2)	117.39(17)
O(2)-Nd(2)-N(2)	51.28(16)
O(1)-Nd(2)-C(35)	87.9(2)
O(2)-Nd(2)-C(35)	124.5(2)
N(2)-Nd(2)-C(35)	130.0(2)
O(1)-Nd(2)-C(27)	112.0(2)
O(2)-Nd(2)-C(27)	146.2(2)
N(2)-Nd(2)-C(27)	116.1(2)
C(35)-Nd(2)-C(27)	88.2(3)
O(1)-Nd(2)-C(34)	117.2(2)
O(2)-Nd(2)-C(34)	136.6(2)
N(2)-Nd(2)-C(34)	111.7(2)
C(35)-Nd(2)-C(34)	29.4(2)
C(27)-Nd(2)-C(34)	75.8(3)
O(1)-Nd(2)-C(28)	84.4(2)
O(2)-Nd(2)-C(28)	125.5(2)
N(2)-Nd(2)-C(28)	125.6(2)
C(35)-Nd(2)-C(28)	97.5(3)
C(27)-Nd(2)-C(28)	29.4(2)
C(34)-Nd(2)-C(28)	97.3(3)
O(1)-Nd(2)-C(30)	110.5(2)
O(2)-Nd(2)-C(30)	99.3(2)

N(2)-Nd(2)-C(30)	77.4(2)
C(35)-Nd(2)-C(30)	136.1(3)
C(27)-Nd(2)-C(30)	48.2(2)
C(34)-Nd(2)-C(30)	116.6(3)
C(28)-Nd(2)-C(30)	48.3(3)
O(1)-Nd(2)-C(26)	131.0(2)
O(2)-Nd(2)-C(26)	124.8(2)
N(2)-Nd(2)-C(26)	86.5(2)
C(35)-Nd(2)-C(26)	109.4(3)
C(27)-Nd(2)-C(26)	29.6(2)
C(34)-Nd(2)-C(26)	87.1(2)
C(28)-Nd(2)-C(26)	49.0(2)
C(30)-Nd(2)-C(26)	29.5(2)
O(1)-Nd(2)-C(29)	83.8(2)
O(2)-Nd(2)-C(29)	100.1(2)
N(2)-Nd(2)-C(29)	100.3(2)
C(35)-Nd(2)-C(29)	126.1(3)
C(27)-Nd(2)-C(29)	47.8(3)
C(34)-Nd(2)-C(29)	123.2(3)
C(28)-Nd(2)-C(29)	28.8(2)
C(30)-Nd(2)-C(29)	29.3(2)
C(26)-Nd(2)-C(29)	48.6(2)
O(1)-Nd(2)-C(36)	78.8(2)
O(2)-Nd(2)-C(36)	95.3(2)
N(2)-Nd(2)-C(36)	109.5(2)
C(35)-Nd(2)-C(36)	29.7(2)
C(27)-Nd(2)-C(36)	117.9(3)
C(34)-Nd(2)-C(36)	48.7(2)
C(28)-Nd(2)-C(36)	123.9(3)
C(30)-Nd(2)-C(36)	164.9(3)
C(26)-Nd(2)-C(36)	135.7(2)
C(29)-Nd(2)-C(36)	149.8(3)
O(1)-Nd(2)-C(33)	126.9(2)
O(2)-Nd(2)-C(33)	110.9(2)
N(2)-Nd(2)-C(33)	84.3(2)
C(35)-Nd(2)-C(33)	48.2(2)
C(27)-Nd(2)-C(33)	96.9(3)
C(34)-Nd(2)-C(33)	29.2(2)
C(28)-Nd(2)-C(33)	123.3(3)
C(30)-Nd(2)-C(33)	121.8(2)
C(26)-Nd(2)-C(33)	95.6(2)
C(29)-Nd(2)-C(33)	142.8(3)
C(36)-Nd(2)-C(33)	48.1(2)
C(5)-C(1)-C(2)	106.9(6)

C(5)-C(1)-C(6)	127.2(7)
C(2)-C(1)-C(6)	125.9(7)
C(5)-C(1)-Nd(1)	73.6(4)
C(2)-C(1)-Nd(1)	75.6(4)
C(6)-C(1)-Nd(1)	117.5(5)
C(3)-C(2)-C(1)	107.5(7)
C(3)-C(2)-Nd(1)	74.3(4)
C(1)-C(2)-Nd(1)	75.0(4)
C(4)-C(3)-C(2)	109.6(7)
C(4)-C(3)-Nd(1)	73.6(5)
C(2)-C(3)-Nd(1)	76.7(4)
C(3)-C(4)-C(5)	107.7(7)
C(3)-C(4)-Nd(1)	77.4(5)
C(5)-C(4)-Nd(1)	76.1(5)
C(4)-C(5)-C(1)	108.3(7)
C(4)-C(5)-Nd(1)	74.0(5)
C(1)-C(5)-Nd(1)	76.9(4)
C(8)-C(7)-C(11)	107.6(8)
C(8)-C(7)-C(12)	131.4(10)
C(11)-C(7)-C(12)	120.9(10)
C(8)-C(7)-Nd(1)	75.4(5)
C(11)-C(7)-Nd(1)	73.9(5)
C(12)-C(7)-Nd(1)	119.2(7)
C(9)-C(8)-C(7)	107.4(8)
C(9)-C(8)-Nd(1)	74.9(5)
C(7)-C(8)-Nd(1)	75.3(5)
C(10)-C(9)-C(8)	108.1(8)
C(10)-C(9)-Nd(1)	74.3(6)
C(8)-C(9)-Nd(1)	75.9(5)
C(11)-C(10)-C(9)	109.5(9)
C(11)-C(10)-Nd(1)	75.8(6)
C(9)-C(10)-Nd(1)	76.8(6)
C(10)-C(11)-C(7)	107.4(8)
C(10)-C(11)-Nd(1)	75.1(6)
C(7)-C(11)-Nd(1)	76.5(5)
C(14)-C(13)-C(18)	119.2(6)
C(14)-C(13)-N(1)	121.9(6)
C(18)-C(13)-N(1)	118.8(6)
C(13)-C(14)-C(15)	121.0(7)
C(16)-C(15)-C(14)	119.1(8)
C(17)-C(16)-C(15)	120.6(8)
C(16)-C(17)-C(18)	120.3(7)
C(17)-C(18)-C(13)	119.8(7)
C(19)-N(1)-C(13)	124.0(6)

N(2)-Nd(2)-C(30)	77.4(2)
C(35)-Nd(2)-C(30)	136.1(3)
C(27)-Nd(2)-C(30)	48.2(2)
C(34)-Nd(2)-C(30)	116.6(3)
C(28)-Nd(2)-C(30)	48.3(3)
O(1)-Nd(2)-C(26)	131.0(2)
O(2)-Nd(2)-C(26)	124.8(2)
N(2)-Nd(2)-C(26)	86.5(2)
C(35)-Nd(2)-C(26)	109.4(3)
C(27)-Nd(2)-C(26)	29.6(2)
C(34)-Nd(2)-C(26)	87.1(2)
C(28)-Nd(2)-C(26)	49.0(2)
C(30)-Nd(2)-C(26)	29.5(2)
O(1)-Nd(2)-C(29)	83.8(2)
O(2)-Nd(2)-C(29)	100.1(2)
N(2)-Nd(2)-C(29)	100.3(2)
C(35)-Nd(2)-C(29)	126.1(3)
C(27)-Nd(2)-C(29)	47.8(3)
C(34)-Nd(2)-C(29)	123.2(3)
C(28)-Nd(2)-C(29)	28.8(2)
C(30)-Nd(2)-C(29)	29.3(2)
C(26)-Nd(2)-C(29)	48.6(2)
O(1)-Nd(2)-C(36)	78.8(2)
O(2)-Nd(2)-C(36)	95.3(2)
N(2)-Nd(2)-C(36)	109.5(2)
C(35)-Nd(2)-C(36)	29.7(2)
C(27)-Nd(2)-C(36)	117.9(3)
C(34)-Nd(2)-C(36)	48.7(2)
C(28)-Nd(2)-C(36)	123.9(3)
C(30)-Nd(2)-C(36)	164.9(3)
C(26)-Nd(2)-C(36)	135.7(2)
C(29)-Nd(2)-C(36)	149.8(3)
O(1)-Nd(2)-C(33)	126.9(2)
O(2)-Nd(2)-C(33)	110.9(2)
N(2)-Nd(2)-C(33)	84.3(2)
C(35)-Nd(2)-C(33)	48.2(2)
C(27)-Nd(2)-C(33)	96.9(3)
C(34)-Nd(2)-C(33)	29.2(2)
C(28)-Nd(2)-C(33)	123.3(3)
C(30)-Nd(2)-C(33)	121.8(2)
C(26)-Nd(2)-C(33)	95.6(2)
C(29)-Nd(2)-C(33)	142.8(3)
C(36)-Nd(2)-C(33)	48.1(2)
C(5)-C(1)-C(2)	106.9(6)

C(5)-C(1)-C(6)	127.2(7)
C(2)-C(1)-C(6)	125.9(7)
C(5)-C(1)-Nd(1)	73.6(4)
C(2)-C(1)-Nd(1)	75.6(4)
C(6)-C(1)-Nd(1)	117.5(5)
C(3)-C(2)-C(1)	107.5(7)
C(3)-C(2)-Nd(1)	74.3(4)
C(1)-C(2)-Nd(1)	75.0(4)
C(4)-C(3)-C(2)	109.6(7)
C(4)-C(3)-Nd(1)	73.6(5)
C(2)-C(3)-Nd(1)	76.7(4)
C(3)-C(4)-C(5)	107.7(7)
C(3)-C(4)-Nd(1)	77.4(5)
C(5)-C(4)-Nd(1)	76.1(5)
C(4)-C(5)-C(1)	108.3(7)
C(4)-C(5)-Nd(1)	74.0(5)
C(1)-C(5)-Nd(1)	76.9(4)
C(8)-C(7)-C(11)	107.6(8)
C(8)-C(7)-C(12)	131.4(10)
C(11)-C(7)-C(12)	120.9(10)
C(8)-C(7)-Nd(1)	75.4(5)
C(11)-C(7)-Nd(1)	73.9(5)
C(12)-C(7)-Nd(1)	119.2(7)
C(9)-C(8)-C(7)	107.4(8)
C(9)-C(8)-Nd(1)	74.9(5)
C(7)-C(8)-Nd(1)	75.3(5)
C(10)-C(9)-C(8)	108.1(8)
C(10)-C(9)-Nd(1)	74.3(6)
C(8)-C(9)-Nd(1)	75.9(5)
C(11)-C(10)-C(9)	109.5(9)
C(11)-C(10)-Nd(1)	75.8(6)
C(9)-C(10)-Nd(1)	76.8(6)
C(10)-C(11)-C(7)	107.4(8)
C(10)-C(11)-Nd(1)	75.1(6)
C(7)-C(11)-Nd(1)	76.5(5)
C(14)-C(13)-C(18)	119.2(6)
C(14)-C(13)-N(1)	121.9(6)
C(18)-C(13)-N(1)	118.8(6)
C(13)-C(14)-C(15)	121.0(7)
C(16)-C(15)-C(14)	119.1(8)
C(17)-C(16)-C(15)	120.6(8)
C(16)-C(17)-C(18)	120.3(7)
C(17)-C(18)-C(13)	119.8(7)
C(19)-N(1)-C(13)	124.0(6)

C(19)-N(1)-Nd(1)	94.7(4)
C(13)-N(1)-Nd(1)	138.2(4)
O(1)-C(19)-N(1)	118.1(6)
O(1)-C(19)-S(1)	114.9(5)
N(1)-C(19)-S(1)	127.0(5)
O(1)-C(19)-Nd(1)	58.9(3)
N(1)-C(19)-Nd(1)	59.3(4)
S(1)-C(19)-Nd(1)	173.6(3)
C(19)-O(1)-Nd(2)	149.8(4)
C(19)-O(1)-Nd(1)	95.5(4)
Nd(2)-O(1)-Nd(1)	114.02(18)
C(20)-S(1)-C(19)	103.8(3)
C(21)-C(20)-C(25)	119.4(7)
C(21)-C(20)-S(1)	121.2(6)
C(25)-C(20)-S(1)	119.2(6)
C(20)-C(21)-C(22)	120.2(7)
C(23)-C(22)-C(21)	118.7(7)
C(24)-C(23)-C(22)	121.9(8)
C(23)-C(24)-C(25)	118.8(8)
C(24)-C(25)-C(20)	120.9(8)
C(30)-C(26)-C(27)	105.5(7)
C(30)-C(26)-C(31)	126.3(8)
C(27)-C(26)-C(31)	128.2(8)
C(30)-C(26)-Nd(2)	74.6(4)
C(27)-C(26)-Nd(2)	74.0(5)
C(31)-C(26)-Nd(2)	118.3(5)
C(28)-C(27)-C(26)	109.5(7)
C(28)-C(27)-Nd(2)	75.4(5)
C(26)-C(27)-Nd(2)	76.4(5)
C(29)-C(28)-C(27)	107.8(7)
C(29)-C(28)-Nd(2)	76.9(5)
C(27)-C(28)-Nd(2)	75.2(5)
C(28)-C(29)-C(30)	108.5(8)
C(28)-C(29)-Nd(2)	74.3(5)
C(30)-C(29)-Nd(2)	74.5(5)
C(29)-C(30)-C(26)	108.8(8)
C(29)-C(30)-Nd(2)	76.2(5)
C(26)-C(30)-Nd(2)	75.9(5)
C(33)-C(32)-C(36)	106.3(7)
C(33)-C(32)-C(37)	127.7(8)
C(36)-C(32)-C(37)	125.9(8)
C(33)-C(32)-Nd(2)	73.9(4)
C(36)-C(32)-Nd(2)	73.5(5)
C(37)-C(32)-Nd(2)	119.7(6)

C(34)-C(33)-C(32)	109.4(7)
C(34)-C(33)-Nd(2)	73.5(4)
C(32)-C(33)-Nd(2)	76.9(4)
C(35)-C(34)-C(33)	108.1(7)
C(35)-C(34)-Nd(2)	75.3(5)
C(33)-C(34)-Nd(2)	77.3(4)
C(34)-C(35)-C(36)	108.3(7)
C(34)-C(35)-Nd(2)	75.3(5)
C(36)-C(35)-Nd(2)	76.7(5)
C(35)-C(36)-C(32)	107.9(7)
C(35)-C(36)-Nd(2)	73.6(5)
C(32)-C(36)-Nd(2)	77.0(5)
C(39)-C(38)-C(43)	120.2(6)
C(39)-C(38)-N(2)	118.4(6)
C(43)-C(38)-N(2)	121.1(6)
C(38)-C(39)-C(40)	119.1(7)
C(41)-C(40)-C(39)	120.6(7)
C(42)-C(41)-C(40)	120.7(8)
C(41)-C(42)-C(43)	119.7(8)
C(38)-C(43)-C(42)	119.8(7)
C(44)-N(2)-C(38)	124.6(6)
C(44)-N(2)-Nd(2)	95.0(4)
C(38)-N(2)-Nd(2)	137.9(4)
O(2)-C(44)-N(2)	117.6(6)
O(2)-C(44)-S(2)	114.2(5)
N(2)-C(44)-S(2)	128.2(5)
O(2)-C(44)-Nd(2)	58.3(3)
N(2)-C(44)-Nd(2)	59.3(4)
S(2)-C(44)-Nd(2)	172.5(4)
C(44)-O(2)-Nd(1)	150.1(4)
C(44)-O(2)-Nd(2)	96.2(4)
Nd(1)-O(2)-Nd(2)	113.07(18)
C(45)-S(2)-C(44)	106.5(3)
C(50)-C(45)-C(46)	121.1(8)
C(50)-C(45)-S(2)	118.6(6)
C(46)-C(45)-S(2)	120.0(6)
C(45)-C(46)-C(47)	117.3(8)
C(48)-C(47)-C(46)	122.4(9)
C(49)-C(48)-C(47)	118.6(10)
C(48)-C(49)-C(50)	120.3(10)
C(45)-C(50)-C(49)	120.2(9)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for complex **2**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Nd(1)	56(1)	66(1)	47(1)	5(1)	4(1)	0(1)
Nd(2)	57(1)	59(1)	47(1)	3(1)	3(1)	1(1)
C(1)	69(5)	70(5)	87(6)	20(4)	14(4)	6(4)
C(2)	94(6)	63(5)	85(6)	13(4)	9(5)	-7(4)
C(3)	74(5)	86(6)	94(7)	21(5)	1(4)	-6(4)
C(4)	76(5)	91(6)	96(7)	30(5)	22(4)	-2(4)
C(5)	91(6)	81(6)	64(5)	15(4)	9(4)	12(4)
C(6)	86(6)	121(8)	120(9)	31(7)	16(6)	16(6)
C(7)	117(7)	91(6)	81(6)	-21(5)	12(5)	-44(6)
C(8)	96(7)	124(9)	113(8)	-61(7)	14(6)	-10(6)
C(9)	127(9)	168(11)	81(7)	-53(7)	12(6)	-49(8)
C(10)	159(11)	138(11)	82(7)	-9(7)	-42(7)	-13(9)
C(11)	76(6)	112(8)	135(10)	-19(8)	-17(6)	-1(6)
C(12)	219(16)	168(15)	240(20)	-26(14)	-8(15)	-68(13)
C(13)	61(4)	63(4)	61(4)	10(3)	7(3)	3(3)
C(14)	73(5)	85(6)	67(5)	1(4)	15(4)	3(4)
C(15)	108(7)	97(7)	77(6)	7(5)	13(5)	24(5)
C(16)	93(6)	106(7)	93(7)	6(6)	24(5)	37(5)
C(17)	64(5)	121(8)	95(7)	19(6)	15(4)	14(5)
C(18)	59(4)	68(5)	86(6)	-2(4)	4(4)	-6(3)
N(1)	50(3)	75(4)	52(3)	4(3)	9(2)	-4(2)
C(19)	64(4)	64(4)	59(4)	7(3)	4(3)	-5(3)
O(1)	58(3)	83(4)	61(3)	11(3)	12(2)	16(2)
S(1)	65(1)	137(2)	59(1)	28(1)	11(1)	12(1)
C(20)	70(4)	73(5)	54(4)	8(3)	16(3)	5(4)
C(21)	80(5)	98(6)	68(5)	-9(5)	15(4)	-7(4)
C(22)	84(6)	124(8)	79(6)	1(6)	34(4)	13(5)
C(23)	84(6)	113(8)	92(7)	9(6)	2(5)	-17(5)
C(24)	134(8)	76(6)	100(7)	10(5)	13(6)	-11(6)
C(25)	104(6)	74(6)	85(6)	9(5)	31(5)	11(5)
C(26)	59(5)	73(5)	115(8)	17(5)	3(4)	3(4)
C(27)	135(8)	70(6)	74(6)	13(5)	16(5)	4(5)
C(28)	99(7)	73(6)	143(10)	18(6)	38(6)	-20(5)
C(29)	88(6)	74(6)	118(8)	4(6)	2(6)	-15(5)

C(30)	98(6)	53(5)	103(7)	10(4)	12(5)	-7(4)
C(31)	93(7)	92(7)	180(12)	45(7)	5(7)	16(5)
C(32)	73(5)	65(5)	91(6)	-15(4)	13(4)	-10(4)
C(33)	72(5)	82(6)	89(6)	-17(5)	-7(4)	-2(4)
C(34)	102(7)	91(7)	71(6)	-6(5)	-21(5)	7(5)
C(35)	96(7)	116(8)	71(6)	-28(5)	10(5)	-17(6)
C(36)	80(6)	92(7)	83(6)	-21(5)	5(4)	2(5)
C(37)	115(7)	86(7)	136(9)	2(7)	26(6)	-16(6)
C(38)	54(4)	63(4)	61(4)	2(3)	5(3)	9(3)
C(39)	64(5)	101(6)	72(5)	1(5)	5(4)	5(4)
C(40)	70(5)	130(9)	85(6)	-7(6)	12(4)	7(5)
C(41)	91(6)	107(7)	85(6)	3(6)	18(5)	32(5)
C(42)	114(7)	85(6)	76(6)	-7(5)	20(5)	23(5)
C(43)	83(5)	81(6)	62(5)	-10(4)	7(4)	7(4)
N(2)	54(3)	72(4)	56(3)	1(3)	9(2)	2(3)
C(44)	69(4)	71(5)	52(4)	1(3)	7(3)	-1(4)
O(2)	56(3)	93(4)	54(3)	13(3)	11(2)	18(2)
S(2)	67(1)	147(2)	57(1)	22(1)	13(1)	19(1)
C(45)	75(5)	92(6)	54(4)	17(4)	17(3)	15(4)
C(46)	93(6)	120(7)	60(5)	16(5)	27(4)	11(5)
C(47)	112(8)	149(11)	94(7)	35(7)	46(6)	32(7)
C(48)	95(8)	152(11)	156(11)	70(9)	36(7)	5(7)
C(49)	109(8)	120(9)	133(10)	34(8)	1(7)	-22(7)
C(50)	108(7)	89(7)	92(7)	24(5)	17(5)	19(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for complex **2**.

	x	y	z	U(eq)
H(2)	11455	1651	2433	97
H(3)	9719	1817	2676	103
H(4)	9666	2074	3958	104
H(5)	11386	2000	4554	94
H(6A)	13172	1622	3190	163
H(6B)	13094	1297	3962	163
H(6C)	13217	2171	3852	163
H(8)	10701	4901	3992	133
H(9)	10887	3875	4904	150
H(10)	12453	3220	4790	156
H(11)	13283	3824	3833	132
H(12A)	13025	4901	3011	316
H(12B)	12473	5578	3339	316
H(12C)	11918	5073	2737	316
H(14)	12173	2164	1276	89
H(15)	13521	1487	955	112
H(16)	15087	1801	1460	116
H(17)	15298	2705	2344	112
H(18)	13963	3414	2634	85
H(21)	13116	3214	198	98
H(22)	14747	3585	115	113
H(23)	15349	4639	728	116
H(24)	14361	5362	1375	124
H(25)	12735	5007	1430	103
H(27)	8573	5404	521	111
H(28)	10316	5365	1034	124
H(29)	10380	5674	2315	113
H(30)	8668	5820	2627	102
H(31A)	6852	5672	994	183
H(31B)	6969	6258	1627	183
H(31C)	6835	5394	1789	183
H(33)	6737	3620	1240	98
H(34)	7664	4167	301	108
H(35)	9244	3478	305	113
H(36)	9323	2507	1276	103
H(37A)	8163	2036	2195	167

H(37B)	7047	2113	1895	167
H(37C)	7517	2690	2470	167
H(39)	6080	4043	2466	95
H(40)	4725	4748	2747	113
H(41)	4924	5710	3565	113
H(42)	6458	5998	4119	109
H(43)	7831	5317	3836	90
H(46)	7055	4334	4981	107
H(47)	5421	4030	5145	139
H(48)	4678	2949	4657	159
H(49)	5532	2196	3923	146
H(50)	7155	2484	3750	115

Table 1. Crystal data and structure refinement for complex **3**.

Identification code	complex **3**
Empirical formula	$C_{29}H_{32}NNdOS_2$
Formula weight	618.92
Temperature	291(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 10.0310(10) Å alpha = 90° b = 23.988(3) Å beta = 95.570(10)° c = 11.685(2) Å gamma = 90°
Volume, Z	2798.4(7) $Å^3$, 4
Density (calculated)	1.469 Mg/m^3
Absorption coefficient	2.025 mm^{-1}
F(000)	1252
Crystal size	0.54 x 0.40 x 0.22 mm
θ range for data collection	1.70 to 24.99°
Limiting indices	$0 \le h \le 11$, $0 \le k \le 28$, $-13 \le l \le 13$
Reflections collected	5584
Independent reflections	4914 (R_{int} = 0.0209)
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.9793 and 0.7380
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4914 / 5 / 310
Goodness-of-fit on F^2	0.793
Final R indices [I>2σ(I)]	R1 = 0.0316, wR2 = 0.0553
R indices (all data)	R1 = 0.0684, wR2 = 0.0604
Extinction coefficient	0.00124(8)
Largest diff. peak and hole	0.509 and -0.475 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for **3** . U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Nd	8511(1)	1591(1)	2805(1)	46(1)
S(1)	7048(1)	560(1)	2484(1)	60(1)
S(2)	9007(1)	-410(1)	2423(1)	71(1)
O	6108(3)	1920(2)	2752(3)	71(1)
N	9656(4)	649(2)	2842(3)	52(1)
C(1)	8661(4)	313(2)	2607(4)	47(1)
C(2)	11011(4)	441(2)	3015(4)	48(1)
C(3)	11556(5)	311(2)	4091(4)	68(2)
C(4)	12873(5)	126(2)	4269(5)	81(2)
C(5)	13632(5)	79(2)	3379(6)	76(2)
C(6)	13092(6)	205(3)	2304(5)	83(2)
C(7)	11772(5)	383(2)	2115(5)	71(2)
C(8)	7407(5)	-704(2)	2099(5)	61(1)
C(9)	6728(7)	-658(3)	1028(5)	94(2)
C(10)	5424(8)	-902(3)	834(6)	109(3)
C(11)	4895(7)	-1173(3)	1676(7)	107(3)
C(12)	5563(6)	-1221(3)	2712(6)	94(2)
C(13)	6825(6)	-988(2)	2928(5)	74(2)
C(14)	7952(6)	1910(2)	543(4)	66(2)
C(15)	8542(6)	2368(2)	1120(4)	70(2)
C(16)	9887(6)	2245(2)	1412(4)	73(2)
C(17)	10123(5)	1711(2)	1032(4)	67(2)
C(18)	8923(5)	1498(2)	480(4)	58(1)
C(19)	8749(6)	953(2)	-142(4)	84(2)
C(20)	9687(9)	1498(3)	5009(5)	132(4)
C(21)	10369(7)	1885(4)	4513(7)	184(7)
C(22)	9667(12)	2352(4)	4311(8)	234(10)
C(23)	8499(9)	2242(3)	4724(6)	113(3)
C(24)	8501(8)	1726(3)	5149(5)	81(2)
C(25)	7420(12)	1466(5)	5712(8)	338(10)
C(26)	4949(7)	1615(3)	2792(8)	163(4)
C(27)	3822(7)	1979(4)	2928(9)	178(5)
C(28)	4337(9)	2523(4)	2974(7)	148(4)
C(29)	5678(7)	2489(3)	2599(6)	119(3)

Table 3. Bond lengths [Å] and angles [°] for complex **3**.

Nd-O	2.531(3)	Nd-N	2.534(4)
Nd-C(21)	2.689(7)	Nd-C(15)	2.713(5)
Nd-C(22)	2.716(9)	Nd-C(16)	2.730(5)
Nd-C(23)	2.734(7)	Nd-C(20)	2.736(6)
Nd-C(14)	2.757(4)	Nd-C(24)	2.759(5)
Nd-C(17)	2.764(5)	Nd-C(18)	2.796(4)
S(1)-C(1)	1.716(4)	S(2)-C(8)	1.760(5)
S(2)-C(1)	1.787(5)	O-C(26)	1.378(7)
O-C(29)	1.438(7)	N-C(1)	1.291(5)
N-C(2)	1.443(5)	C(2)-C(3)	1.358(6)
C(2)-C(7)	1.365(6)	C(3)-C(4)	1.390(6)
C(4)-C(5)	1.351(7)	C(5)-C(6)	1.354(7)
C(6)-C(7)	1.388(6)	C(8)-C(13)	1.361(7)
C(8)-C(9)	1.369(7)	C(9)-C(10)	1.430(8)
C(10)-C(11)	1.332(9)	C(11)-C(12)	1.330(8)
C(12)-C(13)	1.384(7)	C(14)-C(15)	1.390(7)
C(14)-C(18)	1.395(6)	C(15)-C(16)	1.390(7)
C(16)-C(17)	1.384(7)	C(17)-C(18)	1.405(6)
C(18)-C(19)	1.497(6)	C(20)-C(21)	1.321(5)
C(20)-C(24)	1.334(5)	C(21)-C(22)	1.332(6)
C(22)-C(23)	1.336(6)	C(23)-C(24)	1.333(5)
C(24)-C(25)	1.463(9)	C(26)-C(27)	1.448(9)
C(27)-C(28)	1.403(11)	C(28)-C(29)	1.458(9)

O-Nd-N	135.02(12)	O-Nd-C(21)	121.7(2)
N-Nd-C(21)	86.6(2)	O-Nd-C(15)	81.1(2)
N-Nd-C(15)	126.0(2)	C(21)-Nd-C(15)	107.6(2)
O-Nd-C(22)	98.7(3)	N-Nd-C(22)	115.1(2)
C(21)-Nd-C(22)	28.52(13)	C(15)-Nd-C(22)	88.5(2)
O-Nd-C(16)	110.0(2)	N-Nd-C(16)	105.6(2)
C(21)-Nd-C(16)	86.4(2)	C(15)-Nd-C(16)	29.60(14)
C(22)-Nd-C(16)	78.0(2)	O-Nd-C(23)	76.2(2)
N-Nd-C(23)	122.3(2)	C(21)-Nd-C(23)	45.5(3)
C(15)-Nd-C(23)	101.8(2)	C(22)-Nd-C(23)	28.38(12)
C(16)-Nd-C(23)	101.7(2)	O-Nd-C(20)	111.8(2)
N-Nd-C(20)	76.0(2)	C(21)-Nd-C(20)	28.16(12)
C(15)-Nd-C(20)	134.8(2)	C(22)-Nd-C(20)	47.7(2)
C(16)-Nd-C(20)	114.3(2)	C(23)-Nd-C(20)	46.4(2)
O-Nd-C(14)	77.60(14)	N-Nd-C(14)	108.31(14)
C(21)-Nd-C(14)	134.5(2)	C(15)-Nd-C(14)	29.42(14)
C(22)-Nd-C(14)	118.0(2)	C(16)-Nd-C(14)	48.4(2)
C(23)-Nd-C(14)	127.7(2)	C(20)-Nd-C(14)	162.6(2)
O-Nd-C(24)	83.8(2)	N-Nd-C(24)	97.6(2)
C(21)-Nd-C(24)	45.7(2)	C(15)-Nd-C(24)	129.9(2)
C(22)-Nd-C(24)	47.2(2)	C(16)-Nd-C(24)	125.1(2)
C(23)-Nd-C(24)	28.09(11)	C(20)-Nd-C(24)	28.09(11)
C(14)-Nd-C(24)	154.0(2)	O-Nd-C(17)	125.04(14)
N-Nd-C(17)	78.97(14)	C(21)-Nd-C(17)	96.6(2)
C(15)-Nd-C(17)	48.4(2)	C(22)-Nd-C(17)	99.9(3)
C(16)-Nd-C(17)	29.17(14)	C(23)-Nd-C(17)	127.2(2)
C(20)-Nd-C(17)	118.9(2)	C(14)-Nd-C(17)	48.1(2)
C(24)-Nd-C(17)	142.2(2)	O-Nd-C(18)	103.37(13)
N-Nd-C(18)	80.56(14)	C(21)-Nd-C(18)	125.8(2)
C(15)-Nd-C(18)	48.4(2)	C(22)-Nd-C(18)	126.1(2)
C(16)-Nd-C(18)	48.4(2)	C(23)-Nd-C(18)	148.8(2)
C(20)-Nd-C(18)	144.8(2)	C(14)-Nd-C(18)	29.10(13)
C(24)-Nd-C(18)	171.5(2)	C(17)-Nd-C(18)	29.28(14)

C(29)-O-Nd	124.9(4)	C(1)-N-C(2)	120.8(4)
C(1)-N-Nd	102.3(3)	C(2)-N-Nd	136.9(3)
N-C(1)-S(1)	120.4(4)	N-C(1)-S(2)	118.4(3)
S(1)-C(1)-S(2)	121.2(3)	N-C(1)-Nd	53.5(2)
S(1)-C(1)-Nd	67.0(2)	S(2)-C(1)-Nd	170.9(2)
C(3)-C(2)-C(7)	119.0(5)	C(3)-C(2)-N	119.9(4)
C(7)-C(2)-N	121.1(4)	C(2)-C(3)-C(4)	120.2(5)
C(5)-C(4)-C(3)	120.6(5)	C(4)-C(5)-C(6)	119.4(5)
C(5)-C(6)-C(7)	120.4(5)	C(2)-C(7)-C(6)	120.3(5)
C(13)-C(8)-C(9)	118.7(5)	C(13)-C(8)-S(2)	119.4(4)
C(9)-C(8)-S(2)	121.8(5)	C(8)-C(9)-C(10)	118.6(6)
C(11)-C(10)-C(9)	120.4(7)	C(12)-C(11)-C(10)	120.8(7)
C(11)-C(12)-C(13)	120.1(7)	C(8)-C(13)-C(12)	121.3(6)
C(15)-C(14)-C(18)	108.6(5)	C(15)-C(14)-Nd	73.5(3)
C(18)-C(14)-Nd	77.0(3)	C(14)-C(15)-C(16)	108.0(5)
C(14)-C(15)-Nd	77.0(3)	C(16)-C(15)-Nd	75.9(3)
C(17)-C(16)-C(15)	108.0(5)	C(17)-C(16)-Nd	76.8(3)
C(15)-C(16)-Nd	74.5(3)	C(16)-C(17)-C(18)	108.5(5)
C(16)-C(17)-Nd	74.1(3)	C(18)-C(17)-Nd	76.6(3)
C(14)-C(18)-C(17)	106.8(5)	C(14)-C(18)-C(19)	126.5(5)
C(17)-C(18)-C(19)	126.5(5)	C(14)-C(18)-Nd	73.9(3)
C(17)-C(18)-Nd	74.1(3)	C(19)-C(18)-Nd	121.4(3)
C(21)-C(20)-C(24)	105.7(6)	C(21)-C(20)-Nd	73.9(4)
C(24)-C(20)-Nd	76.9(3)	C(20)-C(21)-C(22)	112.4(8)
C(20)-C(21)-Nd	77.9(4)	C(22)-C(21)-Nd	76.9(6)
C(21)-C(22)-C(23)	103.7(8)	C(21)-C(22)-Nd	74.6(6)
C(23)-C(22)-Nd	76.5(5)	C(24)-C(23)-C(22)	110.3(7)
C(24)-C(23)-Nd	77.0(4)	C(22)-C(23)-Nd	75.1(6)
C(23)-C(24)-C(20)	107.8(6)	C(23)-C(24)-C(25)	126.1(10)
C(20)-C(24)-C(25)	126.1(10)	C(23)-C(24)-Nd	74.9(4)
C(20)-C(24)-Nd	75.0(3)	C(25)-C(24)-Nd	118.1(4)
O-C(26)-C(27)	110.8(7)	C(28)-C(27)-C(26)	106.1(8)
C(27)-C(28)-C(29)	106.4(7)	O-C(29)-C(28)	106.9(7)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for complex **3**.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + \ldots + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Nd	41(1)	50(1)	45(1)	-1(1)	-2(1)	-2(1)
S(1)	37(1)	58(1)	83(1)	-3(1)	1(1)	-2(1)
S(2)	53(1)	53(1)	106(1)	-10(1)	4(1)	2(1)
O	52(2)	68(3)	92(3)	-9(2)	6(2)	16(2)
N	39(2)	52(3)	62(3)	2(2)	-3(2)	-1(2)
C(1)	44(3)	51(3)	47(3)	2(2)	5(2)	2(3)
C(2)	36(3)	47(3)	58(3)	0(2)	-2(2)	-1(2)
C(3)	55(3)	86(4)	64(4)	4(3)	4(3)	16(3)
C(4)	61(4)	104(5)	75(4)	7(4)	-13(3)	18(4)
C(5)	36(3)	83(4)	107(5)	-2(4)	0(3)	9(3)
C(6)	58(4)	104(5)	88(4)	10(4)	20(3)	20(4)
C(7)	55(4)	89(4)	69(4)	6(3)	6(3)	15(3)
C(8)	63(4)	46(3)	73(4)	-8(3)	-1(3)	-4(3)
C(9)	108(5)	101(5)	70(4)	-7(4)	-2(4)	-14(4)
C(10)	118(7)	104(6)	96(6)	-22(5)	-43(5)	-6(5)
C(11)	93(6)	70(5)	149(7)	-21(5)	-34(6)	-15(4)
C(12)	71(5)	72(5)	139(7)	11(4)	9(4)	-8(4)
C(13)	68(4)	58(4)	92(4)	-4(3)	-9(3)	1(3)
C(14)	77(4)	75(4)	45(3)	12(3)	-3(3)	19(4)
C(15)	90(5)	56(4)	64(4)	10(3)	13(3)	1(4)
C(16)	70(4)	75(4)	73(4)	12(3)	4(3)	-21(4)
C(17)	56(3)	80(5)	66(3)	14(3)	15(3)	5(3)
C(18)	64(3)	68(4)	44(3)	2(3)	6(2)	9(3)
C(19)	98(5)	97(5)	56(3)	-16(3)	7(3)	16(4)
C(20)	177(8)	134(8)	71(5)	-46(5)	-59(5)	105(7)
C(21)	78(5)	405(20)	70(6)	-73(9)	14(4)	-133(9)
C(22)	509(27)	132(9)	47(5)	4(6)	-54(10)	-202(13)
C(23)	171(9)	79(6)	79(6)	-35(5)	-38(5)	44(6)
C(24)	120(6)	78(5)	46(3)	-17(3)	16(4)	-43(4)
C(25)	406(18)	486(22)	146(9)	-147(11)	155(11)	-333(17)
C(26)	58(4)	138(7)	293(12)	-42(8)	16(6)	9(6)
C(27)	60(6)	192(10)	280(13)	-85(10)	3(6)	32(7)
C(28)	157(9)	195(10)	99(6)	19(6)	48(6)	115(8)
C(29)	111(6)	125(7)	122(6)	3(5)	9(5)	56(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for complex **3**.

	x	y	z	U(eq)
H(3)	11046(5)	345(2)	4711(4)	82
H(4)	13236(5)	35(2)	5008(5)	97
H(5)	14517(5)	-40(2)	3505(6)	91
H(6)	13608(6)	172(3)	1688(5)	99
H(7)	11404(5)	463(2)	1371(5)	85
H(9)	7106(7)	-473(3)	440(5)	113
H(10)	4943(8)	-871(3)	116(6)	131
H(11)	4047(7)	-1330(3)	1539(7)	128
H(12)	5182(6)	-1412(3)	3292(6)	113
H(13)	7285(6)	-1026(2)	3654(5)	89
H(14)	7059(6)	1884(2)	248(4)	79
H(15)	8112(6)	2698(2)	1282(4)	84
H(16)	10517(6)	2481(2)	1795(4)	87
H(17)	10939(5)	1524(2)	1127(4)	80
H(19A)	8736(32)	1016(3)	-955(5)	101
H(19B)	7919(16)	785(6)	20(21)	101
H(19C)	9478(17)	710(5)	108(20)	101
H(20)	9975(9)	1140(3)	5218(5)	158
H(21)	11242(7)	1837(4)	4325(7)	220
H(22)	9928(12)	2678(4)	3964(8)	281
H(23)	7785(9)	2490(3)	4716(6)	135
H(25A)	6611(30)	1471(47)	5200(42)	405
H(25B)	7283(87)	1668(32)	6400(59)	405
H(25C)	7655(53)	1087(17)	5904(96)	405
H(26A)	5059(7)	1356(3)	3431(8)	196
H(26B)	4776(7)	1402(3)	2089(8)	196
H(27A)	3144(7)	1938(4)	2283(9)	214
H(27B)	3425(7)	1890(4)	3631(9)	214
H(28A)	4374(9)	2668(4)	3752(7)	178
H(28B)	3776(9)	2767(4)	2471(7)	178
H(29A)	5664(7)	2596(3)	1797(6)	143
H(29B)	6284(7)	2736(3)	3054(6)	143