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Supplemental Information

Thiocyanate complexes of the lanthanides, Am and Cm.

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Experimental Details

Caution! ^{243}Am and ^{248}Cm and their associated decay daughters are α,β,γ-emitting radionuclides. ^{248}Cm decays by spontaneous fission and is a neutron emitter. All experiments described here were performed in a laboratory specially designed for the handling of radionuclides including radiological fume hoods and gloveboxes under the supervision of health physics personnel.

General Methods. All chemicals and solvents, unless otherwise noted, were obtained from commercial sources and used as received. $[Et_4N][NCS]$ was prepared by combining ethanolic solutions of commercially available KNCS and $[Et_4N]Cl$ (in a 1:1 ratio) and removing the resulting KCl precipitate by filtration. The solution was then evaporated to dryness using a rotary evaporator to give $[Et_4N][NCS]$ as a white powder which was used for use in synthesis and spectroscopic studies.

^{243}Am Stock Solution: Americium in acidic solution was converted to nitrate form by adding 15 M HNO_3 and evaporating to near dryness twice. The residue was then dissolved in 2 M HNO_3 (30 ml) and 1 ml ascorbic acid was added. The solution was loaded onto a 10 ml bed volume of TRU resin which had been conditioned with HNO_3. Once loaded on the column the Am was rinsed with 30 ml of a 2 M HNO_3/0.3 M ascorbic acid solution. Followed by 70 ml of 2 M HNO_3. 11 ml of 9 M HCl was then used to convert the column to Cl^- form, and the Am eluted with 4 M HCl. The HCl solution containing the Am was then passed through a column containing Amberlyte XAD-7 resin and filtered through a 0.45 μm syringe filter. The solution was then evaporated to near dryness, and converted to the nitrate form by dissolving in nitric acid and evaporating to near dryness twice. The residue was dissolved in 2 M HNO_3 and

precipitated using 50% NaOH solution (wt/wt). The resulting precipitate was then washed 3 times with 3 ml of water and dissolved in 3 M HOTf. The HOTf solution was allowed to evaporate until crystals of $[Am(H_2O)_9][OTf]_3$ had formed. The crystals were removed from the supernatant and allowed to dry for 6 h before being dissolved in MeOH. The solution concentration was then determined by scintillation counting.

^{248}Cm Stock Solution: The ^{248}Cm was first precipitated from a 0.1 M $HClO_4$ solution by the addition of aqueous sodium hydroxide. The precipitate was washed three times with dionized water and redissolved in 3 M HOTf. The HOTf solution was allowed to evaporate until crystals of $[Cm(H_2O)_9][OTf]_3$ had formed. The crystals were removed from the supernatant and allowed to dry for 6 hours before being dissolved in MeOH. The solution concentration was determined by scintillation counting.

Synthesis of $[An(NCS)_7(H_2O)][Et_4N]_4$ An: Am, Cm: 150 µl of a 10 mM stock solution of $[An(H_2O)_9][OTf]_3$ in MeOH was combined with 500 µl (125 eq.) of a 0.38 M stock solution of $[Et_4N][NCS]$ in MeOH and diluted with 300 µl of additional MeOH. This solution was placed in a 5 ml shell vial, which was lowered into a 20 ml scintillation vial with 10 ml diethyl ether. The larger vial was capped and allowed to stand at room temperature until pink crystals of Am-NCS or yellow crystals of Cm-NCS had formed.

Synthesis of $[Ln(NCS)_7(H_2O)][Et_4N]_4$ (Ln-NCS, Ln = La-Nd, Sm-Lu): The Ln-NCS compounds were all prepared in the same manner. In each case, crystalline $[Ln(H_2O)_n]Cl_3$ (n = 7 for La-Pr and n = 6 for Nd-Lu) was dissolved in methanol at a concentration of 0.3 M. To 50 µl (15 mmol Ln^{III}) of this solution was added 400 µl (150 mmol, 10 eq.) of a 0.38 M solution of $[Et_4N][NCS]$ dissolved in methanol. The resulting mixture was then diluted with 1 ml additional

methanol. The sample was covered loosely with parafilm and left in a Drierite® desiccator until evaporation was complete. The resulting crystalline blocks obtained at this stage were suitable for X-ray diffraction and collection of Raman spectroscopy data. However, the product can be obtained free of additional salts by washing 2 x 1 ml with dichloromethane and allowing to dry for 2 h. The remaining solid is then dissolved in 1 ml methanol and allowed to crystallize open to the air until almost dry.

Previously reported diffraction data for La/Pr-NCS were solved in the space group Pm-3.[1] The structures we obtained, however, contained the additional symmetry elements of the space group Pm-3m. Additionally, structural data for Nd/Dy/Er-NCS were included in the same report and solved in I4/m. The structures we obtained, however, contained the additional symmetry elements of the space group I4/mmm. For this reason, we elected to resolve these structures in the correct space groups.

Single Crystal X-ray Diffraction. Crystals were mounted on glass fibers using a heavy oil. Full spheres of data were collected at 100 K on a Bruker Apex II diffractometer using Mo Kα radiation. The data were corrected for absorption using SADABS, Structure refinement was carried out using SHELXL software.[2, 3] Both the cubic and tetragonal structures contained Et_4N^+ cations in which the carbon atoms were disordered about special positions. As all unique orientations of these carbon atoms were crystallographically equivalent, the occupancy was fixed such that each unique atom had a total occupancy of one. We previously reported a coordinated water molecule disordered over all eight ligand sites at the metal center for the Ce compound, as supported by IR data and the thiocyanate ligands and coordinated water molecule were allowed to freely refine resulting in net occupancies near 7/8 and 1/8 respectively.[4] However, the difference maps did not support the inclusion of the water molecule in the data here, and we

instead refined the structures using only a 7/8 occupied thiocyanate. The inclusion of the water molecule would there for have been arbitrary. Hydrogen atoms could not be located in the difference map, and a suitable combination of constraints could not be identified to assign hydrogen atoms in riding positions at the disordered cations. Hydrogen atoms were therefore omitted from the structure refinements.

Raman Spectroscopy. Raman spectra of the Ln-NCS compounds were collected on randomly oriented single crystals utilizing a Renishaw inVia Raman microscope using circularly polarized light from a 532 or 785 nm diode laser. Spectra of Am-NCS were collected using a 442 nm diode laser, and the Cm data were collected using 532 nm radiation. Single crystals were spread on a glass slide, and several crystals were examined to ensure sample homogeneity. Radioactive samples were mounted on a glass drop-slide and covered with a glass coverslip affixed with epoxy. Data were collected from 100 to 4000 cm^{-1}. Representative full spectra of La-NCS and Lu-NCS as well as the low frequency and C=N stretching region for all reported compounds are shown in the supporting information.

FT-IR Spectroscopy. IR spectra were collected on a Nicolet Nexus 870 FTIR spectrometer. Samples were ground with KBr and pressed into pellets. Data were collected using 32 scans over 4000-400 cm^{-1} with a resolution of 2 cm^{-1}.

Electron Microscopy: Single crystals were mounted on carbon tape for analysis. A JEOL JSM-6010LA scanning electron microscope was used at beam voltage of 5kV and 20 kV to reveal the L-emission lines in the lighter lanthanides La-Sm. EDS spectra were collected using an acquisition time of 120 seconds.

Table 1. Crystal data and structure refinement for LaSCN.

Identification code	pm3m	
Empirical formula	C39 H0 La N11 O0 S7	
Formula weight	985.83	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Cubic	
Space group	Pm-3m	
Unit cell dimensions	a = 11.4263(5) Å	α= 90°.
	b = 11.4263(5) Å	β= 90°.
	c = 11.4263(5) Å	γ = 90°.
Volume	1491.8(2) $Å^3$	
Z	1	
Density (calculated)	1.097 Mg/m^3	
Absorption coefficient	0.991 mm^{-1}	
F(000)	480	
Crystal size	0.650 x 0.362 x 0.128 mm^3	
Theta range for data collection	1.782 to 33.080°.	
Index ranges	-16<=h<=16, -17<=k<=17, -17<=l<=17	
Reflections collected	25943	
Independent reflections	625 [R(int) = 0.0454]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.4351 and 0.3127	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	625 / 1 / 29	
Goodness-of-fit on F^2	1.148	
Final R indices [I>2sigma(I)]	R1 = 0.0533, wR2 = 0.1469	
R indices (all data)	R1 = 0.0533, wR2 = 0.1469	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.140 and -2.261 $e.Å^{-3}$	

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

	x	y	z	U(eq)
La(1)	0	0	0	21(1)
N(2)	0	0	5000	199(18)
C(2)	0	1080(30)	4161(11)	181(14)
N(3)	5000	5000	5000	34(2)
C(3)	0	2300(20)	5000	157(5)
C(4)	4066(14)	4066(14)	5000	78(5)
C(5)	3001(11)	5000	5000	78(5)
S(1)	2634(2)	2634(2)	2634(2)	106(2)
C(1)	1848(5)	1848(5)	1848(5)	70(3)
N(1)	1274(5)	1274(5)	1274(5)	89(4)

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

La(1)-N(1)#1	2.520(9)
La(1)-N(1)#2	2.520(9)
La(1)-N(1)#3	2.520(9)
La(1)-N(1)#4	2.520(9)
La(1)-N(1)#5	2.520(9)
La(1)-N(1)#6	2.520(9)
La(1)-N(1)#7	2.520(9)
La(1)-N(1)	2.521(9)
N(2)-C(2)#8	1.57(2)
N(2)-C(2)#9	1.57(2)
N(2)-C(2)#10	1.57(2)
N(2)-C(2)#6	1.57(2)
N(2)-C(2)#11	1.57(2)
N(2)-C(2)#12	1.57(2)
N(2)-C(2)#13	1.57(2)
N(2)-C(2)	1.57(2)
C(2)-C(2)#8	1.75(4)
C(2)-C(2)#11	1.75(4)
C(2)-C(3)	1.69(3)
C(2)-C(2)#10	1.92(3)
N(3)-C(4)	1.51(2)
N(3)-C(4)#14	1.51(2)
N(3)-C(4)#15	1.51(2)
N(3)-C(4)#16	1.51(2)
N(3)-C(4)#17	1.51(2)
N(3)-C(4)#18	1.51(2)
N(3)-C(4)#19	1.51(2)
N(3)-C(4)#20	1.51(2)
N(3)-C(4)#21	1.51(2)
N(3)-C(4)#22	1.51(2)
N(3)-C(4)#23	1.51(2)
N(3)-C(4)#24	1.51(2)
C(3)-C(2)#10	1.69(3)
C(4)-C(4)#24	1.51(2)

C(4)-C(4)#21	1.51(2)
C(4)-C(4)#16	1.51(2)
C(4)-C(4)#18	1.51(2)
C(4)-C(5)	1.618(9)
C(4)-C(5)#18	1.618(9)
C(5)-C(4)#24	1.618(9)
C(5)-C(4)#22	1.618(9)
C(5)-C(4)#16	1.618(9)
S(1)-C(1)	1.555(10)
C(1)-N(1)	1.137(12)

N(1)#1-La(1)-N(1)#2	109.471(1)
N(1)#1-La(1)-N(1)#3	70.529(1)
N(1)#2-La(1)-N(1)#3	180.0(2)
N(1)#1-La(1)-N(1)#4	109.5
N(1)#2-La(1)-N(1)#4	109.5
N(1)#3-La(1)-N(1)#4	70.5
N(1)#1-La(1)-N(1)#5	70.5
N(1)#2-La(1)-N(1)#5	70.5
N(1)#3-La(1)-N(1)#5	109.5
N(1)#4-La(1)-N(1)#5	180.0(2)
N(1)#1-La(1)-N(1)#6	70.5
N(1)#2-La(1)-N(1)#6	70.5
N(1)#3-La(1)-N(1)#6	109.5
N(1)#4-La(1)-N(1)#6	70.5
N(1)#5-La(1)-N(1)#6	109.5
N(1)#1-La(1)-N(1)#7	109.5
N(1)#2-La(1)-N(1)#7	109.5
N(1)#3-La(1)-N(1)#7	70.5
N(1)#4-La(1)-N(1)#7	109.5
N(1)#5-La(1)-N(1)#7	70.5
N(1)#6-La(1)-N(1)#7	180.0(4)
N(1)#1-La(1)-N(1)	180.0(6)
N(1)#2-La(1)-N(1)	70.529(1)
N(1)#3-La(1)-N(1)	109.5
N(1)#4-La(1)-N(1)	70.5

N(1)#5-La(1)-N(1)	109.5
N(1)#6-La(1)-N(1)	109.5
N(1)#7-La(1)-N(1)	70.5
C(2)#8-N(2)-C(2)#9	180.0(7)
C(2)#8-N(2)-C(2)#10	112.0(9)
C(2)#9-N(2)-C(2)#10	68.0(9)
C(2)#8-N(2)-C(2)#6	68.0(9)
C(2)#9-N(2)-C(2)#6	112.0(9)
C(2)#10-N(2)-C(2)#6	180.0
C(2)#8-N(2)-C(2)#11	104.5(17)
C(2)#9-N(2)-C(2)#11	75.5(17)
C(2)#10-N(2)-C(2)#11	112.0(9)
C(2)#6-N(2)-C(2)#11	68.0(9)
C(2)#8-N(2)-C(2)#12	112.0(9)
C(2)#9-N(2)-C(2)#12	68.0(9)
C(2)#10-N(2)-C(2)#12	104.5(17)
C(2)#6-N(2)-C(2)#12	75.5(17)
C(2)#11-N(2)-C(2)#12	112.0(9)
C(2)#8-N(2)-C(2)#13	75.5(17)
C(2)#9-N(2)-C(2)#13	104.5(17)
C(2)#10-N(2)-C(2)#13	68.0(9)
C(2)#6-N(2)-C(2)#13	112.0(9)
C(2)#11-N(2)-C(2)#13	180.0
C(2)#12-N(2)-C(2)#13	68.0(9)
C(2)#8-N(2)-C(2)	68.0(9)
C(2)#9-N(2)-C(2)	112.0(9)
C(2)#10-N(2)-C(2)	75.5(17)
C(2)#6-N(2)-C(2)	104.5(17)
C(2)#11-N(2)-C(2)	68.0(9)
C(2)#12-N(2)-C(2)	180.0
C(2)#13-N(2)-C(2)	112.0(9)
N(2)-C(2)-C(2)#8	56.0(4)
N(2)-C(2)-C(2)#11	56.0(4)
C(2)#8-C(2)-C(2)#11	90.000(1)
N(2)-C(2)-C(3)	107.7(10)
C(2)#8-C(2)-C(3)	125.7(3)

C(2)#11-C(2)-C(3)	125.7(3)
N(2)-C(2)-C(2)#10	52.2(9)
C(2)#8-C(2)-C(2)#10	89.999(1)
C(2)#11-C(2)-C(2)#10	89.999(1)
C(3)-C(2)-C(2)#10	55.5(6)
C(4)-N(3)-C(4)#14	120.0
C(4)-N(3)-C(4)#15	180.0
C(4)#14-N(3)-C(4)#15	60.000(1)
C(4)-N(3)-C(4)#16	60.000(1)
C(4)#14-N(3)-C(4)#16	180.0
C(4)#15-N(3)-C(4)#16	120.0
C(4)-N(3)-C(4)#17	120.000(1)
C(4)#14-N(3)-C(4)#17	60.0
C(4)#15-N(3)-C(4)#17	60.0
C(4)#16-N(3)-C(4)#17	120.0
C(4)-N(3)-C(4)#18	60.000(1)
C(4)#14-N(3)-C(4)#18	120.000(1)
C(4)#15-N(3)-C(4)#18	120.000(1)
C(4)#16-N(3)-C(4)#18	60.000(1)
C(4)#17-N(3)-C(4)#18	180.0
C(4)-N(3)-C(4)#19	120.0
C(4)#14-N(3)-C(4)#19	90.000(2)
C(4)#15-N(3)-C(4)#19	60.000(1)
C(4)#16-N(3)-C(4)#19	90.000(1)
C(4)#17-N(3)-C(4)#19	120.000(1)
C(4)#18-N(3)-C(4)#19	60.000(1)
C(4)-N(3)-C(4)#20	120.000(1)
C(4)#14-N(3)-C(4)#20	120.000(1)
C(4)#15-N(3)-C(4)#20	60.0
C(4)#16-N(3)-C(4)#20	60.0
C(4)#17-N(3)-C(4)#20	90.000(3)
C(4)#18-N(3)-C(4)#20	90.000(1)
C(4)#19-N(3)-C(4)#20	60.0
C(4)-N(3)-C(4)#21	60.0
C(4)#14-N(3)-C(4)#21	60.0
C(4)#15-N(3)-C(4)#21	120.000(1)

C(4)#16-N(3)-C(4)#21	120.000(1)
C(4)#17-N(3)-C(4)#21	90.000(1)
C(4)#18-N(3)-C(4)#21	90.000(3)
C(4)#19-N(3)-C(4)#21	120.000(1)
C(4)#20-N(3)-C(4)#21	180.0
C(4)-N(3)-C(4)#22	90.000(2)
C(4)#14-N(3)-C(4)#22	120.000(1)
C(4)#15-N(3)-C(4)#22	90.0
C(4)#16-N(3)-C(4)#22	60.000(1)
C(4)#17-N(3)-C(4)#22	60.000(1)
C(4)#18-N(3)-C(4)#22	120.000(1)
C(4)#19-N(3)-C(4)#22	120.000(1)
C(4)#20-N(3)-C(4)#22	60.000(1)
C(4)#21-N(3)-C(4)#22	120.000(1)
C(4)-N(3)-C(4)#23	90.0
C(4)#14-N(3)-C(4)#23	60.0
C(4)#15-N(3)-C(4)#23	90.000(2)
C(4)#16-N(3)-C(4)#23	120.000(1)
C(4)#17-N(3)-C(4)#23	120.000(1)
C(4)#18-N(3)-C(4)#23	60.0
C(4)#19-N(3)-C(4)#23	60.0
C(4)#20-N(3)-C(4)#23	120.000(1)
C(4)#21-N(3)-C(4)#23	60.0
C(4)#22-N(3)-C(4)#23	180.0
C(4)-N(3)-C(4)#24	60.000(1)
C(4)#14-N(3)-C(4)#24	90.000(1)
C(4)#15-N(3)-C(4)#24	120.0
C(4)#16-N(3)-C(4)#24	90.000(2)
C(4)#17-N(3)-C(4)#24	60.000(1)
C(4)#18-N(3)-C(4)#24	120.000(1)
C(4)#19-N(3)-C(4)#24	180.0
C(4)#20-N(3)-C(4)#24	120.000(1)
C(4)#21-N(3)-C(4)#24	60.000(1)
C(4)#22-N(3)-C(4)#24	60.000(1)
C(4)#23-N(3)-C(4)#24	120.000(1)
C(2)#10-C(3)-C(2)	69.0(13)

N(3)-C(4)-C(4)#24	60.000(3)
N(3)-C(4)-C(4)#21	60.000(3)
C(4)#24-C(4)-C(4)#21	60.000(1)
N(3)-C(4)-C(4)#16	60.000(3)
C(4)#24-C(4)-C(4)#16	90.000(6)
C(4)#21-C(4)-C(4)#16	120.000(12)
N(3)-C(4)-C(4)#18	60.000(4)
C(4)#24-C(4)-C(4)#18	120.000(12)
C(4)#21-C(4)-C(4)#18	90.000(9)
C(4)#16-C(4)-C(4)#18	60.000(1)
N(3)-C(4)-C(5)	93.8(8)
C(4)#24-C(4)-C(5)	62.2(5)
C(4)#21-C(4)-C(5)	122.1(4)
C(4)#16-C(4)-C(5)	62.2(5)
C(4)#18-C(4)-C(5)	122.1(4)
N(3)-C(4)-C(5)#18	93.8(8)
C(4)#24-C(4)-C(5)#18	122.1(4)
C(4)#21-C(4)-C(5)#18	62.2(5)
C(4)#16-C(4)-C(5)#18	122.1(4)
C(4)#18-C(4)-C(5)#18	62.2(5)
C(5)-C(4)-C(5)#18	172.5(16)
C(4)#24-C(5)-C(4)#22	55.6(10)
C(4)#24-C(5)-C(4)#16	82.5(16)
C(4)#22-C(5)-C(4)#16	55.6(10)
C(4)#24-C(5)-C(4)	55.6(10)
C(4)#22-C(5)-C(4)	82.5(16)
C(4)#16-C(5)-C(4)	55.6(10)
N(1)-C(1)-S(1)	180.0(12)
C(1)-N(1)-La(1)	180.0(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -x,y,z #3 x,-y,-z #4 x,-y,z

#5 -x,y,-z #6 -x,-y,z #7 x,y,-z #8 -y,-x,z

#9 y,x,-z+1 #10 x,y,-z+1 #11 y,x,z #12 -x,-y,-z+1

#13 -y,-x,-z+1 #14 -y+1,-z+1,-x+1 #15 -x+1,-y+1,-z+1

#16 y,z,x #17 -z+1,-x+1,-y+1 #18 z,x,y #19 -y+1,z,x

#20 -z+1,-x+1,y #21 z,x,-y+1 #22 x,-y+1,z

#23 -x+1,y,-z+1 #24 y,-z+1,-x+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for LaSCN. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
La(1)	21(1)	21(1)	21(1)	0	0	0
N(2)	280(30)	280(30)	38(9)	0	0	0
C(2)	190(30)	290(30)	64(9)	79(16)	0	0
N(3)	34(2)	34(2)	34(2)	0	0	0
C(3)	168(17)	168(18)	135(14)	0	0	0
C(4)	95(8)	95(8)	43(7)	0	0	-23(15)
C(5)	95(8)	95(8)	43(7)	0	0	-23(15)
S(1)	106(2)	106(2)	106(2)	-36(1)	-36(1)	-36(1)
C(1)	70(3)	70(3)	70(3)	-18(2)	-18(2)	-18(2)
N(1)	89(4)	89(4)	89(4)	-27(3)	-27(3)	-27(3)

Table 5. Crystal data and structure refinement for CeSCN.

Identification code	pm3m	
Empirical formula	C39 H0 Ce N11 O0 S7	
Formula weight	987.04	
Temperature	173 K	
Wavelength	0.71073 Å	
Crystal system	Cubic	
Space group	Pm-3m	
Unit cell dimensions	a = 11.3981(7) Å	α= 90°.
	b = 11.3981(7) Å	β= 90°.
	c = 11.3981(7) Å	γ = 90°.
Volume	1480.8(3) $Å^3$	
Z	1	
Density (calculated)	1.107 Mg/m^3	
Absorption coefficient	1.046 mm^{-1}	
F(000)	481	
Crystal size	0.206 x 0.152 x 0.094 mm^3	
Theta range for data collection	1.787 to 30.563°.	
Index ranges	-16<=h<=16, -15<=k<=15, -16<=l<=15	
Reflections collected	21416	
Independent reflections	512 [R(int) = 0.0226]	
Completeness to theta = 25.242°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	512 / 1 / 27	
Goodness-of-fit on F^2	1.076	
Final R indices [I>2sigma(I)]	R1 = 0.0560, wR2 = 0.1590	
R indices (all data)	R1 = 0.0560, wR2 = 0.1590	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.183 and -1.901 $e.Å^{-3}$	

Table 6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for CeSCN. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ce(1)	0	0	0	22(1)
N(2)	0	0	5000	156(15)
C(2)	0	1060(30)	4155(17)	173(9)
N(3)	5000	5000	5000	36(4)
C(3)	0	2290(30)	5000	173(9)
C(4)	4070(20)	4070(20)	5000	88(6)
C(5)	3026(11)	5000	5000	88(6)
S(1)	2630(2)	2630(2)	2630(2)	113(2)
C(1)	1838(6)	1838(6)	1838(6)	75(4)
N(1)	1265(6)	1265(6)	1265(6)	96(5)

Table 7. Bond lengths [Å] and angles [°] for CeSCN.

Ce(1)-N(1)	2.497(12)
Ce(1)-N(1)#1	2.497(12)
Ce(1)-N(1)#2	2.497(12)
Ce(1)-N(1)#3	2.497(12)
Ce(1)-N(1)#4	2.497(12)
Ce(1)-N(1)#5	2.497(12)
Ce(1)-N(1)#6	2.497(12)
Ce(1)-N(1)#7	2.497(12)
N(2)-C(2)#8	1.55(2)
N(2)-C(2)#9	1.55(2)
N(2)-C(2)#10	1.55(2)
N(2)-C(2)#3	1.55(2)
N(2)-C(2)#11	1.55(2)
N(2)-C(2)#12	1.55(2)
N(2)-C(2)#13	1.55(2)
N(2)-C(2)	1.55(2)
C(2)-C(3)	1.70(3)
C(2)-C(2)#8	1.71(5)
C(2)-C(2)#11	1.71(5)
C(2)-C(2)#10	1.93(4)
N(3)-C(4)	1.51(3)
N(3)-C(4)#14	1.51(3)
N(3)-C(4)#15	1.51(3)
N(3)-C(4)#16	1.51(3)
N(3)-C(4)#17	1.51(3)
N(3)-C(4)#18	1.51(3)
N(3)-C(4)#19	1.51(3)
N(3)-C(4)#20	1.51(3)
N(3)-C(4)#21	1.51(3)
N(3)-C(4)#22	1.51(3)
N(3)-C(4)#23	1.51(3)
N(3)-C(4)#24	1.51(3)
C(3)-C(2)#10	1.70(3)
C(4)-C(4)#24	1.51(3)

C(4)-C(4)#21	1.51(3)
C(4)-C(4)#16	1.51(3)
C(4)-C(4)#18	1.51(3)
C(4)-C(5)#18	1.593(10)
C(4)-C(5)	1.593(10)
C(5)-C(4)#24	1.593(10)
C(5)-C(4)#22	1.593(10)
C(5)-C(4)#16	1.593(10)
S(1)-C(1)	1.564(13)
C(1)-N(1)	1.131(16)

N(1)-Ce(1)-N(1)#1	180.0(3)
N(1)-Ce(1)-N(1)#2	70.5
N(1)#1-Ce(1)-N(1)#2	109.5
N(1)-Ce(1)-N(1)#3	109.5
N(1)#1-Ce(1)-N(1)#3	70.5
N(1)#2-Ce(1)-N(1)#3	180.0(3)
N(1)-Ce(1)-N(1)#4	70.529(1)
N(1)#1-Ce(1)-N(1)#4	109.5
N(1)#2-Ce(1)-N(1)#4	109.5
N(1)#3-Ce(1)-N(1)#4	70.5
N(1)-Ce(1)-N(1)#5	109.5
N(1)#1-Ce(1)-N(1)#5	70.5
N(1)#2-Ce(1)-N(1)#5	70.5
N(1)#3-Ce(1)-N(1)#5	109.5
N(1)#4-Ce(1)-N(1)#5	70.5
N(1)-Ce(1)-N(1)#6	70.5
N(1)#1-Ce(1)-N(1)#6	109.5
N(1)#2-Ce(1)-N(1)#6	109.5
N(1)#3-Ce(1)-N(1)#6	70.5
N(1)#4-Ce(1)-N(1)#6	109.5
N(1)#5-Ce(1)-N(1)#6	180.0(3)
N(1)-Ce(1)-N(1)#7	109.5
N(1)#1-Ce(1)-N(1)#7	70.529(1)
N(1)#2-Ce(1)-N(1)#7	70.5
N(1)#3-Ce(1)-N(1)#7	109.5

N(1)#4-Ce(1)-N(1)#7	180.0
N(1)#5-Ce(1)-N(1)#7	109.5
N(1)#6-Ce(1)-N(1)#7	70.5
C(2)#8-N(2)-C(2)#9	180.0(12)
C(2)#8-N(2)-C(2)#10	112.8(11)
C(2)#9-N(2)-C(2)#10	67.2(11)
C(2)#8-N(2)-C(2)#3	67.2(11)
C(2)#9-N(2)-C(2)#3	112.8(11)
C(2)#10-N(2)-C(2)#3	180.0
C(2)#8-N(2)-C(2)#11	103(2)
C(2)#9-N(2)-C(2)#11	77(2)
C(2)#10-N(2)-C(2)#11	112.8(11)
C(2)#3-N(2)-C(2)#11	67.2(11)
C(2)#8-N(2)-C(2)#12	112.8(11)
C(2)#9-N(2)-C(2)#12	67.2(11)
C(2)#10-N(2)-C(2)#12	103(2)
C(2)#3-N(2)-C(2)#12	77(2)
C(2)#11-N(2)-C(2)#12	112.8(11)
C(2)#8-N(2)-C(2)#13	77(2)
C(2)#9-N(2)-C(2)#13	103(2)
C(2)#10-N(2)-C(2)#13	67.2(11)
C(2)#3-N(2)-C(2)#13	112.8(11)
C(2)#11-N(2)-C(2)#13	180.0
C(2)#12-N(2)-C(2)#13	67.2(11)
C(2)#8-N(2)-C(2)	67.2(11)
C(2)#9-N(2)-C(2)	112.8(11)
C(2)#10-N(2)-C(2)	77(2)
C(2)#3-N(2)-C(2)	103(2)
C(2)#11-N(2)-C(2)	67.2(11)
C(2)#12-N(2)-C(2)	180.0
C(2)#13-N(2)-C(2)	112.8(11)
N(2)-C(2)-C(3)	107.1(15)
N(2)-C(2)-C(2)#8	56.4(6)
C(3)-C(2)-C(2)#8	125.7(5)
N(2)-C(2)-C(2)#11	56.4(6)
C(3)-C(2)-C(2)#11	125.7(5)

C(2)#8-C(2)-C(2)#11	89.999(1)
N(2)-C(2)-C(2)#10	51.5(11)
C(3)-C(2)-C(2)#10	55.6(9)
C(2)#8-C(2)-C(2)#10	90.000(3)
C(2)#11-C(2)-C(2)#10	90.000(1)
C(4)-N(3)-C(4)#14	120.0
C(4)-N(3)-C(4)#15	180.0
C(4)#14-N(3)-C(4)#15	60.000(2)
C(4)-N(3)-C(4)#16	60.000(2)
C(4)#14-N(3)-C(4)#16	180.0
C(4)#15-N(3)-C(4)#16	120.000(1)
C(4)-N(3)-C(4)#17	120.000(2)
C(4)#14-N(3)-C(4)#17	60.000(1)
C(4)#15-N(3)-C(4)#17	60.000(1)
C(4)#16-N(3)-C(4)#17	120.000(1)
C(4)-N(3)-C(4)#18	60.000(2)
C(4)#14-N(3)-C(4)#18	120.000(2)
C(4)#15-N(3)-C(4)#18	120.000(2)
C(4)#16-N(3)-C(4)#18	60.000(1)
C(4)#17-N(3)-C(4)#18	180.0
C(4)-N(3)-C(4)#19	120.000(1)
C(4)#14-N(3)-C(4)#19	90.000(3)
C(4)#15-N(3)-C(4)#19	60.000(2)
C(4)#16-N(3)-C(4)#19	90.000(2)
C(4)#17-N(3)-C(4)#19	120.000(1)
C(4)#18-N(3)-C(4)#19	60.000(2)
C(4)-N(3)-C(4)#20	120.000(2)
C(4)#14-N(3)-C(4)#20	120.000(2)
C(4)#15-N(3)-C(4)#20	60.000(1)
C(4)#16-N(3)-C(4)#20	60.0
C(4)#17-N(3)-C(4)#20	90.000(3)
C(4)#18-N(3)-C(4)#20	90.000(2)
C(4)#19-N(3)-C(4)#20	60.000(1)
C(4)-N(3)-C(4)#21	60.000(1)
C(4)#14-N(3)-C(4)#21	60.000(1)
C(4)#15-N(3)-C(4)#21	120.000(2)

C(4)#16-N(3)-C(4)#21	120.000(2)
C(4)#17-N(3)-C(4)#21	90.000(2)
C(4)#18-N(3)-C(4)#21	90.000(3)
C(4)#19-N(3)-C(4)#21	120.000(1)
C(4)#20-N(3)-C(4)#21	180.0
C(4)-N(3)-C(4)#22	90.000(3)
C(4)#14-N(3)-C(4)#22	120.000(2)
C(4)#15-N(3)-C(4)#22	90.000(1)
C(4)#16-N(3)-C(4)#22	60.000(2)
C(4)#17-N(3)-C(4)#22	60.000(2)
C(4)#18-N(3)-C(4)#22	120.000(2)
C(4)#19-N(3)-C(4)#22	120.000(1)
C(4)#20-N(3)-C(4)#22	60.000(2)
C(4)#21-N(3)-C(4)#22	120.000(2)
C(4)-N(3)-C(4)#23	90.000(1)
C(4)#14-N(3)-C(4)#23	60.000(1)
C(4)#15-N(3)-C(4)#23	90.000(3)
C(4)#16-N(3)-C(4)#23	120.000(2)
C(4)#17-N(3)-C(4)#23	120.000(2)
C(4)#18-N(3)-C(4)#23	60.0
C(4)#19-N(3)-C(4)#23	60.000(2)
C(4)#20-N(3)-C(4)#23	120.000(2)
C(4)#21-N(3)-C(4)#23	60.0
C(4)#22-N(3)-C(4)#23	180.0
C(4)-N(3)-C(4)#24	60.000(2)
C(4)#14-N(3)-C(4)#24	90.000(2)
C(4)#15-N(3)-C(4)#24	120.0
C(4)#16-N(3)-C(4)#24	90.000(4)
C(4)#17-N(3)-C(4)#24	60.000(2)
C(4)#18-N(3)-C(4)#24	120.000(2)
C(4)#19-N(3)-C(4)#24	180.0
C(4)#20-N(3)-C(4)#24	120.000(2)
C(4)#21-N(3)-C(4)#24	60.000(2)
C(4)#22-N(3)-C(4)#24	60.000(2)
C(4)#23-N(3)-C(4)#24	120.000(2)
C(2)-C(3)-C(2)#10	68.9(18)

N(3)-C(4)-C(4)#24	60.001(4)
N(3)-C(4)-C(4)#21	60.001(4)
C(4)#24-C(4)-C(4)#21	60.001(1)
N(3)-C(4)-C(4)#16	60.001(4)
C(4)#24-C(4)-C(4)#16	90.001(9)
C(4)#21-C(4)-C(4)#16	120.003(16)
N(3)-C(4)-C(4)#18	60.001(5)
C(4)#24-C(4)-C(4)#18	120.003(18)
C(4)#21-C(4)-C(4)#18	90.002(13)
C(4)#16-C(4)-C(4)#18	60.001(1)
N(3)-C(4)-C(5)#18	93.1(12)
C(4)#24-C(4)-C(5)#18	121.7(7)
C(4)#21-C(4)-C(5)#18	61.8(7)
C(4)#16-C(4)-C(5)#18	121.7(7)
C(4)#18-C(4)-C(5)#18	61.8(7)
N(3)-C(4)-C(5)	93.1(12)
C(4)#24-C(4)-C(5)	61.8(7)
C(4)#21-C(4)-C(5)	121.7(7)
C(4)#16-C(4)-C(5)	61.8(7)
C(4)#18-C(4)-C(5)	121.7(7)
C(5)#18-C(4)-C(5)	174(2)
C(4)#24-C(5)-C(4)#22	56.4(14)
C(4)#24-C(5)-C(4)#16	84(2)
C(4)#22-C(5)-C(4)#16	56.4(14)
C(4)#24-C(5)-C(4)	56.4(14)
C(4)#22-C(5)-C(4)	84(2)
C(4)#16-C(5)-C(4)	56.4(14)
N(1)-C(1)-S(1)	180.0(16)
C(1)-N(1)-Ce(1)	180.0(14)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 x,y,-z #3 -x,-y,z #4 -x,y,z

#5 -x,y,-z #6 x,-y,z #7 x,-y,-z #8 -y,-x,z

#9 y,x,-z+1 #10 x,y,-z+1 #11 y,x,z #12 -x,-y,-z+1

#13 -y,-x,-z+1 #14 -y+1,-z+1,-x+1 #15 -x+1,-y+1,-z+1

#16 y,z,x #17 -z+1,-x+1,-y+1 #18 z,x,y #19 -y+1,z,x

#20 -z+1,-x+1,y #21 z,x,-y+1 #22 x,-y+1,z

#23 -x+1,y,-z+1 #24 y,-z+1,-x+1

Table 8. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for CeSCN. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ce(1)	22(1)	22(1)	22(1)	0	0	0
N(2)	210(30)	210(30)	50(12)	0	0	0
C(2)	169(13)	250(20)	105(12)	86(17)	0	0
N(3)	36(4)	36(4)	36(4)	0	0	0
C(3)	169(13)	250(20)	105(12)	86(17)	0	0
C(4)	102(12)	102(12)	60(12)	0	0	-20(20)
C(5)	102(12)	102(12)	60(12)	0	0	-20(20)
S(1)	113(2)	113(2)	113(2)	-39(1)	-39(1)	-39(1)
C(1)	75(4)	75(4)	75(4)	-21(3)	-21(3)	-21(3)
N(1)	96(5)	96(5)	96(5)	-30(4)	-30(4)	-30(4)

Table 9. Crystal data and structure refinement for PrSCN.

Identification code	pm3m	
Empirical formula	C39 H82 N11 O Pr S7	
Formula weight	1086.48	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Cubic	
Space group	Pm-3m	
Unit cell dimensions	a = 11.4242(9) Å	α= 90°.
	b = 11.4242(9) Å	β= 90°.
	c = 11.4242(9) Å	γ = 90°.
Volume	1491.0(4) $Å^3$	
Z	1	
Density (calculated)	1.210 Mg/m^3	
Absorption coefficient	1.098 mm^{-1}	
F(000)	572	
Crystal size	0.365 x 0.124 x 0.120 mm^3	
Theta range for data collection	1.783 to 33.087°.	
Index ranges	-17<=h<=16, -17<=k<=17, -17<=l<=17	
Reflections collected	25892	
Independent reflections	626 [R(int) = 0.0257]	
Completeness to theta = 25.242°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	626 / 1 / 29	
Goodness-of-fit on F^2	1.022	
Final R indices [I>2sigma(I)]	R1 = 0.0514, wR2 = 0.1448	
R indices (all data)	R1 = 0.0514, wR2 = 0.1448	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.489 and -2.440 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Pr(1)	0	0	0	18(1)
N(2)	0	0	5000	149(13)
C(2)	0	1060(20)	4162(12)	160(12)
N(3)	5000	5000	5000	29(2)
C(3)	0	2280(20)	5000	155(7)
C(4)	4056(17)	4056(17)	5000	76(5)
C(5)	3007(11)	5000	5000	76(5)
S(1)	2624(2)	2624(2)	2624(2)	93(1)
C(1)	1835(5)	1835(5)	1835(5)	61(3)
N(1)	1260(5)	1260(5)	1260(5)	78(3)

Table 11. Bond lengths [Å] and angles [°] for PrSCN.

Pr(1)-N(1)#1	2.493(9)
Pr(1)-N(1)#2	2.493(9)
Pr(1)-N(1)#3	2.493(9)
Pr(1)-N(1)#4	2.493(9)
Pr(1)-N(1)#5	2.493(9)
Pr(1)-N(1)#6	2.493(9)
Pr(1)-N(1)#7	2.493(9)
Pr(1)-N(1)	2.493(9)
N(2)-C(2)#8	1.55(2)
N(2)-C(2)#9	1.55(2)
N(2)-C(2)#10	1.55(2)
N(2)-C(2)#6	1.55(2)
N(2)-C(2)#11	1.55(2)
N(2)-C(2)#12	1.55(2)
N(2)-C(2)#13	1.55(2)
N(2)-C(2)	1.55(2)
C(2)-C(2)#8	1.72(4)
C(2)-C(2)#11	1.72(4)
C(2)-C(3)	1.69(3)
C(2)-C(2)#10	1.91(3)
N(3)-C(4)	1.53(3)
N(3)-C(4)#14	1.53(3)
N(3)-C(4)#15	1.53(3)
N(3)-C(4)#16	1.53(3)
N(3)-C(4)#17	1.53(3)
N(3)-C(4)#18	1.53(3)
N(3)-C(4)#19	1.53(3)
N(3)-C(4)#20	1.53(3)
N(3)-C(4)#21	1.53(3)
N(3)-C(4)#22	1.53(3)
N(3)-C(4)#23	1.53(3)
N(3)-C(4)#24	1.53(3)
C(3)-C(2)#10	1.69(3)
C(4)-C(4)#24	1.53(3)

C(4)-C(4)#21	1.53(3)
C(4)-C(4)#16	1.53(3)
C(4)-C(4)#18	1.53(3)
C(4)-C(5)	1.612(9)
C(4)-C(5)#18	1.612(9)
C(5)-C(4)#24	1.612(9)
C(5)-C(4)#22	1.612(9)
C(5)-C(4)#16	1.612(9)
S(1)-C(1)	1.561(11)
C(1)-N(1)	1.138(12)

N(1)#1-Pr(1)-N(1)#2	109.471(1)
N(1)#1-Pr(1)-N(1)#3	70.529(1)
N(1)#2-Pr(1)-N(1)#3	180.0(4)
N(1)#1-Pr(1)-N(1)#4	109.5
N(1)#2-Pr(1)-N(1)#4	109.5
N(1)#3-Pr(1)-N(1)#4	70.5
N(1)#1-Pr(1)-N(1)#5	70.5
N(1)#2-Pr(1)-N(1)#5	70.5
N(1)#3-Pr(1)-N(1)#5	109.5
N(1)#4-Pr(1)-N(1)#5	180.0(6)
N(1)#1-Pr(1)-N(1)#6	70.5
N(1)#2-Pr(1)-N(1)#6	70.5
N(1)#3-Pr(1)-N(1)#6	109.5
N(1)#4-Pr(1)-N(1)#6	70.5
N(1)#5-Pr(1)-N(1)#6	109.5
N(1)#1-Pr(1)-N(1)#7	109.5
N(1)#2-Pr(1)-N(1)#7	109.5
N(1)#3-Pr(1)-N(1)#7	70.5
N(1)#4-Pr(1)-N(1)#7	109.5
N(1)#5-Pr(1)-N(1)#7	70.5
N(1)#6-Pr(1)-N(1)#7	180.0(6)
N(1)#1-Pr(1)-N(1)	180.0(6)
N(1)#2-Pr(1)-N(1)	70.529(1)
N(1)#3-Pr(1)-N(1)	109.5
N(1)#4-Pr(1)-N(1)	70.5

N(1)#5-Pr(1)-N(1)	109.5
N(1)#6-Pr(1)-N(1)	109.5
N(1)#7-Pr(1)-N(1)	70.529(1)
C(2)#8-N(2)-C(2)#9	180.0(8)
C(2)#8-N(2)-C(2)#10	112.5(9)
C(2)#9-N(2)-C(2)#10	67.5(9)
C(2)#8-N(2)-C(2)#6	67.5(9)
C(2)#9-N(2)-C(2)#6	112.5(9)
C(2)#10-N(2)-C(2)#6	180.0
C(2)#8-N(2)-C(2)#11	103.5(17)
C(2)#9-N(2)-C(2)#11	76.5(17)
C(2)#10-N(2)-C(2)#11	112.5(9)
C(2)#6-N(2)-C(2)#11	67.5(9)
C(2)#8-N(2)-C(2)#12	112.5(9)
C(2)#9-N(2)-C(2)#12	67.5(9)
C(2)#10-N(2)-C(2)#12	103.5(17)
C(2)#6-N(2)-C(2)#12	76.5(17)
C(2)#11-N(2)-C(2)#12	112.5(9)
C(2)#8-N(2)-C(2)#13	76.5(17)
C(2)#9-N(2)-C(2)#13	103.5(17)
C(2)#10-N(2)-C(2)#13	67.5(9)
C(2)#6-N(2)-C(2)#13	112.5(9)
C(2)#11-N(2)-C(2)#13	180.0
C(2)#12-N(2)-C(2)#13	67.5(9)
C(2)#8-N(2)-C(2)	67.5(9)
C(2)#9-N(2)-C(2)	112.5(9)
C(2)#10-N(2)-C(2)	76.5(17)
C(2)#6-N(2)-C(2)	103.5(17)
C(2)#11-N(2)-C(2)	67.5(9)
C(2)#12-N(2)-C(2)	180.0
C(2)#13-N(2)-C(2)	112.5(9)
N(2)-C(2)-C(2)#8	56.3(5)
N(2)-C(2)-C(2)#11	56.3(5)
C(2)#8-C(2)-C(2)#11	90.000(2)
N(2)-C(2)-C(3)	107.2(11)
C(2)#8-C(2)-C(3)	125.6(3)

C(2)#11-C(2)-C(3)	125.6(3)
N(2)-C(2)-C(2)#10	51.8(9)
C(2)#8-C(2)-C(2)#10	89.999(2)
C(2)#11-C(2)-C(2)#10	89.999(1)
C(3)-C(2)-C(2)#10	55.4(7)
C(4)-N(3)-C(4)#14	120.0
C(4)-N(3)-C(4)#15	180.0
C(4)#14-N(3)-C(4)#15	60.000(1)
C(4)-N(3)-C(4)#16	60.000(2)
C(4)#14-N(3)-C(4)#16	180.0
C(4)#15-N(3)-C(4)#16	120.0
C(4)-N(3)-C(4)#17	120.000(1)
C(4)#14-N(3)-C(4)#17	60.0
C(4)#15-N(3)-C(4)#17	60.0
C(4)#16-N(3)-C(4)#17	120.0
C(4)-N(3)-C(4)#18	60.000(1)
C(4)#14-N(3)-C(4)#18	120.000(2)
C(4)#15-N(3)-C(4)#18	120.000(2)
C(4)#16-N(3)-C(4)#18	60.000(1)
C(4)#17-N(3)-C(4)#18	180.0
C(4)-N(3)-C(4)#19	120.0
C(4)#14-N(3)-C(4)#19	90.000(3)
C(4)#15-N(3)-C(4)#19	60.000(2)
C(4)#16-N(3)-C(4)#19	90.000(1)
C(4)#17-N(3)-C(4)#19	120.000(2)
C(4)#18-N(3)-C(4)#19	60.000(1)
C(4)-N(3)-C(4)#20	120.000(2)
C(4)#14-N(3)-C(4)#20	120.000(1)
C(4)#15-N(3)-C(4)#20	60.0
C(4)#16-N(3)-C(4)#20	60.0
C(4)#17-N(3)-C(4)#20	90.000(3)
C(4)#18-N(3)-C(4)#20	90.000(1)
C(4)#19-N(3)-C(4)#20	60.0
C(4)-N(3)-C(4)#21	60.0
C(4)#14-N(3)-C(4)#21	60.0
C(4)#15-N(3)-C(4)#21	120.000(1)

C(4)#16-N(3)-C(4)#21	120.000(2)
C(4)#17-N(3)-C(4)#21	90.000(1)
C(4)#18-N(3)-C(4)#21	90.000(3)
C(4)#19-N(3)-C(4)#21	120.000(1)
C(4)#20-N(3)-C(4)#21	180.0
C(4)-N(3)-C(4)#22	90.000(3)
C(4)#14-N(3)-C(4)#22	120.000(1)
C(4)#15-N(3)-C(4)#22	90.0
C(4)#16-N(3)-C(4)#22	60.000(1)
C(4)#17-N(3)-C(4)#22	60.000(1)
C(4)#18-N(3)-C(4)#22	120.000(1)
C(4)#19-N(3)-C(4)#22	120.000(1)
C(4)#20-N(3)-C(4)#22	60.000(1)
C(4)#21-N(3)-C(4)#22	120.000(1)
C(4)-N(3)-C(4)#23	90.0
C(4)#14-N(3)-C(4)#23	60.000(1)
C(4)#15-N(3)-C(4)#23	90.000(3)
C(4)#16-N(3)-C(4)#23	120.000(1)
C(4)#17-N(3)-C(4)#23	120.000(2)
C(4)#18-N(3)-C(4)#23	60.0
C(4)#19-N(3)-C(4)#23	60.000(1)
C(4)#20-N(3)-C(4)#23	120.000(2)
C(4)#21-N(3)-C(4)#23	60.0
C(4)#22-N(3)-C(4)#23	180.0
C(4)-N(3)-C(4)#24	60.000(2)
C(4)#14-N(3)-C(4)#24	90.000(1)
C(4)#15-N(3)-C(4)#24	120.0
C(4)#16-N(3)-C(4)#24	90.000(3)
C(4)#17-N(3)-C(4)#24	60.000(1)
C(4)#18-N(3)-C(4)#24	120.000(2)
C(4)#19-N(3)-C(4)#24	180.0
C(4)#20-N(3)-C(4)#24	120.000(2)
C(4)#21-N(3)-C(4)#24	60.000(1)
C(4)#22-N(3)-C(4)#24	60.000(2)
C(4)#23-N(3)-C(4)#24	120.000(2)
C(2)#10-C(3)-C(2)	69.2(13)

N(3)-C(4)-C(4)#24	60.000(3)
N(3)-C(4)-C(4)#21	60.000(4)
C(4)#24-C(4)-C(4)#21	60.0
N(3)-C(4)-C(4)#16	60.000(3)
C(4)#24-C(4)-C(4)#16	90.000(5)
C(4)#21-C(4)-C(4)#16	120.000(13)
N(3)-C(4)-C(4)#18	60.000(4)
C(4)#24-C(4)-C(4)#18	120.000(14)
C(4)#21-C(4)-C(4)#18	90.000(10)
C(4)#16-C(4)-C(4)#18	60.000(1)
N(3)-C(4)-C(5)	93.0(10)
C(4)#24-C(4)-C(5)	61.8(6)
C(4)#21-C(4)-C(5)	121.7(5)
C(4)#16-C(4)-C(5)	61.8(6)
C(4)#18-C(4)-C(5)	121.7(5)
N(3)-C(4)-C(5)#18	93.0(10)
C(4)#24-C(4)-C(5)#18	121.7(5)
C(4)#21-C(4)-C(5)#18	61.8(6)
C(4)#16-C(4)-C(5)#18	121.7(5)
C(4)#18-C(4)-C(5)#18	61.8(6)
C(5)-C(4)-C(5)#18	174.0(19)
C(4)#24-C(5)-C(4)#22	56.5(11)
C(4)#24-C(5)-C(4)#16	84.0(19)
C(4)#22-C(5)-C(4)#16	56.5(11)
C(4)#24-C(5)-C(4)	56.5(11)
C(4)#22-C(5)-C(4)	84.0(19)
C(4)#16-C(5)-C(4)	56.5(11)
N(1)-C(1)-S(1)	180.0(13)
C(1)-N(1)-Pr(1)	180.0(11)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -x,y,z #3 x,-y,-z #4 x,-y,z

#5 -x,y,-z #6 -x,-y,z #7 x,y,-z #8 -y,-x,z

#9 y,x,-z+1 #10 x,y,-z+1 #11 y,x,z #12 -x,-y,-z+1

#13 -y,-x,-z+1 #14 -y+1,-z+1,-x+1 #15 -x+1,-y+1,-z+1

#16 y,z,x #17 -z+1,-x+1,-y+1 #18 z,x,y #19 -y+1,z,x

#20 -z+1,-x+1,y #21 z,x,-y+1 #22 x,-y+1,z

#23 -x+1,y,-z+1 #24 y,-z+1,-x+1

Table 12. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for PrSCN. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pr(1)	18(1)	18(1)	18(1)	0	0	0
N(2)	210(20)	210(20)	35(8)	0	0	0
C(2)	160(20)	260(30)	55(8)	74(14)	0	0
N(3)	29(2)	29(2)	29(2)	0	0	0
C(3)	157(17)	159(18)	150(17)	0	0	0
C(4)	93(9)	93(9)	41(7)	0	0	-22(17)
C(5)	93(9)	93(9)	41(7)	0	0	-22(17)
S(1)	93(1)	93(1)	93(1)	-31(1)	-31(1)	-31(1)
C(1)	61(3)	61(3)	61(3)	-15(2)	-15(2)	-15(2)
N(1)	78(3)	78(3)	78(3)	-24(3)	-24(3)	-24(3)

Table 13. Crystal data and structure refinement for NdSCN.

Identification code	pm3m	
Empirical formula	C39 H0 N11 Nd O0 S7	
Formula weight	991.16	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Cubic	
Space group	Pm-3m	
Unit cell dimensions	a = 11.3976(4) Å	α= 90°.
	b = 11.3976(4) Å	β= 90°.
	c = 11.3976(4) Å	γ = 90°.
Volume	1480.61(16) $Å^3$	
Z	1	
Density (calculated)	1.112 Mg/m^3	
Absorption coefficient	1.154 mm^{-1}	
F(000)	483	
Crystal size	0.270 x 0.109 x 0.058 mm^3	
Theta range for data collection	1.787 to 33.113°.	
Index ranges	-17<=h<=17, -17<=k<=17, -17<=l<=17	
Reflections collected	25898	
Independent reflections	625 [R(int) = 0.0183]	
Completeness to theta = 25.242°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	625 / 1 / 29	
Goodness-of-fit on F^2	0.973	
Final R indices [I>2sigma(I)]	R1 = 0.0502, wR2 = 0.1414	
R indices (all data)	R1 = 0.0502, wR2 = 0.1414	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.573 and -2.412 $e.Å^{-3}$	

Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for NdSCN. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Nd(1)	0	0	0	18(1)
N(2)	0	0	5000	141(13)
C(2)	0	1040(20)	4165(13)	158(12)
N(3)	5000	5000	5000	28(3)
C(3)	0	2280(20)	5000	155(7)
C(4)	4053(18)	4053(18)	5000	76(5)
C(5)	3003(11)	5000	5000	76(5)
S(1)	2622(2)	2622(2)	2622(2)	95(1)
C(1)	1831(5)	1831(5)	1831(5)	63(3)
N(1)	1253(5)	1253(5)	1253(5)	80(4)

Table 15. Bond lengths [Å] and angles [°] for NdSCN.

Nd(1)-N(1)	2.473(10)
Nd(1)-N(1)#1	2.473(10)
Nd(1)-N(1)#2	2.473(10)
Nd(1)-N(1)#3	2.473(10)
Nd(1)-N(1)#4	2.473(10)
Nd(1)-N(1)#5	2.473(10)
Nd(1)-N(1)#6	2.473(10)
Nd(1)-N(1)#7	2.473(10)
N(2)-C(2)	1.52(2)
N(2)-C(2)#8	1.52(2)
N(2)-C(2)#9	1.52(2)
N(2)-C(2)#3	1.52(2)
N(2)-C(2)#10	1.52(2)
N(2)-C(2)#11	1.52(2)
N(2)-C(2)#12	1.52(2)
N(2)-C(2)#13	1.52(2)
C(2)-C(2)#8	1.68(4)
C(2)-C(2)#11	1.68(4)
C(2)-C(3)	1.70(3)
C(2)-C(2)#10	1.90(3)
N(3)-C(4)#14	1.53(3)
N(3)-C(4)#15	1.53(3)
N(3)-C(4)#16	1.53(3)
N(3)-C(4)#17	1.53(3)
N(3)-C(4)#18	1.53(3)
N(3)-C(4)#19	1.53(3)
N(3)-C(4)#20	1.53(3)
N(3)-C(4)#21	1.53(3)
N(3)-C(4)#22	1.53(3)
N(3)-C(4)#23	1.53(3)
N(3)-C(4)#24	1.53(3)
N(3)-C(4)	1.53(3)
C(3)-C(2)#10	1.70(3)
C(4)-C(4)#24	1.53(3)

C(4)-C(4)#22	1.53(3)
C(4)-C(4)#15	1.53(3)
C(4)-C(4)#18	1.53(3)
C(4)-C(5)#18	1.612(9)
C(4)-C(5)	1.612(9)
C(5)-C(4)#20	1.612(9)
C(5)-C(4)#24	1.612(9)
C(5)-C(4)#15	1.612(9)
S(1)-C(1)	1.561(11)
C(1)-N(1)	1.141(13)

N(1)-Nd(1)-N(1)#1	180.0(4)
N(1)-Nd(1)-N(1)#2	70.5
N(1)#1-Nd(1)-N(1)#2	109.5
N(1)-Nd(1)-N(1)#3	109.5
N(1)#1-Nd(1)-N(1)#3	70.5
N(1)#2-Nd(1)-N(1)#3	70.5
N(1)-Nd(1)-N(1)#4	70.5
N(1)#1-Nd(1)-N(1)#4	109.5
N(1)#2-Nd(1)-N(1)#4	109.5
N(1)#3-Nd(1)-N(1)#4	180.0(6)
N(1)-Nd(1)-N(1)#5	109.5
N(1)#1-Nd(1)-N(1)#5	70.5
N(1)#2-Nd(1)-N(1)#5	70.5
N(1)#3-Nd(1)-N(1)#5	109.5
N(1)#4-Nd(1)-N(1)#5	70.5
N(1)-Nd(1)-N(1)#6	70.5
N(1)#1-Nd(1)-N(1)#6	109.5
N(1)#2-Nd(1)-N(1)#6	109.5
N(1)#3-Nd(1)-N(1)#6	70.5
N(1)#4-Nd(1)-N(1)#6	109.5
N(1)#5-Nd(1)-N(1)#6	180.0(6)
N(1)-Nd(1)-N(1)#7	109.5
N(1)#1-Nd(1)-N(1)#7	70.5
N(1)#2-Nd(1)-N(1)#7	180.0(4)
N(1)#3-Nd(1)-N(1)#7	109.5

N(1)#4-Nd(1)-N(1)#7	70.5
N(1)#5-Nd(1)-N(1)#7	109.5
N(1)#6-Nd(1)-N(1)#7	70.5
C(2)-N(2)-C(2)#8	67.0(10)
C(2)-N(2)-C(2)#9	113.0(10)
C(2)#8-N(2)-C(2)#9	180.0(8)
C(2)-N(2)-C(2)#3	102.6(18)
C(2)#8-N(2)-C(2)#3	67.0(10)
C(2)#9-N(2)-C(2)#3	113.0(10)
C(2)-N(2)-C(2)#10	77.4(18)
C(2)#8-N(2)-C(2)#10	113.0(10)
C(2)#9-N(2)-C(2)#10	67.0(10)
C(2)#3-N(2)-C(2)#10	180.0(8)
C(2)-N(2)-C(2)#11	67.0(10)
C(2)#8-N(2)-C(2)#11	102.6(18)
C(2)#9-N(2)-C(2)#11	77.4(18)
C(2)#3-N(2)-C(2)#11	67.0(10)
C(2)#10-N(2)-C(2)#11	113.0(10)
C(2)-N(2)-C(2)#12	180.0
C(2)#8-N(2)-C(2)#12	113.0(10)
C(2)#9-N(2)-C(2)#12	67.0(10)
C(2)#3-N(2)-C(2)#12	77.4(18)
C(2)#10-N(2)-C(2)#12	102.6(18)
C(2)#11-N(2)-C(2)#12	113.0(10)
C(2)-N(2)-C(2)#13	113.0(10)
C(2)#8-N(2)-C(2)#13	77.4(18)
C(2)#9-N(2)-C(2)#13	102.6(18)
C(2)#3-N(2)-C(2)#13	113.0(10)
C(2)#10-N(2)-C(2)#13	67.0(10)
C(2)#11-N(2)-C(2)#13	180.0(13)
C(2)#12-N(2)-C(2)#13	67.0(10)
N(2)-C(2)-C(2)#8	56.5(5)
N(2)-C(2)-C(2)#11	56.5(5)
C(2)#8-C(2)-C(2)#11	90.001(1)
N(2)-C(2)-C(3)	107.2(11)
C(2)#8-C(2)-C(3)	125.9(3)

C(2)#11-C(2)-C(3)	125.9(3)
N(2)-C(2)-C(2)#10	51.3(9)
C(2)#8-C(2)-C(2)#10	90.001(2)
C(2)#11-C(2)-C(2)#10	90.001(1)
C(3)-C(2)-C(2)#10	55.9(7)
C(4)#14-N(3)-C(4)#15	180.0
C(4)#14-N(3)-C(4)#16	60.000(1)
C(4)#15-N(3)-C(4)#16	120.000(1)
C(4)#14-N(3)-C(4)#17	60.0
C(4)#15-N(3)-C(4)#17	120.0
C(4)#16-N(3)-C(4)#17	60.0
C(4)#14-N(3)-C(4)#18	120.000(2)
C(4)#15-N(3)-C(4)#18	60.000(1)
C(4)#16-N(3)-C(4)#18	120.000(2)
C(4)#17-N(3)-C(4)#18	180.0
C(4)#14-N(3)-C(4)#19	90.000(3)
C(4)#15-N(3)-C(4)#19	90.000(1)
C(4)#16-N(3)-C(4)#19	60.000(2)
C(4)#17-N(3)-C(4)#19	120.000(2)
C(4)#18-N(3)-C(4)#19	60.000(2)
C(4)#14-N(3)-C(4)#20	120.000(1)
C(4)#15-N(3)-C(4)#20	60.0
C(4)#16-N(3)-C(4)#20	90.0
C(4)#17-N(3)-C(4)#20	60.000(1)
C(4)#18-N(3)-C(4)#20	120.000(1)
C(4)#19-N(3)-C(4)#20	120.0
C(4)#14-N(3)-C(4)#21	120.000(2)
C(4)#15-N(3)-C(4)#21	60.0
C(4)#16-N(3)-C(4)#21	60.0
C(4)#17-N(3)-C(4)#21	90.000(3)
C(4)#18-N(3)-C(4)#21	90.000(1)
C(4)#19-N(3)-C(4)#21	60.0
C(4)#20-N(3)-C(4)#21	60.0
C(4)#14-N(3)-C(4)#22	60.0
C(4)#15-N(3)-C(4)#22	120.000(2)
C(4)#16-N(3)-C(4)#22	120.000(1)

C(4)#17-N(3)-C(4)#22	90.000(1)
C(4)#18-N(3)-C(4)#22	90.000(3)
C(4)#19-N(3)-C(4)#22	120.000(1)
C(4)#20-N(3)-C(4)#22	120.000(1)
C(4)#21-N(3)-C(4)#22	180.0
C(4)#14-N(3)-C(4)#23	60.0
C(4)#15-N(3)-C(4)#23	120.000(1)
C(4)#16-N(3)-C(4)#23	90.000(3)
C(4)#17-N(3)-C(4)#23	120.000(2)
C(4)#18-N(3)-C(4)#23	60.0
C(4)#19-N(3)-C(4)#23	60.0
C(4)#20-N(3)-C(4)#23	180.0
C(4)#21-N(3)-C(4)#23	120.000(2)
C(4)#22-N(3)-C(4)#23	60.0
C(4)#14-N(3)-C(4)#24	90.000(1)
C(4)#15-N(3)-C(4)#24	90.000(3)
C(4)#16-N(3)-C(4)#24	120.0
C(4)#17-N(3)-C(4)#24	60.000(1)
C(4)#18-N(3)-C(4)#24	120.000(2)
C(4)#19-N(3)-C(4)#24	180.0
C(4)#20-N(3)-C(4)#24	60.000(1)
C(4)#21-N(3)-C(4)#24	120.000(2)
C(4)#22-N(3)-C(4)#24	60.000(1)
C(4)#23-N(3)-C(4)#24	120.000(1)
C(4)#14-N(3)-C(4)	120.000(2)
C(4)#15-N(3)-C(4)	60.000(2)
C(4)#16-N(3)-C(4)	180.0
C(4)#17-N(3)-C(4)	120.000(2)
C(4)#18-N(3)-C(4)	60.000(1)
C(4)#19-N(3)-C(4)	120.000(2)
C(4)#20-N(3)-C(4)	90.000(3)
C(4)#21-N(3)-C(4)	120.000(1)
C(4)#22-N(3)-C(4)	60.000(2)
C(4)#23-N(3)-C(4)	90.000(3)
C(4)#24-N(3)-C(4)	60.000(2)
C(2)#10-C(3)-C(2)	68.1(13)

C(4)#24-C(4)-C(4)#22	59.999(1)
C(4)#24-C(4)-C(4)#15	89.999(8)
C(4)#22-C(4)-C(4)#15	119.998(13)
C(4)#24-C(4)-C(4)#18	119.998(14)
C(4)#22-C(4)-C(4)#18	89.999(12)
C(4)#15-C(4)-C(4)#18	59.999(1)
C(4)#24-C(4)-N(3)	59.999(4)
C(4)#22-C(4)-N(3)	59.999(3)
C(4)#15-C(4)-N(3)	59.999(4)
C(4)#18-C(4)-N(3)	59.999(3)
C(4)#24-C(4)-C(5)#18	121.7(6)
C(4)#22-C(4)-C(5)#18	61.7(6)
C(4)#15-C(4)-C(5)#18	121.7(6)
C(4)#18-C(4)-C(5)#18	61.7(6)
N(3)-C(4)-C(5)#18	92.9(10)
C(4)#24-C(4)-C(5)	61.7(6)
C(4)#22-C(4)-C(5)	121.7(6)
C(4)#15-C(4)-C(5)	61.7(6)
C(4)#18-C(4)-C(5)	121.7(6)
N(3)-C(4)-C(5)	92.9(10)
C(5)#18-C(4)-C(5)	174(2)
C(4)-C(5)-C(4)#20	84(2)
C(4)-C(5)-C(4)#24	56.6(12)
C(4)#20-C(5)-C(4)#24	56.6(12)
C(4)-C(5)-C(4)#15	56.6(12)
C(4)#20-C(5)-C(4)#15	56.6(12)
C(4)#24-C(5)-C(4)#15	84(2)
N(1)-C(1)-S(1)	180.0(13)
C(1)-N(1)-Nd(1)	180.0(11)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -x,y,z #3 -x,-y,z #4 x,y,-z

#5 -x,y,-z #6 x,-y,z #7 x,-y,-z #8 -y,-x,z

#9 y,x,-z+1 #10 x,y,-z+1 #11 y,x,z #12 -x,-y,-z+1

#13 -y,-x,-z+1 #14 -y+1,-z+1,-x+1 #15 y,z,x

#16 -x+1,-y+1,-z+1 #17 -z+1,-x+1,-y+1 #18 z,x,y

#19 -y+1,z,x #20 x,-y+1,z #21 -z+1,-x+1,y

#22 z,x,-y+1 #23 -x+1,y,-z+1 #24 y,-z+1,-x+1

Table 16. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for NdSCN. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Nd(1)	18(1)	18(1)	18(1)	0	0	0
N(2)	200(20)	200(20)	33(8)	0	0	0
C(2)	150(19)	270(30)	57(8)	78(14)	0	0
N(3)	28(3)	28(3)	28(3)	0	0	0
C(3)	147(17)	157(18)	161(18)	0	0	0
C(4)	92(9)	92(9)	44(8)	0	0	-23(17)
C(5)	92(9)	92(9)	44(8)	0	0	-23(17)
S(1)	95(1)	95(1)	95(1)	-32(1)	-32(1)	-32(1)
C(1)	63(3)	63(3)	63(3)	-17(3)	-17(3)	-17(3)
N(1)	80(4)	80(4)	80(4)	-25(3)	-25(3)	-25(3)

Table 17. Crystal data and structure refinement for SmSCN.

Identification code	pm3m	
Empirical formula	C39 H0 N11 O0 S7 Sm	
Formula weight	997.27	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Cubic	
Space group	Pm-3m	
Unit cell dimensions	a = 11.3772(6) Å	α= 90°.
	b = 11.3772(6) Å	β= 90°.
	c = 11.3772(6) Å	γ = 90°.
Volume	1472.7(2) $Å^3$	
Z	1	
Density (calculated)	1.124 Mg/m^3	
Absorption coefficient	1.276 mm^{-1}	
F(000)	485	
Crystal size	0.128 x 0.070 x 0.058 mm^3	
Theta range for data collection	1.790 to 33.058°.	
Index ranges	-16<=h<=16, -17<=k<=17, -16<=l<=16	
Reflections collected	25736	
Independent reflections	615 [R(int) = 0.0366]	
Completeness to theta = 25.242°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	615 / 0 / 32	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0392, wR2 = 0.1136	
R indices (all data)	R1 = 0.0392, wR2 = 0.1136	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.383 and -0.827 $e.Å^{-3}$	

Table 18. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for SmSCN. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Sm(1)	0	0	0	17(1)
N(2)	0	0	5000	141(11)
C(2)	0	1000(20)	4152(12)	157(10)
N(3)	5000	5000	5000	30(2)
C(3)	0	2200(20)	5000	175(8)
C(4)	4063(9)	4063(9)	5000	54(5)
C(5)	2742(12)	5000	5000	59(3)
S(1)	2617(2)	2617(2)	2617(2)	98(1)
C(1)	1823(5)	1823(5)	1823(5)	64(3)
N(1)	1244(4)	1244(4)	1244(4)	80(3)

Table 19. Bond lengths [Å] and angles [°] for SmSCN.

Sm(1)-N(1)	2.452(8)
Sm(1)-N(1)#1	2.452(8)
Sm(1)-N(1)#2	2.452(8)
Sm(1)-N(1)#3	2.452(8)
Sm(1)-N(1)#4	2.452(8)
Sm(1)-N(1)#5	2.452(8)
Sm(1)-N(1)#6	2.452(8)
Sm(1)-N(1)#7	2.452(8)
N(2)-C(2)#8	1.490(18)
N(2)-C(2)#9	1.490(18)
N(2)-C(2)#10	1.490(18)
N(2)-C(2)#3	1.490(18)
N(2)-C(2)#11	1.490(18)
N(2)-C(2)#12	1.490(18)
N(2)-C(2)#13	1.490(18)
N(2)-C(2)	1.490(18)
C(2)-C(2)#8	1.61(3)
C(2)-C(2)#11	1.61(3)
C(2)-C(3)	1.67(2)
C(2)-C(2)#10	1.93(3)
N(3)-C(4)#14	1.508(15)
N(3)-C(4)	1.508(15)
N(3)-C(4)#15	1.508(15)
N(3)-C(4)#16	1.508(15)
N(3)-C(4)#17	1.508(14)
N(3)-C(4)#18	1.508(14)
N(3)-C(4)#19	1.508(15)
N(3)-C(4)#20	1.508(14)
N(3)-C(4)#21	1.508(14)
N(3)-C(4)#22	1.508(14)
N(3)-C(4)#23	1.508(15)
N(3)-C(4)#24	1.508(15)
C(3)-C(2)#10	1.67(2)
C(4)-C(4)#24	1.508(14)

C(4)-C(4)#21	1.508(14)
C(4)-C(4)#16	1.508(14)
C(4)-C(4)#18	1.508(14)
C(4)-C(5)	1.843(11)
C(4)-C(5)#18	1.843(11)
C(5)-C(4)#22	1.843(11)
C(5)-C(4)#24	1.843(11)
C(5)-C(4)#16	1.843(11)
S(1)-C(1)	1.566(10)
C(1)-N(1)	1.140(11)

N(1)-Sm(1)-N(1)#1	180.0(4)
N(1)-Sm(1)-N(1)#2	70.529(1)
N(1)#1-Sm(1)-N(1)#2	109.471(1)
N(1)-Sm(1)-N(1)#3	109.5
N(1)#1-Sm(1)-N(1)#3	70.529(1)
N(1)#2-Sm(1)-N(1)#3	70.5
N(1)-Sm(1)-N(1)#4	70.5
N(1)#1-Sm(1)-N(1)#4	109.5
N(1)#2-Sm(1)-N(1)#4	109.5
N(1)#3-Sm(1)-N(1)#4	180.0(6)
N(1)-Sm(1)-N(1)#5	109.5
N(1)#1-Sm(1)-N(1)#5	70.529(1)
N(1)#2-Sm(1)-N(1)#5	70.5
N(1)#3-Sm(1)-N(1)#5	109.5
N(1)#4-Sm(1)-N(1)#5	70.5
N(1)-Sm(1)-N(1)#6	70.5
N(1)#1-Sm(1)-N(1)#6	109.5
N(1)#2-Sm(1)-N(1)#6	109.5
N(1)#3-Sm(1)-N(1)#6	70.5
N(1)#4-Sm(1)-N(1)#6	109.5
N(1)#5-Sm(1)-N(1)#6	180.0(6)
N(1)-Sm(1)-N(1)#7	109.471(1)
N(1)#1-Sm(1)-N(1)#7	70.529(1)
N(1)#2-Sm(1)-N(1)#7	180.0(4)
N(1)#3-Sm(1)-N(1)#7	109.5

N(1)#4-Sm(1)-N(1)#7	70.5
N(1)#5-Sm(1)-N(1)#7	109.5
N(1)#6-Sm(1)-N(1)#7	70.5
C(2)#8-N(2)-C(2)#9	180.0(8)
C(2)#8-N(2)-C(2)#10	114.8(9)
C(2)#9-N(2)-C(2)#10	65.2(9)
C(2)#8-N(2)-C(2)#3	65.2(9)
C(2)#9-N(2)-C(2)#3	114.8(9)
C(2)#10-N(2)-C(2)#3	180.0
C(2)#8-N(2)-C(2)#11	99.3(17)
C(2)#9-N(2)-C(2)#11	80.7(17)
C(2)#10-N(2)-C(2)#11	114.8(9)
C(2)#3-N(2)-C(2)#11	65.2(9)
C(2)#8-N(2)-C(2)#12	114.8(9)
C(2)#9-N(2)-C(2)#12	65.2(9)
C(2)#10-N(2)-C(2)#12	99.3(17)
C(2)#3-N(2)-C(2)#12	80.7(17)
C(2)#11-N(2)-C(2)#12	114.8(9)
C(2)#8-N(2)-C(2)#13	80.7(17)
C(2)#9-N(2)-C(2)#13	99.3(17)
C(2)#10-N(2)-C(2)#13	65.2(9)
C(2)#3-N(2)-C(2)#13	114.8(9)
C(2)#11-N(2)-C(2)#13	180.0
C(2)#12-N(2)-C(2)#13	65.2(9)
C(2)#8-N(2)-C(2)	65.2(9)
C(2)#9-N(2)-C(2)	114.8(9)
C(2)#10-N(2)-C(2)	80.7(17)
C(2)#3-N(2)-C(2)	99.3(17)
C(2)#11-N(2)-C(2)	65.2(9)
C(2)#12-N(2)-C(2)	180.0
C(2)#13-N(2)-C(2)	114.8(9)
N(2)-C(2)-C(2)#8	57.4(5)
N(2)-C(2)-C(2)#11	57.4(5)
C(2)#8-C(2)-C(2)#11	90.0
N(2)-C(2)-C(3)	104.4(11)
C(2)#8-C(2)-C(3)	125.3(3)

C(2)#11-C(2)-C(3)	125.3(3)
N(2)-C(2)-C(2)#10	49.6(8)
C(2)#8-C(2)-C(2)#10	90.000(2)
C(2)#11-C(2)-C(2)#10	90.000(1)
C(3)-C(2)-C(2)#10	54.7(6)
C(4)#14-N(3)-C(4)	120.000(1)
C(4)#14-N(3)-C(4)#15	60.000(1)
C(4)-N(3)-C(4)#15	180.0(6)
C(4)#14-N(3)-C(4)#16	180.0
C(4)-N(3)-C(4)#16	60.000(1)
C(4)#15-N(3)-C(4)#16	120.0
C(4)#14-N(3)-C(4)#17	60.0
C(4)-N(3)-C(4)#17	120.0
C(4)#15-N(3)-C(4)#17	60.0
C(4)#16-N(3)-C(4)#17	120.0
C(4)#14-N(3)-C(4)#18	120.000(1)
C(4)-N(3)-C(4)#18	60.000(1)
C(4)#15-N(3)-C(4)#18	120.000(1)
C(4)#16-N(3)-C(4)#18	60.000(1)
C(4)#17-N(3)-C(4)#18	180.0
C(4)#14-N(3)-C(4)#19	90.000(2)
C(4)-N(3)-C(4)#19	120.0
C(4)#15-N(3)-C(4)#19	60.000(1)
C(4)#16-N(3)-C(4)#19	90.000(1)
C(4)#17-N(3)-C(4)#19	120.000(1)
C(4)#18-N(3)-C(4)#19	60.000(1)
C(4)#14-N(3)-C(4)#20	120.000(1)
C(4)-N(3)-C(4)#20	120.000(1)
C(4)#15-N(3)-C(4)#20	60.0
C(4)#16-N(3)-C(4)#20	60.0
C(4)#17-N(3)-C(4)#20	90.000(1)
C(4)#18-N(3)-C(4)#20	90.000(1)
C(4)#19-N(3)-C(4)#20	60.0
C(4)#14-N(3)-C(4)#21	60.0
C(4)-N(3)-C(4)#21	60.0
C(4)#15-N(3)-C(4)#21	120.000(1)

C(4)#16-N(3)-C(4)#21	120.000(1)
C(4)#17-N(3)-C(4)#21	90.000(1)
C(4)#18-N(3)-C(4)#21	90.000(2)
C(4)#19-N(3)-C(4)#21	120.000(1)
C(4)#20-N(3)-C(4)#21	180.0
C(4)#14-N(3)-C(4)#22	120.0
C(4)-N(3)-C(4)#22	90.000(2)
C(4)#15-N(3)-C(4)#22	90.0
C(4)#16-N(3)-C(4)#22	60.0
C(4)#17-N(3)-C(4)#22	60.000(1)
C(4)#18-N(3)-C(4)#22	120.000(1)
C(4)#19-N(3)-C(4)#22	120.0
C(4)#20-N(3)-C(4)#22	60.0
C(4)#21-N(3)-C(4)#22	120.000(1)
C(4)#14-N(3)-C(4)#23	60.0
C(4)-N(3)-C(4)#23	90.0
C(4)#15-N(3)-C(4)#23	90.000(1)
C(4)#16-N(3)-C(4)#23	120.0
C(4)#17-N(3)-C(4)#23	120.000(1)
C(4)#18-N(3)-C(4)#23	60.0
C(4)#19-N(3)-C(4)#23	60.0
C(4)#20-N(3)-C(4)#23	120.000(1)
C(4)#21-N(3)-C(4)#23	60.0
C(4)#22-N(3)-C(4)#23	180.0
C(4)#14-N(3)-C(4)#24	90.000(1)
C(4)-N(3)-C(4)#24	60.000(1)
C(4)#15-N(3)-C(4)#24	120.0
C(4)#16-N(3)-C(4)#24	90.000(2)
C(4)#17-N(3)-C(4)#24	60.000(1)
C(4)#18-N(3)-C(4)#24	120.000(1)
C(4)#19-N(3)-C(4)#24	180.0
C(4)#20-N(3)-C(4)#24	120.000(1)
C(4)#21-N(3)-C(4)#24	60.000(1)
C(4)#22-N(3)-C(4)#24	60.000(1)
C(4)#23-N(3)-C(4)#24	120.000(1)
C(2)-C(3)-C(2)#10	70.5(13)

C(4)#24-C(4)-N(3)	60.000(2)
C(4)#24-C(4)-C(4)#21	60.0
N(3)-C(4)-C(4)#21	60.000(2)
C(4)#24-C(4)-C(4)#16	90.000(4)
N(3)-C(4)-C(4)#16	60.000(2)
C(4)#21-C(4)-C(4)#16	120.000(7)
C(4)#24-C(4)-C(4)#18	120.000(8)
N(3)-C(4)-C(4)#18	60.000(2)
C(4)#21-C(4)-C(4)#18	90.000(6)
C(4)#16-C(4)-C(4)#18	60.0
C(4)#24-C(4)-C(5)	65.9(3)
N(3)-C(4)-C(5)	99.7(5)
C(4)#21-C(4)-C(5)	125.2(2)
C(4)#16-C(4)-C(5)	65.9(3)
C(4)#18-C(4)-C(5)	125.2(2)
C(4)#24-C(4)-C(5)#18	125.2(2)
N(3)-C(4)-C(5)#18	99.7(5)
C(4)#21-C(4)-C(5)#18	65.9(3)
C(4)#16-C(4)-C(5)#18	125.2(2)
C(4)#18-C(4)-C(5)#18	65.9(3)
C(5)-C(4)-C(5)#18	160.7(10)
C(4)#22-C(5)-C(4)#24	48.3(6)
C(4)#22-C(5)-C(4)	70.7(10)
C(4)#24-C(5)-C(4)	48.3(6)
C(4)#22-C(5)-C(4)#16	48.3(6)
C(4)#24-C(5)-C(4)#16	70.7(10)
C(4)-C(5)-C(4)#16	48.3(6)
N(1)-C(1)-S(1)	180.0(11)
C(1)-N(1)-Sm(1)	180.0(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -x,y,z #3 -x,-y,z #4 x,y,-z

#5 -x,y,-z #6 x,-y,z #7 x,-y,-z #8 -y,-x,z

#9 y,x,-z+1 #10 x,y,-z+1 #11 y,x,z #12 -x,-y,-z+1

#13 -y,-x,-z+1 #14 -y+1,-z+1,-x+1 #15 -x+1,-y+1,-z+1

#16 y,z,x #17 -z+1,-x+1,-y+1 #18 z,x,y #19 -y+1,z,x

#20 -z+1,-x+1,y #21 z,x,-y+1 #22 x,-y+1,z

#23 -x+1,y,-z+1 #24 y,-z+1,-x+1

Table 20. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for SmSCN. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Sm(1)	17(1)	17(1)	17(1)	0	0	0
N(2)	197(17)	197(17)	28(6)	0	0	0
C(2)	143(16)	260(30)	65(8)	77(13)	0	0
N(3)	30(2)	30(2)	30(2)	0	0	0
C(3)	124(13)	190(20)	210(20)	0	0	0
C(4)	63(7)	63(7)	36(7)	0	0	-38(9)
C(5)	28(5)	74(6)	74(6)	0	0	0
S(1)	98(1)	98(1)	98(1)	-34(1)	-34(1)	-34(1)
C(1)	64(3)	64(3)	64(3)	-17(2)	-17(2)	-17(2)
N(1)	80(3)	80(3)	80(3)	-25(2)	-25(2)	-25(2)

Table 21. Crystal data and structure refinement for EuSCN.

Identification code	i4mmm	
Empirical formula	C39 H82 Eu N11 O S7	
Formula weight	1097.53	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	I4/mmm	
Unit cell dimensions	a = 11.3876(5) Å	α= 90°.
	b = 11.3876(5) Å	β= 90°.
	c = 22.5539(11) Å	γ = 90°.
Volume	2924.7(3) $Å^3$	
Z	2	
Density (calculated)	1.246 Mg/m^3	
Absorption coefficient	1.359 mm^{-1}	
F(000)	1152	
Crystal size	0.107 x 0.080 x 0.033 mm^3	
Theta range for data collection	1.806 to 33.198°.	
Index ranges	-17<=h<=16, -16<=k<=16, -33<=l<=34	
Reflections collected	25799	
Independent reflections	1605 [R(int) = 0.0288]	
Completeness to theta = 25.242°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1605 / 0 / 60	
Goodness-of-fit on F^2	1.063	
Final R indices [I>2sigma(I)]	R1 = 0.0533, wR2 = 0.1489	
R indices (all data)	R1 = 0.0544, wR2 = 0.1513	
Extinction coefficient	n/a	
Largest diff. peak and hole	4.928 and -1.769 $e.Å^{-3}$	

Table 22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for EuSCN. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Eu(1)	0	0	0	29(1)
S(1)	2591(1)	2591(1)	1320(1)	77(1)
C(1)	1806(4)	1806(4)	914(4)	65(2)
N(1)	1237(5)	1237(5)	607(4)	99(3)
N(2)	0	5000	0	81(3)
C(2)	0	5786(16)	-524(12)	145(9)
C(3)	0	5000	-1134(8)	146(7)
C(4)	-1010(30)	5798(16)	0	145(9)
C(5)	-2220(30)	5000	0	171(11)
N(3)	0	0	2515(6)	81(3)
C(6)	1090(20)	0	2110(6)	93(6)
C(7)	1051(10)	0	2924(5)	54(2)
C(8)	2267(9)	0	2533(7)	100(3)

Table 23. Bond lengths [Å] and angles [°] for EuSCN.

Eu(1)-N(1)#1	2.417(7)
Eu(1)-N(1)#2	2.417(7)
Eu(1)-N(1)#3	2.417(7)
Eu(1)-N(1)#4	2.417(7)
Eu(1)-N(1)#5	2.417(7)
Eu(1)-N(1)#6	2.417(7)
Eu(1)-N(1)#7	2.417(7)
Eu(1)-N(1)	2.417(7)
S(1)-C(1)	1.561(7)
C(1)-N(1)	1.148(9)
N(2)-C(4)#8	1.47(3)
N(2)-C(4)#9	1.47(3)
N(2)-C(4)#10	1.47(3)
N(2)-C(4)	1.47(3)
N(2)-C(2)#11	1.482(19)
N(2)-C(2)#2	1.482(19)
N(2)-C(2)#10	1.482(19)
N(2)-C(2)	1.482(19)
C(2)-C(3)	1.64(3)
C(2)-C(4)#9	1.65(3)
C(2)-C(4)	1.65(3)
C(2)-C(2)#11	1.79(4)
C(3)-C(2)#11	1.64(3)
C(4)-C(2)#2	1.65(3)
C(4)-C(5)	1.65(4)
C(4)-C(4)#8	1.82(4)
C(5)-C(4)#8	1.65(4)
N(3)-C(7)#6	1.511(13)
N(3)-C(7)#5	1.511(13)
N(3)-C(7)#3	1.511(13)
N(3)-C(7)	1.511(13)
N(3)-C(6)	1.543(18)
N(3)-C(6)#5	1.543(18)
N(3)-C(6)#3	1.543(18)

N(3)-C(6)#6	1.543(18)
C(6)-C(8)	1.64(3)
C(6)-C(6)#5	1.76(3)
C(6)-C(6)#6	1.76(3)
C(6)-C(7)	1.836(15)
C(7)-C(8)	1.642(15)
C(7)-C(7)#5	1.692(17)
C(7)-C(7)#6	1.692(17)

N(1)#1-Eu(1)-N(1)#2	111.0(5)
N(1)#1-Eu(1)-N(1)#3	69.0(5)
N(1)#2-Eu(1)-N(1)#3	180.0(5)
N(1)#1-Eu(1)-N(1)#4	71.3(2)
N(1)#2-Eu(1)-N(1)#4	71.3(2)
N(1)#3-Eu(1)-N(1)#4	108.7(2)
N(1)#1-Eu(1)-N(1)#5	108.7(2)
N(1)#2-Eu(1)-N(1)#5	108.7(2)
N(1)#3-Eu(1)-N(1)#5	71.3(2)
N(1)#4-Eu(1)-N(1)#5	180.0(5)
N(1)#1-Eu(1)-N(1)#6	108.7(2)
N(1)#2-Eu(1)-N(1)#6	108.7(2)
N(1)#3-Eu(1)-N(1)#6	71.3(2)
N(1)#4-Eu(1)-N(1)#6	69.0(5)
N(1)#5-Eu(1)-N(1)#6	111.0(5)
N(1)#1-Eu(1)-N(1)#7	71.3(2)
N(1)#2-Eu(1)-N(1)#7	71.3(2)
N(1)#3-Eu(1)-N(1)#7	108.7(2)
N(1)#4-Eu(1)-N(1)#7	111.0(5)
N(1)#5-Eu(1)-N(1)#7	69.0(5)
N(1)#6-Eu(1)-N(1)#7	180.0(4)
N(1)#1-Eu(1)-N(1)	180.0
N(1)#2-Eu(1)-N(1)	69.0(5)
N(1)#3-Eu(1)-N(1)	111.0(5)
N(1)#4-Eu(1)-N(1)	108.7(2)
N(1)#5-Eu(1)-N(1)	71.3(2)
N(1)#6-Eu(1)-N(1)	71.3(2)

N(1)#7-Eu(1)-N(1)	108.7(2)
N(1)-C(1)-S(1)	178.9(9)
C(1)-N(1)-Eu(1)	177.5(9)
C(4)#8-N(2)-C(4)#9	180.0(11)
C(4)#8-N(2)-C(4)#10	103(2)
C(4)#9-N(2)-C(4)#10	77(2)
C(4)#8-N(2)-C(4)	77(2)
C(4)#9-N(2)-C(4)	103(2)
C(4)#10-N(2)-C(4)	180.0
C(4)#8-N(2)-C(2)#11	68.0(7)
C(4)#9-N(2)-C(2)#11	112.0(7)
C(4)#10-N(2)-C(2)#11	68.0(7)
C(4)-N(2)-C(2)#11	112.0(7)
C(4)#8-N(2)-C(2)#2	112.0(7)
C(4)#9-N(2)-C(2)#2	68.0(7)
C(4)#10-N(2)-C(2)#2	112.0(7)
C(4)-N(2)-C(2)#2	68.0(7)
C(2)#11-N(2)-C(2)#2	180.0(12)
C(4)#8-N(2)-C(2)#10	68.0(7)
C(4)#9-N(2)-C(2)#10	112.0(7)
C(4)#10-N(2)-C(2)#10	68.0(7)
C(4)-N(2)-C(2)#10	112.0(7)
C(2)#11-N(2)-C(2)#10	106(2)
C(2)#2-N(2)-C(2)#10	74(2)
C(4)#8-N(2)-C(2)	112.0(7)
C(4)#9-N(2)-C(2)	68.0(7)
C(4)#10-N(2)-C(2)	112.0(7)
C(4)-N(2)-C(2)	68.0(7)
C(2)#11-N(2)-C(2)	74(2)
C(2)#2-N(2)-C(2)	106(2)
C(2)#10-N(2)-C(2)	180.0
N(2)-C(2)-C(3)	109.9(13)
N(2)-C(2)-C(4)#9	55.5(11)
C(3)-C(2)-C(4)#9	127.3(13)
N(2)-C(2)-C(4)	55.5(11)
C(3)-C(2)-C(4)	127.3(13)

C(4)#9-C(2)-C(4)	88(2)
N(2)-C(2)-C(2)#11	52.9(10)
C(3)-C(2)-C(2)#11	57.0(6)
C(4)#9-C(2)-C(2)#11	90.5(9)
C(4)-C(2)-C(2)#11	90.5(9)
C(2)-C(3)-C(2)#11	66.0(12)
N(2)-C(4)-C(2)#2	56.5(12)
N(2)-C(4)-C(2)	56.5(12)
C(2)#2-C(4)-C(2)	92(2)
N(2)-C(4)-C(5)	108.3(14)
C(2)#2-C(4)-C(5)	125.3(13)
C(2)-C(4)-C(5)	125.3(13)
N(2)-C(4)-C(4)#8	51.7(11)
C(2)#2-C(4)-C(4)#8	89.5(9)
C(2)-C(4)-C(4)#8	89.5(9)
C(5)-C(4)-C(4)#8	56.6(10)
C(4)#8-C(5)-C(4)	66.8(19)
C(7)#6-N(3)-C(7)#5	104.7(12)
C(7)#6-N(3)-C(7)#3	68.1(6)
C(7)#5-N(3)-C(7)#3	68.1(6)
C(7)#6-N(3)-C(7)	68.1(6)
C(7)#5-N(3)-C(7)	68.1(6)
C(7)#3-N(3)-C(7)	104.7(12)
C(7)#6-N(3)-C(6)	111.2(4)
C(7)#5-N(3)-C(6)	111.2(4)
C(7)#3-N(3)-C(6)	178.7(13)
C(7)-N(3)-C(6)	73.9(8)
C(7)#6-N(3)-C(6)#5	178.7(13)
C(7)#5-N(3)-C(6)#5	73.9(8)
C(7)#3-N(3)-C(6)#5	111.2(4)
C(7)-N(3)-C(6)#5	111.2(4)
C(6)-N(3)-C(6)#5	69.5(9)
C(7)#6-N(3)-C(6)#3	111.2(4)
C(7)#5-N(3)-C(6)#3	111.2(4)
C(7)#3-N(3)-C(6)#3	73.9(8)
C(7)-N(3)-C(6)#3	178.7(13)

C(6)-N(3)-C(6)#3	107.4(18)
C(6)#5-N(3)-C(6)#3	69.5(9)
C(7)#6-N(3)-C(6)#6	73.9(8)
C(7)#5-N(3)-C(6)#6	178.7(13)
C(7)#3-N(3)-C(6)#6	111.2(4)
C(7)-N(3)-C(6)#6	111.2(4)
C(6)-N(3)-C(6)#6	69.5(9)
C(6)#5-N(3)-C(6)#6	107.4(18)
C(6)#3-N(3)-C(6)#6	69.5(9)
N(3)-C(6)-C(8)	108.2(10)
N(3)-C(6)-C(6)#5	55.3(5)
C(8)-C(6)-C(6)#5	125.2(3)
N(3)-C(6)-C(6)#6	55.3(5)
C(8)-C(6)-C(6)#6	125.2(3)
C(6)#5-C(6)-C(6)#6	90.002(1)
N(3)-C(6)-C(7)	52.2(7)
C(8)-C(6)-C(7)	56.0(8)
C(6)#5-C(6)-C(7)	89.0(6)
C(6)#6-C(6)-C(7)	89.0(6)
N(3)-C(7)-C(8)	109.9(8)
N(3)-C(7)-C(7)#5	55.9(3)
C(8)-C(7)-C(7)#5	126.6(3)
N(3)-C(7)-C(7)#6	55.9(3)
C(8)-C(7)-C(7)#6	126.6(3)
C(7)#5-C(7)-C(7)#6	89.999(1)
N(3)-C(7)-C(6)	53.8(9)
C(8)-C(7)-C(6)	56.1(10)
C(7)#5-C(7)-C(6)	91.0(6)
C(7)#6-C(7)-C(6)	91.0(6)
C(7)-C(8)-C(6)	67.9(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 x,y,-z #3 -x,-y,z #4 -y,x,-z

#5 y,-x,z #6 -y,x,z #7 y,-x,-z #8 x,-y+1,z

#9 -x,y,-z #10 -x,-y+1,-z #11 -x,-y+1,z

Table 24. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for EuSCN. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Eu(1)	25(1)	25(1)	36(1)	0	0	0
S(1)	86(1)	86(1)	60(1)	-6(1)	-6(1)	-39(1)
C(1)	60(2)	60(2)	75(4)	-10(2)	-10(2)	-18(3)
N(1)	77(3)	77(3)	144(8)	-32(4)	-32(4)	-16(4)
N(2)	152(11)	34(3)	57(4)	0	0	0
C(2)	230(30)	55(6)	149(15)	55(9)	0	0
C(3)	190(20)	150(20)	97(10)	0	0	0
C(4)	230(30)	55(6)	149(15)	55(9)	0	0
C(5)	230(30)	210(30)	71(7)	0	0	0
N(3)	152(11)	34(3)	57(4)	0	0	0
C(6)	155(18)	53(6)	71(7)	0	58(10)	0
C(7)	48(5)	64(6)	51(4)	0	-7(4)	0
C(8)	74(5)	84(6)	143(7)	0	27(6)	0

Table 25. Crystal data and structure refinement for GdSCN.

Identification code	i4mmm	
Empirical formula	C39 H0 Gd N11 O S7	
Formula weight	1020.17	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	I4/mmm	
Unit cell dimensions	a = 11.418(2) Å	α= 90°.
	b = 11.418(2) Å	β= 90°.
	c = 22.504(4) Å	γ = 90°.
Volume	2934.1(12) $Å^3$	
Z	2	
Density (calculated)	1.155 Mg/m^3	
Absorption coefficient	1.412 mm^{-1}	
F(000)	990	
Crystal size	0.120 x 0.100 x 0.090 mm^3	
Theta range for data collection	1.810 to 32.961°.	
Index ranges	-17<=h<=17, -17<=k<=17, -34<=l<=34	
Reflections collected	24130	
Independent reflections	1592 [R(int) = 0.0501]	
Completeness to theta = 25.242°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1592 / 0 / 59	
Goodness-of-fit on F^2	1.295	
Final R indices [I>2sigma(I)]	R1 = 0.0647, wR2 = 0.1727	
R indices (all data)	R1 = 0.0655, wR2 = 0.1738	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.434 and -1.532 $e.Å^{-3}$	

Table 26. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for GdSCN. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Gd(1)	0	0	0	29(1)
S(1)	2575(2)	2575(2)	1322(1)	75(1)
C(1)	1803(5)	1803(5)	916(4)	61(2)
N(1)	1227(5)	1227(5)	611(5)	91(3)
N(2)	0	5000	0	80(5)
C(2)	0	5800(20)	-561(16)	126(8)
C(3)	0	5000	-1097(14)	163(10)
C(4)	-950(30)	5820(20)	0	126(8)
C(5)	-2090(50)	5000	0	240(20)
N(3)	0	0	2515(5)	54(2)
C(6)	1100(20)	0	2125(7)	73(3)
C(7)	1050(20)	0	2933(7)	73(3)
C(8)	2236(12)	0	2553(8)	110(4)
OW1	-5000	5000	0	12(1)

Table 27. Bond lengths [Å] and angles [°] for GdSCN.

Gd(1)-N(1)#1	2.412(8)
Gd(1)-N(1)#2	2.412(8)
Gd(1)-N(1)#3	2.412(8)
Gd(1)-N(1)#4	2.412(8)
Gd(1)-N(1)#5	2.412(8)
Gd(1)-N(1)#6	2.412(8)
Gd(1)-N(1)#7	2.412(8)
Gd(1)-N(1)	2.412(8)
S(1)-C(1)	1.545(7)
C(1)-N(1)	1.156(10)
N(2)-C(4)	1.43(3)
N(2)-C(4)#8	1.43(3)
N(2)-C(4)#9	1.43(3)
N(2)-C(4)#10	1.43(3)
N(2)-C(2)#11	1.56(2)
N(2)-C(2)#2	1.56(2)
N(2)-C(2)#10	1.56(2)
N(2)-C(2)	1.56(2)
C(2)-C(3)	1.52(3)
C(2)-C(4)	1.66(3)
C(2)-C(4)#9	1.66(3)
C(2)-C(2)#11	1.84(5)
C(3)-C(2)#11	1.52(3)
C(4)-C(5)	1.60(4)
C(4)-C(2)#2	1.66(3)
C(4)-C(4)#8	1.87(5)
C(5)-C(4)#8	1.60(4)
N(3)-C(7)#6	1.52(2)
N(3)-C(7)#5	1.52(2)
N(3)-C(7)#3	1.52(2)
N(3)-C(7)	1.52(2)
N(3)-C(6)	1.53(2)
N(3)-C(6)#5	1.53(2)
N(3)-C(6)#3	1.53(2)

N(3)-C(6)#6	1.53(2)
C(6)-C(8)	1.62(3)
C(6)-C(6)#5	1.77(3)
C(6)-C(6)#6	1.77(3)
C(6)-C(7)	1.821(19)
C(7)-C(8)	1.60(2)
C(7)-C(7)#5	1.69(3)
C(7)-C(7)#6	1.69(3)

N(1)#1-Gd(1)-N(1)#2	110.5(6)
N(1)#1-Gd(1)-N(1)#3	69.5(6)
N(1)#2-Gd(1)-N(1)#3	180.0(6)
N(1)#1-Gd(1)-N(1)#4	71.1(3)
N(1)#2-Gd(1)-N(1)#4	71.1(3)
N(1)#3-Gd(1)-N(1)#4	108.9(3)
N(1)#1-Gd(1)-N(1)#5	108.9(3)
N(1)#2-Gd(1)-N(1)#5	108.9(3)
N(1)#3-Gd(1)-N(1)#5	71.1(3)
N(1)#4-Gd(1)-N(1)#5	180.0(6)
N(1)#1-Gd(1)-N(1)#6	108.9(3)
N(1)#2-Gd(1)-N(1)#6	108.9(3)
N(1)#3-Gd(1)-N(1)#6	71.1(3)
N(1)#4-Gd(1)-N(1)#6	69.5(6)
N(1)#5-Gd(1)-N(1)#6	110.5(6)
N(1)#1-Gd(1)-N(1)#7	71.1(3)
N(1)#2-Gd(1)-N(1)#7	71.1(3)
N(1)#3-Gd(1)-N(1)#7	108.9(3)
N(1)#4-Gd(1)-N(1)#7	110.5(6)
N(1)#5-Gd(1)-N(1)#7	69.5(6)
N(1)#6-Gd(1)-N(1)#7	180.0(4)
N(1)#1-Gd(1)-N(1)	180.0
N(1)#2-Gd(1)-N(1)	69.5(6)
N(1)#3-Gd(1)-N(1)	110.5(6)
N(1)#4-Gd(1)-N(1)	108.9(3)
N(1)#5-Gd(1)-N(1)	71.1(3)
N(1)#6-Gd(1)-N(1)	71.1(3)

N(1)#7-Gd(1)-N(1)	108.9(3)
N(1)-C(1)-S(1)	179.7(11)
C(1)-N(1)-Gd(1)	178.2(10)
C(4)-N(2)-C(4)#8	81(3)
C(4)-N(2)-C(4)#9	99(3)
C(4)#8-N(2)-C(4)#9	180.0(14)
C(4)-N(2)-C(4)#10	180.0
C(4)#8-N(2)-C(4)#10	99(3)
C(4)#9-N(2)-C(4)#10	81(3)
C(4)-N(2)-C(2)#11	112.6(9)
C(4)#8-N(2)-C(2)#11	67.4(9)
C(4)#9-N(2)-C(2)#11	112.6(9)
C(4)#10-N(2)-C(2)#11	67.4(9)
C(4)-N(2)-C(2)#2	67.4(9)
C(4)#8-N(2)-C(2)#2	112.6(9)
C(4)#9-N(2)-C(2)#2	67.4(9)
C(4)#10-N(2)-C(2)#2	112.6(9)
C(2)#11-N(2)-C(2)#2	180.0(15)
C(4)-N(2)-C(2)#10	112.6(9)
C(4)#8-N(2)-C(2)#10	67.4(9)
C(4)#9-N(2)-C(2)#10	112.6(9)
C(4)#10-N(2)-C(2)#10	67.4(9)
C(2)#11-N(2)-C(2)#10	108(3)
C(2)#2-N(2)-C(2)#10	72(3)
C(4)-N(2)-C(2)	67.4(9)
C(4)#8-N(2)-C(2)	112.6(9)
C(4)#9-N(2)-C(2)	67.4(9)
C(4)#10-N(2)-C(2)	112.6(9)
C(2)#11-N(2)-C(2)	72(3)
C(2)#2-N(2)-C(2)	108(3)
C(2)#10-N(2)-C(2)	180.0
C(3)-C(2)-N(2)	106.7(18)
C(3)-C(2)-C(4)	127.5(17)
N(2)-C(2)-C(4)	52.5(13)
C(3)-C(2)-C(4)#9	127.5(17)
N(2)-C(2)-C(4)#9	52.5(13)

C(4)-C(2)-C(4)#9	81(3)
C(3)-C(2)-C(2)#11	52.7(10)
N(2)-C(2)-C(2)#11	53.9(13)
C(4)-C(2)-C(2)#11	90.5(12)
C(4)#9-C(2)-C(2)#11	90.5(12)
C(2)-C(3)-C(2)#11	74.6(19)
N(2)-C(4)-C(5)	104(2)
N(2)-C(4)-C(2)#2	60.0(13)
C(5)-C(4)-C(2)#2	121.7(17)
N(2)-C(4)-C(2)	60.0(13)
C(5)-C(4)-C(2)	121.7(17)
C(2)#2-C(4)-C(2)	99(3)
N(2)-C(4)-C(4)#8	49.3(13)
C(5)-C(4)-C(4)#8	54.4(13)
C(2)#2-C(4)-C(4)#8	89.5(12)
C(2)-C(4)-C(4)#8	89.5(12)
C(4)#8-C(5)-C(4)	71(3)
C(7)#6-N(3)-C(7)#5	103.6(15)
C(7)#6-N(3)-C(7)#3	67.5(8)
C(7)#5-N(3)-C(7)#3	67.5(8)
C(7)#6-N(3)-C(7)	67.5(8)
C(7)#5-N(3)-C(7)	67.5(8)
C(7)#3-N(3)-C(7)	103.6(15)
C(7)#6-N(3)-C(6)	110.8(5)
C(7)#5-N(3)-C(6)	110.8(5)
C(7)#3-N(3)-C(6)	176.9(13)
C(7)-N(3)-C(6)	73.3(9)
C(7)#6-N(3)-C(6)#5	176.9(13)
C(7)#5-N(3)-C(6)#5	73.3(9)
C(7)#3-N(3)-C(6)#5	110.8(5)
C(7)-N(3)-C(6)#5	110.8(5)
C(6)-N(3)-C(6)#5	70.7(8)
C(7)#6-N(3)-C(6)#3	110.8(5)
C(7)#5-N(3)-C(6)#3	110.8(5)
C(7)#3-N(3)-C(6)#3	73.3(9)
C(7)-N(3)-C(6)#3	176.9(13)

C(6)-N(3)-C(6)#3	109.8(16)
C(6)#5-N(3)-C(6)#3	70.7(8)
C(7)#6-N(3)-C(6)#6	73.3(9)
C(7)#5-N(3)-C(6)#6	176.9(13)
C(7)#3-N(3)-C(6)#6	110.8(5)
C(7)-N(3)-C(6)#6	110.8(5)
C(6)-N(3)-C(6)#6	70.7(8)
C(6)#5-N(3)-C(6)#6	109.8(16)
C(6)#3-N(3)-C(6)#6	70.7(8)
N(3)-C(6)-C(8)	108.4(10)
N(3)-C(6)-C(6)#5	54.6(4)
C(8)-C(6)-C(6)#5	124.6(4)
N(3)-C(6)-C(6)#6	54.6(4)
C(8)-C(6)-C(6)#6	124.6(4)
C(6)#5-C(6)-C(6)#6	89.998(1)
N(3)-C(6)-C(7)	53.2(10)
C(8)-C(6)-C(7)	55.2(11)
C(6)#5-C(6)-C(7)	88.8(8)
C(6)#6-C(6)-C(7)	88.8(8)
N(3)-C(7)-C(8)	109.6(11)
N(3)-C(7)-C(7)#5	56.2(4)
C(8)-C(7)-C(7)#5	126.7(4)
N(3)-C(7)-C(7)#6	56.2(4)
C(8)-C(7)-C(7)#6	126.7(4)
C(7)#5-C(7)-C(7)#6	90.000(1)
N(3)-C(7)-C(6)	53.5(10)
C(8)-C(7)-C(6)	56.0(11)
C(7)#5-C(7)-C(6)	91.2(8)
C(7)#6-C(7)-C(6)	91.2(8)
C(7)-C(8)-C(6)	68.7(9)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 x,y,-z #3 -x,-y,z #4 -y,x,-z

#5 y,-x,z #6 -y,x,z #7 y,-x,-z #8 x,-y+1,z

#9 -x,y,-z #10 -x,-y+1,-z #11 -x,-y+1,z

Table 28. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for GdSCN. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Gd(1)	22(1)	22(1)	41(1)	0	0	0
S(1)	78(1)	78(1)	68(1)	-10(1)	-10(1)	-30(1)
C(1)	55(2)	55(2)	73(4)	-13(2)	-13(2)	-16(3)
N(1)	66(3)	66(3)	141(9)	-30(4)	-30(4)	-13(4)
N(2)	121(17)	46(7)	73(8)	0	0	0
C(2)	150(20)	66(10)	159(19)	60(13)	0	0
C(3)	120(20)	200(30)	170(20)	0	0	0
C(4)	150(20)	66(10)	159(19)	60(13)	0	0
C(5)	330(70)	270(50)	118(18)	0	0	0
N(3)	56(4)	56(4)	51(5)	0	0	0
C(6)	93(9)	66(6)	61(4)	0	12(5)	0
C(7)	93(9)	66(6)	61(4)	0	12(5)	0
C(8)	79(8)	88(8)	164(11)	0	30(9)	0
OW1	16(1)	16(1)	5(1)	0	0	0

Table 29. Crystal data and structure refinement for TbSCN.

Identification code	i4mmm	
Empirical formula	C39 H0 N11 O0 S7 Tb	
Formula weight	1005.84	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	I4/mmm	
Unit cell dimensions	a = 11.3933(6) Å	α= 90°.
	b = 11.3933(6) Å	β= 90°.
	c = 22.4759(12) Å	γ = 90°.
Volume	2917.5(3) $Å^3$	
Z	2	
Density (calculated)	1.145 Mg/m^3	
Absorption coefficient	1.494 mm^{-1}	
F(000)	976	
Crystal size	0.177 x 0.118 x 0.065 mm^3	
Theta range for data collection	1.812 to 33.129°.	
Index ranges	-16<=h<=16, -16<=k<=17, -33<=l<=33	
Reflections collected	25720	
Independent reflections	1580 [R(int) = 0.0261]	
Completeness to theta = 25.242°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1580 / 12 / 58	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0466, wR2 = 0.1344	
R indices (all data)	R1 = 0.0469, wR2 = 0.1349	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.031 and -0.901 $e.Å^{-3}$	

Table 30. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for TbSCN. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Tb(1)	0	0	0	30(1)
S(1)	2575(1)	2575(1)	1317(1)	73(1)
C(1)	1792(4)	1792(4)	912(3)	64(2)
N(1)	1221(4)	1221(4)	604(4)	95(3)
N(2)	0	5000	0	97(6)
C(2)	0	5795(12)	-531(7)	132(7)
C(3)	0	5000	-1134(7)	151(5)
C(4)	-1053(16)	5801(12)	0	132(7)
C(5)	-2250(20)	5000	0	151(5)
N(3)	0	0	2519(4)	57(2)
C(6)	1080(13)	0	2116(5)	89(5)
C(7)	1049(8)	0	2934(4)	54(2)
C(8)	2256(8)	0	2540(6)	101(3)

Table 31. Bond lengths [Å] and angles [°] for TbSCN.

Tb(1)-N(1)#1	2.391(7)
Tb(1)-N(1)#2	2.391(7)
Tb(1)-N(1)#3	2.391(7)
Tb(1)-N(1)#4	2.391(7)
Tb(1)-N(1)#5	2.391(7)
Tb(1)-N(1)#6	2.391(7)
Tb(1)-N(1)#7	2.391(7)
Tb(1)-N(1)	2.391(7)
S(1)-C(1)	1.557(6)
C(1)-N(1)	1.150(8)
N(2)-C(2)#7	1.499(12)
N(2)-C(2)#8	1.499(12)
N(2)-C(2)#9	1.499(12)
N(2)-C(2)	1.499(12)
N(2)-C(4)#10	1.507(14)
N(2)-C(4)#11	1.507(14)
N(2)-C(4)#9	1.507(14)
N(2)-C(4)	1.507(14)
C(2)-C(3)	1.630(15)
C(2)-C(4)#11	1.693(19)
C(2)-C(4)	1.693(19)
C(2)-C(2)#8	1.81(3)
C(3)-C(2)#8	1.630(15)
C(4)-C(5)	1.637(16)
C(4)-C(2)#7	1.693(19)
C(4)-C(4)#10	1.82(3)
C(5)-C(4)#10	1.637(16)
N(3)-C(7)#5	1.516(9)
N(3)-C(7)#3	1.516(9)
N(3)-C(7)#6	1.516(9)
N(3)-C(7)	1.516(9)
N(3)-C(6)#6	1.528(11)
N(3)-C(6)#3	1.528(11)
N(3)-C(6)#5	1.528(11)

N(3)-C(6)	1.528(11)
C(6)-C(8)	1.643(14)
C(6)-C(6)#3	1.74(2)
C(6)-C(6)#5	1.74(2)
C(6)-C(7)	1.839(13)
C(7)-C(8)	1.636(11)
C(7)-C(7)#3	1.690(13)
C(7)-C(7)#5	1.690(13)

N(1)#1-Tb(1)-N(1)#2	71.2(2)
N(1)#1-Tb(1)-N(1)#3	108.8(2)
N(1)#2-Tb(1)-N(1)#3	180.0(5)
N(1)#1-Tb(1)-N(1)#4	71.2(2)
N(1)#2-Tb(1)-N(1)#4	110.8(4)
N(1)#3-Tb(1)-N(1)#4	69.2(4)
N(1)#1-Tb(1)-N(1)#5	108.8(2)
N(1)#2-Tb(1)-N(1)#5	69.2(4)
N(1)#3-Tb(1)-N(1)#5	110.8(4)
N(1)#4-Tb(1)-N(1)#5	180.0(5)
N(1)#1-Tb(1)-N(1)#6	69.2(4)
N(1)#2-Tb(1)-N(1)#6	108.8(2)
N(1)#3-Tb(1)-N(1)#6	71.2(2)
N(1)#4-Tb(1)-N(1)#6	108.8(2)
N(1)#5-Tb(1)-N(1)#6	71.2(2)
N(1)#1-Tb(1)-N(1)#7	110.8(4)
N(1)#2-Tb(1)-N(1)#7	71.2(2)
N(1)#3-Tb(1)-N(1)#7	108.8(2)
N(1)#4-Tb(1)-N(1)#7	71.2(2)
N(1)#5-Tb(1)-N(1)#7	108.8(2)
N(1)#6-Tb(1)-N(1)#7	180.0(5)
N(1)#1-Tb(1)-N(1)	180.0
N(1)#2-Tb(1)-N(1)	108.8(2)
N(1)#3-Tb(1)-N(1)	71.2(2)
N(1)#4-Tb(1)-N(1)	108.8(2)
N(1)#5-Tb(1)-N(1)	71.2(2)
N(1)#6-Tb(1)-N(1)	110.8(4)

N(1)#7-Tb(1)-N(1)	69.2(4)
N(1)-C(1)-S(1)	178.9(8)
C(1)-N(1)-Tb(1)	177.7(8)
C(2)#7-N(2)-C(2)#8	180.0(9)
C(2)#7-N(2)-C(2)#9	74.4(13)
C(2)#8-N(2)-C(2)#9	105.6(13)
C(2)#7-N(2)-C(2)	105.6(13)
C(2)#8-N(2)-C(2)	74.4(13)
C(2)#9-N(2)-C(2)	180.0
C(2)#7-N(2)-C(4)#10	111.5(5)
C(2)#8-N(2)-C(4)#10	68.5(5)
C(2)#9-N(2)-C(4)#10	68.5(5)
C(2)-N(2)-C(4)#10	111.5(5)
C(2)#7-N(2)-C(4)#11	68.5(5)
C(2)#8-N(2)-C(4)#11	111.5(5)
C(2)#9-N(2)-C(4)#11	111.5(5)
C(2)-N(2)-C(4)#11	68.5(5)
C(4)#10-N(2)-C(4)#11	180.0
C(2)#7-N(2)-C(4)#9	111.5(5)
C(2)#8-N(2)-C(4)#9	68.5(5)
C(2)#9-N(2)-C(4)#9	68.5(5)
C(2)-N(2)-C(4)#9	111.5(5)
C(4)#10-N(2)-C(4)#9	105.5(14)
C(4)#11-N(2)-C(4)#9	74.5(14)
C(2)#7-N(2)-C(4)	68.5(5)
C(2)#8-N(2)-C(4)	111.5(5)
C(2)#9-N(2)-C(4)	111.5(5)
C(2)-N(2)-C(4)	68.5(5)
C(4)#10-N(2)-C(4)	74.5(14)
C(4)#11-N(2)-C(4)	105.5(14)
C(4)#9-N(2)-C(4)	180.0
N(2)-C(2)-C(3)	109.1(10)
N(2)-C(2)-C(4)#11	56.0(5)
C(3)-C(2)-C(4)#11	126.1(8)
N(2)-C(2)-C(4)	56.0(5)
C(3)-C(2)-C(4)	126.1(8)

C(4)#11-C(2)-C(4)	90.3(10)
N(2)-C(2)-C(2)#8	52.8(7)
C(3)-C(2)-C(2)#8	56.2(5)
C(4)#11-C(2)-C(2)#8	90.2(7)
C(4)-C(2)-C(2)#8	90.2(7)
C(2)-C(3)-C(2)#8	67.5(10)
N(2)-C(4)-C(5)	108.9(11)
N(2)-C(4)-C(2)#7	55.5(5)
C(5)-C(4)-C(2)#7	125.9(9)
N(2)-C(4)-C(2)	55.5(5)
C(5)-C(4)-C(2)	125.9(9)
C(2)#7-C(4)-C(2)	89.7(10)
N(2)-C(4)-C(4)#10	52.8(7)
C(5)-C(4)-C(4)#10	56.1(6)
C(2)#7-C(4)-C(4)#10	89.8(7)
C(2)-C(4)-C(4)#10	89.8(7)
C(4)-C(5)-C(4)#10	67.7(13)
C(7)#5-N(3)-C(7)#3	104.0(9)
C(7)#5-N(3)-C(7)#6	67.7(5)
C(7)#3-N(3)-C(7)#6	67.7(5)
C(7)#5-N(3)-C(7)	67.7(5)
C(7)#3-N(3)-C(7)	67.7(5)
C(7)#6-N(3)-C(7)	104.0(9)
C(7)#5-N(3)-C(6)#6	111.4(3)
C(7)#3-N(3)-C(6)#6	111.4(3)
C(7)#6-N(3)-C(6)#6	74.3(6)
C(7)-N(3)-C(6)#6	178.4(9)
C(7)#5-N(3)-C(6)#3	178.3(9)
C(7)#3-N(3)-C(6)#3	74.3(6)
C(7)#6-N(3)-C(6)#3	111.4(3)
C(7)-N(3)-C(6)#3	111.4(3)
C(6)#6-N(3)-C(6)#3	69.4(7)
C(7)#5-N(3)-C(6)#5	74.3(6)
C(7)#3-N(3)-C(6)#5	178.3(9)
C(7)#6-N(3)-C(6)#5	111.4(3)
C(7)-N(3)-C(6)#5	111.4(3)

C(6)#6-N(3)-C(6)#5	69.4(7)
C(6)#3-N(3)-C(6)#5	107.3(13)
C(7)#5-N(3)-C(6)	111.4(3)
C(7)#3-N(3)-C(6)	111.4(3)
C(7)#6-N(3)-C(6)	178.4(9)
C(7)-N(3)-C(6)	74.3(6)
C(6)#6-N(3)-C(6)	107.3(13)
C(6)#3-N(3)-C(6)	69.4(7)
C(6)#5-N(3)-C(6)	69.4(7)
N(3)-C(6)-C(8)	108.3(7)
N(3)-C(6)-C(6)#3	55.3(3)
C(8)-C(6)-C(6)#3	125.2(3)
N(3)-C(6)-C(6)#5	55.3(3)
C(8)-C(6)-C(6)#5	125.2(3)
C(6)#3-C(6)-C(6)#5	90.002(2)
N(3)-C(6)-C(7)	52.5(5)
C(8)-C(6)-C(7)	55.7(5)
C(6)#3-C(6)-C(7)	89.2(4)
C(6)#5-C(6)-C(7)	89.2(4)
N(3)-C(7)-C(8)	109.2(6)
N(3)-C(7)-C(7)#3	56.1(2)
C(8)-C(7)-C(7)#3	126.5(3)
N(3)-C(7)-C(7)#5	56.1(2)
C(8)-C(7)-C(7)#5	126.5(3)
C(7)#3-C(7)-C(7)#5	89.999(1)
N(3)-C(7)-C(6)	53.1(5)
C(8)-C(7)-C(6)	56.1(5)
C(7)#3-C(7)-C(6)	90.8(4)
C(7)#5-C(7)-C(6)	90.8(4)
C(7)-C(8)-C(6)	68.2(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -y,x,-z #3 y,-x,z #4 y,-x,-z

#5 -y,x,z #6 -x,-y,z #7 x,y,-z #8 -x,-y+1,z

#9 -x,-y+1,-z #10 x,-y+1,z #11 -x,y,-z

Table 32. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for TbSCN. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Tb(1)	26(1)	26(1)	37(1)	0	0	0
S(1)	78(1)	78(1)	62(1)	-5(1)	-5(1)	-33(1)
C(1)	59(2)	59(2)	75(3)	-10(2)	-10(2)	-16(3)
N(1)	73(3)	73(3)	139(7)	-28(3)	-28(3)	-14(4)
N(2)	176(18)	37(5)	79(7)	0	0	0
C(2)	200(20)	54(6)	145(13)	50(8)	0	0
C(3)	179(16)	180(15)	94(6)	0	0	0
C(4)	200(20)	54(6)	145(13)	50(8)	0	0
C(5)	179(16)	180(15)	94(6)	0	0	0
N(3)	62(3)	62(3)	48(4)	0	0	0
C(6)	146(15)	51(6)	71(7)	0	53(9)	0
C(7)	49(4)	63(5)	49(4)	0	-7(3)	0
C(8)	70(5)	81(5)	151(7)	0	26(6)	0

Table 33. Crystal data and structure refinement for DySCN.

Identification code	i4mmm	
Empirical formula	C39 H0 Dy N11 O0 S7	
Formula weight	1009.42	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	I4/mmm	
Unit cell dimensions	a = 11.4134(6) Å	α= 90°.
	b = 11.4134(6) Å	β= 90°.
	c = 22.6144(11) Å	γ = 90°.
Volume	2945.9(3) $Å^3$	
Z	2	
Density (calculated)	1.138 Mg/m^3	
Absorption coefficient	1.547 mm^{-1}	
F(000)	978	
Crystal size	0.147 x 0.125 x 0.060 mm^3	
Theta range for data collection	1.801 to 30.465°.	
Index ranges	-16<=h<=16, -16<=k<=16, -31<=l<=31	
Reflections collected	21181	
Independent reflections	1310 [R(int) = 0.0172]	
Completeness to theta = 25.242°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1310 / 12 / 58	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2sigma(I)]	R1 = 0.0393, wR2 = 0.1132	
R indices (all data)	R1 = 0.0393, wR2 = 0.1132	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.906 and -0.802 $e.Å^{-3}$	

Table 34. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for DySCN. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Dy(1)	0	0	0	28(1)
S(1)	2564(1)	2564(1)	1320(1)	73(1)
C(1)	1779(4)	1779(4)	916(3)	61(1)
N(1)	1215(4)	1215(4)	615(3)	80(2)
N(2)	0	5000	0	104(6)
C(2)	0	5799(12)	-528(7)	133(6)
C(3)	0	5000	-1124(7)	147(5)
C(4)	-1058(15)	5805(12)	0	133(6)
C(5)	-2240(18)	5000	0	147(5)
N(3)	0	0	2534(4)	55(2)
C(6)	1081(12)	0	2133(4)	86(5)
C(7)	1060(8)	0	2942(3)	52(2)
C(8)	2259(7)	0	2548(5)	92(2)

Table 35. Bond lengths [Å] and angles [°] for DySCN.

Dy(1)-N(1)	2.403(6)
Dy(1)-N(1)#1	2.404(6)
Dy(1)-N(1)#2	2.404(6)
Dy(1)-N(1)#3	2.404(6)
Dy(1)-N(1)#4	2.404(6)
Dy(1)-N(1)#5	2.404(6)
Dy(1)-N(1)#6	2.404(6)
Dy(1)-N(1)#7	2.404(6)
S(1)-C(1)	1.563(6)
C(1)-N(1)	1.136(7)
N(2)-C(2)#4	1.502(12)
N(2)-C(2)#8	1.502(12)
N(2)-C(2)#9	1.502(12)
N(2)-C(2)	1.502(12)
N(2)-C(4)#10	1.518(14)
N(2)-C(4)#11	1.518(14)
N(2)-C(4)#9	1.518(14)
N(2)-C(4)	1.518(14)
C(2)-C(3)	1.628(14)
C(2)-C(4)#11	1.698(18)
C(2)-C(4)	1.698(18)
C(2)-C(2)#8	1.82(3)
C(3)-C(2)#8	1.628(14)
C(4)-C(5)	1.632(15)
C(4)-C(2)#4	1.698(18)
C(4)-C(4)#10	1.84(3)
C(5)-C(4)#10	1.632(15)
N(3)-C(7)#5	1.520(9)
N(3)-C(7)	1.520(9)
N(3)-C(7)#7	1.520(9)
N(3)-C(7)#3	1.520(9)
N(3)-C(6)#3	1.531(10)
N(3)-C(6)#7	1.531(10)
N(3)-C(6)#5	1.531(10)

N(3)-C(6)	1.531(10)
C(6)-C(8)	1.640(13)
C(6)-C(6)#7	1.745(19)
C(6)-C(6)#5	1.745(19)
C(6)-C(7)	1.828(11)
C(7)-C(8)	1.633(10)
C(7)-C(7)#7	1.710(12)
C(7)-C(7)#5	1.710(12)

N(1)-Dy(1)-N(1)#1	180.0
N(1)-Dy(1)-N(1)#2	109.55(16)
N(1)#1-Dy(1)-N(1)#2	70.45(16)
N(1)-Dy(1)-N(1)#3	109.3(3)
N(1)#1-Dy(1)-N(1)#3	70.7(3)
N(1)#2-Dy(1)-N(1)#3	109.55(16)
N(1)-Dy(1)-N(1)#4	70.7(3)
N(1)#1-Dy(1)-N(1)#4	109.3(3)
N(1)#2-Dy(1)-N(1)#4	70.45(16)
N(1)#3-Dy(1)-N(1)#4	180.0(4)
N(1)-Dy(1)-N(1)#5	70.45(16)
N(1)#1-Dy(1)-N(1)#5	109.55(16)
N(1)#2-Dy(1)-N(1)#5	70.7(3)
N(1)#3-Dy(1)-N(1)#5	70.45(16)
N(1)#4-Dy(1)-N(1)#5	109.55(16)
N(1)-Dy(1)-N(1)#6	109.55(16)
N(1)#1-Dy(1)-N(1)#6	70.45(16)
N(1)#2-Dy(1)-N(1)#6	109.3(3)
N(1)#3-Dy(1)-N(1)#6	109.55(16)
N(1)#4-Dy(1)-N(1)#6	70.45(16)
N(1)#5-Dy(1)-N(1)#6	180.0(3)
N(1)-Dy(1)-N(1)#7	70.45(16)
N(1)#1-Dy(1)-N(1)#7	109.55(16)
N(1)#2-Dy(1)-N(1)#7	180.0(4)
N(1)#3-Dy(1)-N(1)#7	70.45(16)
N(1)#4-Dy(1)-N(1)#7	109.55(16)
N(1)#5-Dy(1)-N(1)#7	109.3(3)

N(1)#6-Dy(1)-N(1)#7	70.7(3)
N(1)-C(1)-S(1)	179.1(7)
C(1)-N(1)-Dy(1)	178.6(6)
C(2)#4-N(2)-C(2)#8	180.0(8)
C(2)#4-N(2)-C(2)#9	74.8(13)
C(2)#8-N(2)-C(2)#9	105.2(13)
C(2)#4-N(2)-C(2)	105.2(13)
C(2)#8-N(2)-C(2)	74.8(13)
C(2)#9-N(2)-C(2)	180.0
C(2)#4-N(2)-C(4)#10	111.6(5)
C(2)#8-N(2)-C(4)#10	68.4(5)
C(2)#9-N(2)-C(4)#10	68.4(5)
C(2)-N(2)-C(4)#10	111.6(5)
C(2)#4-N(2)-C(4)#11	68.4(5)
C(2)#8-N(2)-C(4)#11	111.6(5)
C(2)#9-N(2)-C(4)#11	111.6(5)
C(2)-N(2)-C(4)#11	68.4(5)
C(4)#10-N(2)-C(4)#11	180.0(8)
C(2)#4-N(2)-C(4)#9	111.6(5)
C(2)#8-N(2)-C(4)#9	68.4(5)
C(2)#9-N(2)-C(4)#9	68.4(5)
C(2)-N(2)-C(4)#9	111.6(5)
C(4)#10-N(2)-C(4)#9	105.5(13)
C(4)#11-N(2)-C(4)#9	74.5(13)
C(2)#4-N(2)-C(4)	68.4(5)
C(2)#8-N(2)-C(4)	111.6(5)
C(2)#9-N(2)-C(4)	111.6(5)
C(2)-N(2)-C(4)	68.4(5)
C(4)#10-N(2)-C(4)	74.5(13)
C(4)#11-N(2)-C(4)	105.5(13)
C(4)#9-N(2)-C(4)	180.0
N(2)-C(2)-C(3)	108.5(10)
N(2)-C(2)-C(4)#11	56.2(5)
C(3)-C(2)-C(4)#11	125.8(8)
N(2)-C(2)-C(4)	56.2(5)
C(3)-C(2)-C(4)	125.8(8)

C(4)#11-C(2)-C(4)	90.7(10)
N(2)-C(2)-C(2)#8	52.6(7)
C(3)-C(2)-C(2)#8	55.9(5)
C(4)#11-C(2)-C(2)#8	90.2(7)
C(4)-C(2)-C(2)#8	90.2(7)
C(2)-C(3)-C(2)#8	68.1(10)
N(2)-C(4)-C(5)	108.5(11)
N(2)-C(4)-C(2)#4	55.3(5)
C(5)-C(4)-C(2)#4	125.8(9)
N(2)-C(4)-C(2)	55.3(5)
C(5)-C(4)-C(2)	125.8(9)
C(2)#4-C(4)-C(2)	89.3(10)
N(2)-C(4)-C(4)#10	52.7(6)
C(5)-C(4)-C(4)#10	55.7(6)
C(2)#4-C(4)-C(4)#10	89.8(7)
C(2)-C(4)-C(4)#10	89.8(7)
C(4)-C(5)-C(4)#10	68.6(12)
C(7)#5-N(3)-C(7)	68.4(4)
C(7)#5-N(3)-C(7)#7	105.4(9)
C(7)-N(3)-C(7)#7	68.4(4)
C(7)#5-N(3)-C(7)#3	68.4(4)
C(7)-N(3)-C(7)#3	105.4(9)
C(7)#7-N(3)-C(7)#3	68.4(4)
C(7)#5-N(3)-C(6)#3	111.0(3)
C(7)-N(3)-C(6)#3	179.0(8)
C(7)#7-N(3)-C(6)#3	111.0(3)
C(7)#3-N(3)-C(6)#3	73.6(6)
C(7)#5-N(3)-C(6)#7	179.0(8)
C(7)-N(3)-C(6)#7	111.0(3)
C(7)#7-N(3)-C(6)#7	73.6(6)
C(7)#3-N(3)-C(6)#7	111.0(3)
C(6)#3-N(3)-C(6)#7	69.5(6)
C(7)#5-N(3)-C(6)#5	73.6(6)
C(7)-N(3)-C(6)#5	111.0(3)
C(7)#7-N(3)-C(6)#5	179.0(8)
C(7)#3-N(3)-C(6)#5	111.0(3)

C(6)#3-N(3)-C(6)#5	69.5(6)
C(6)#7-N(3)-C(6)#5	107.4(11)
C(7)#5-N(3)-C(6)	111.0(3)
C(7)-N(3)-C(6)	73.6(6)
C(7)#7-N(3)-C(6)	111.0(3)
C(7)#3-N(3)-C(6)	179.0(8)
C(6)#3-N(3)-C(6)	107.4(11)
C(6)#7-N(3)-C(6)	69.5(6)
C(6)#5-N(3)-C(6)	69.5(6)
N(3)-C(6)-C(8)	108.8(6)
N(3)-C(6)-C(6)#7	55.3(3)
C(8)-C(6)-C(6)#7	125.4(2)
N(3)-C(6)-C(6)#5	55.3(3)
C(8)-C(6)-C(6)#5	125.4(2)
C(6)#7-C(6)-C(6)#5	89.998(1)
N(3)-C(6)-C(7)	52.9(4)
C(8)-C(6)-C(7)	55.9(5)
C(6)#7-C(6)-C(7)	89.5(4)
C(6)#5-C(6)-C(7)	89.5(4)
N(3)-C(7)-C(8)	109.7(6)
N(3)-C(7)-C(7)#7	55.8(2)
C(8)-C(7)-C(7)#7	126.4(2)
N(3)-C(7)-C(7)#5	55.8(2)
C(8)-C(7)-C(7)#5	126.4(2)
C(7)#7-C(7)-C(7)#5	90.001(1)
N(3)-C(7)-C(6)	53.5(5)
C(8)-C(7)-C(6)	56.2(5)
C(7)#7-C(7)-C(6)	90.5(4)
C(7)#5-C(7)-C(6)	90.5(4)
C(7)-C(8)-C(6)	67.9(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -y,x,-z #3 -x,-y,z #4 x,y,-z

#5 -y,x,z #6 y,-x,-z #7 y,-x,z #8 -x,-y+1,z

#9 -x,-y+1,-z #10 x,-y+1,z #11 -x,y,-z

Table 36. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for DySCN. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Dy(1)	26(1)	26(1)	31(1)	0	0	0
S(1)	78(1)	78(1)	64(1)	-6(1)	-6(1)	-30(1)
C(1)	60(2)	60(2)	62(3)	-9(2)	-9(2)	-16(3)
N(1)	73(2)	73(2)	94(4)	-16(2)	-16(2)	-18(3)
N(2)	177(18)	37(5)	99(9)	0	0	0
C(2)	181(18)	54(5)	164(14)	54(9)	0	0
C(3)	163(13)	167(13)	112(7)	0	0	0
C(4)	181(18)	54(5)	164(14)	54(9)	0	0
C(5)	163(13)	167(13)	112(7)	0	0	0
N(3)	60(3)	60(3)	44(3)	0	0	0
C(6)	147(14)	51(5)	59(5)	0	50(8)	0
C(7)	46(4)	66(5)	44(4)	0	-9(3)	0
C(8)	65(4)	79(4)	132(6)	0	18(5)	0

Table 37. Crystal data and structure refinement for HoSCN.

Identification code	i4mmm	
Empirical formula	C39 H0 Ho N11 O0 S7	
Formula weight	1011.85	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	I4/mmm	
Unit cell dimensions	a = 11.4039(4) Å	α= 90°.
	b = 11.4039(4) Å	β= 90°.
	c = 22.5714(8) Å	γ = 90°.
Volume	2935.4(2) $Å^3$	
Z	2	
Density (calculated)	1.145 Mg/m^3	
Absorption coefficient	1.628 mm^{-1}	
F(000)	980	
Crystal size	0.150 x 0.110 x 0.044 mm^3	
Theta range for data collection	1.804 to 33.092°.	
Index ranges	-16<=h<=17, -17<=k<=17, -34<=l<=33	
Reflections collected	25910	
Independent reflections	1615 [R(int) = 0.0196]	
Completeness to theta = 25.242°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1615 / 12 / 58	
Goodness-of-fit on F^2	0.987	
Final R indices [I>2sigma(I)]	R1 = 0.0398, wR2 = 0.1151	
R indices (all data)	R1 = 0.0398, wR2 = 0.1151	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.017 and -0.932 $e.Å^{-3}$	

Table 38. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for HoSCN. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ho(1)	0	0	0	27(1)
S(1)	2563(1)	2563(1)	1319(1)	72(1)
C(1)	1782(3)	1782(3)	917(3)	58(1)
N(1)	1210(3)	1210(3)	612(3)	75(2)
N(2)	0	5000	0	102(6)
C(2)	0	5801(11)	-524(7)	131(6)
C(3)	0	5000	-1123(7)	150(5)
C(4)	-1054(15)	5809(12)	0	131(6)
C(5)	-2238(19)	5000	0	150(5)
N(3)	0	0	2533(3)	53(2)
C(6)	1081(11)	0	2132(4)	84(5)
C(7)	1056(7)	0	2944(3)	49(2)
C(8)	2259(6)	0	2551(5)	91(2)

Table 39. Bond lengths [Å] and angles [°] for HoSCN.

Ho(1)-N(1)	2.391(5)
Ho(1)-N(1)#1	2.391(5)
Ho(1)-N(1)#2	2.391(5)
Ho(1)-N(1)#3	2.391(5)
Ho(1)-N(1)#4	2.391(5)
Ho(1)-N(1)#5	2.391(5)
Ho(1)-N(1)#6	2.391(5)
Ho(1)-N(1)#7	2.391(5)
S(1)-C(1)	1.551(6)
C(1)-N(1)	1.152(7)
N(2)-C(2)#4	1.495(12)
N(2)-C(2)#8	1.495(12)
N(2)-C(2)#9	1.495(12)
N(2)-C(2)	1.495(12)
N(2)-C(4)#10	1.515(14)
N(2)-C(4)#11	1.515(14)
N(2)-C(4)#9	1.515(14)
N(2)-C(4)	1.515(14)
C(2)-C(3)	1.632(14)
C(2)-C(4)#11	1.687(18)
C(2)-C(4)	1.687(18)
C(2)-C(2)#8	1.83(3)
C(3)-C(2)#8	1.632(14)
C(4)-C(5)	1.635(16)
C(4)-C(2)#4	1.687(18)
C(4)-C(4)#10	1.85(3)
C(5)-C(4)#10	1.635(16)
N(3)-C(7)#5	1.519(8)
N(3)-C(7)#7	1.519(8)
N(3)-C(7)#3	1.519(8)
N(3)-C(7)	1.519(8)
N(3)-C(6)#3	1.529(10)
N(3)-C(6)#7	1.529(10)
N(3)-C(6)#5	1.529(10)

N(3)-C(6)	1.529(10)
C(6)-C(8)	1.643(13)
C(6)-C(6)#7	1.743(19)
C(6)-C(6)#5	1.743(19)
C(6)-C(7)	1.832(11)
C(7)-C(8)	1.634(10)
C(7)-C(7)#7	1.702(12)
C(7)-C(7)#5	1.702(12)

N(1)-Ho(1)-N(1)#1	180.0
N(1)-Ho(1)-N(1)#2	109.48(16)
N(1)#1-Ho(1)-N(1)#2	70.52(16)
N(1)-Ho(1)-N(1)#3	109.4(3)
N(1)#1-Ho(1)-N(1)#3	70.6(3)
N(1)#2-Ho(1)-N(1)#3	109.48(16)
N(1)-Ho(1)-N(1)#4	70.6(3)
N(1)#1-Ho(1)-N(1)#4	109.4(3)
N(1)#2-Ho(1)-N(1)#4	70.52(16)
N(1)#3-Ho(1)-N(1)#4	180.0(4)
N(1)-Ho(1)-N(1)#5	70.52(16)
N(1)#1-Ho(1)-N(1)#5	109.48(16)
N(1)#2-Ho(1)-N(1)#5	70.6(3)
N(1)#3-Ho(1)-N(1)#5	70.52(16)
N(1)#4-Ho(1)-N(1)#5	109.48(16)
N(1)-Ho(1)-N(1)#6	109.48(16)
N(1)#1-Ho(1)-N(1)#6	70.52(16)
N(1)#2-Ho(1)-N(1)#6	109.4(3)
N(1)#3-Ho(1)-N(1)#6	109.48(16)
N(1)#4-Ho(1)-N(1)#6	70.52(16)
N(1)#5-Ho(1)-N(1)#6	180.0(3)
N(1)-Ho(1)-N(1)#7	70.52(16)
N(1)#1-Ho(1)-N(1)#7	109.48(16)
N(1)#2-Ho(1)-N(1)#7	180.0(4)
N(1)#3-Ho(1)-N(1)#7	70.52(16)
N(1)#4-Ho(1)-N(1)#7	109.48(16)
N(1)#5-Ho(1)-N(1)#7	109.4(3)

N(1)#6-Ho(1)-N(1)#7	70.6(3)
N(1)-C(1)-S(1)	179.0(7)
C(1)-N(1)-Ho(1)	178.5(6)
C(2)#4-N(2)-C(2)#8	180.0(8)
C(2)#4-N(2)-C(2)#9	75.3(13)
C(2)#8-N(2)-C(2)#9	104.7(13)
C(2)#4-N(2)-C(2)	104.7(13)
C(2)#8-N(2)-C(2)	75.3(13)
C(2)#9-N(2)-C(2)	180.0
C(2)#4-N(2)-C(4)#10	111.9(5)
C(2)#8-N(2)-C(4)#10	68.1(5)
C(2)#9-N(2)-C(4)#10	68.1(5)
C(2)-N(2)-C(4)#10	111.9(5)
C(2)#4-N(2)-C(4)#11	68.1(5)
C(2)#8-N(2)-C(4)#11	111.9(5)
C(2)#9-N(2)-C(4)#11	111.9(5)
C(2)-N(2)-C(4)#11	68.1(5)
C(4)#10-N(2)-C(4)#11	180.0(8)
C(2)#4-N(2)-C(4)#9	111.9(5)
C(2)#8-N(2)-C(4)#9	68.1(5)
C(2)#9-N(2)-C(4)#9	68.1(5)
C(2)-N(2)-C(4)#9	111.9(5)
C(4)#10-N(2)-C(4)#9	105.0(13)
C(4)#11-N(2)-C(4)#9	75.0(13)
C(2)#4-N(2)-C(4)	68.1(5)
C(2)#8-N(2)-C(4)	111.9(5)
C(2)#9-N(2)-C(4)	111.9(5)
C(2)-N(2)-C(4)	68.1(5)
C(4)#10-N(2)-C(4)	75.0(13)
C(4)#11-N(2)-C(4)	105.0(13)
C(4)#9-N(2)-C(4)	180.0(8)
N(2)-C(2)-C(3)	108.3(10)
N(2)-C(2)-C(4)#11	56.5(5)
C(3)-C(2)-C(4)#11	125.8(8)
N(2)-C(2)-C(4)	56.5(5)
C(3)-C(2)-C(4)	125.8(8)

C(4)#11-C(2)-C(4)	90.9(10)
N(2)-C(2)-C(2)#8	52.3(6)
C(3)-C(2)-C(2)#8	55.9(5)
C(4)#11-C(2)-C(2)#8	90.3(6)
C(4)-C(2)-C(2)#8	90.3(6)
C(2)-C(3)-C(2)#8	68.1(9)
N(2)-C(4)-C(5)	108.1(11)
N(2)-C(4)-C(2)#4	55.4(5)
C(5)-C(4)-C(2)#4	125.8(9)
N(2)-C(4)-C(2)	55.4(5)
C(5)-C(4)-C(2)	125.8(9)
C(2)#4-C(4)-C(2)	89.1(10)
N(2)-C(4)-C(4)#10	52.5(6)
C(5)-C(4)-C(4)#10	55.7(6)
C(2)#4-C(4)-C(4)#10	89.7(6)
C(2)-C(4)-C(4)#10	89.7(6)
C(4)-C(5)-C(4)#10	68.7(12)
C(7)#5-N(3)-C(7)#7	104.8(8)
C(7)#5-N(3)-C(7)#3	68.2(4)
C(7)#7-N(3)-C(7)#3	68.2(4)
C(7)#5-N(3)-C(7)	68.2(4)
C(7)#7-N(3)-C(7)	68.2(4)
C(7)#3-N(3)-C(7)	104.8(8)
C(7)#5-N(3)-C(6)#3	111.2(3)
C(7)#7-N(3)-C(6)#3	111.2(3)
C(7)#3-N(3)-C(6)#3	73.9(6)
C(7)-N(3)-C(6)#3	178.7(8)
C(7)#5-N(3)-C(6)#7	178.7(8)
C(7)#7-N(3)-C(6)#7	73.9(6)
C(7)#3-N(3)-C(6)#7	111.2(3)
C(7)-N(3)-C(6)#7	111.2(3)
C(6)#3-N(3)-C(6)#7	69.5(6)
C(7)#5-N(3)-C(6)#5	73.9(6)
C(7)#7-N(3)-C(6)#5	178.7(8)
C(7)#3-N(3)-C(6)#5	111.2(3)
C(7)-N(3)-C(6)#5	111.2(3)

C(6)#3-N(3)-C(6)#5	69.5(6)
C(6)#7-N(3)-C(6)#5	107.4(11)
C(7)#5-N(3)-C(6)	111.2(3)
C(7)#7-N(3)-C(6)	111.2(3)
C(7)#3-N(3)-C(6)	178.7(8)
C(7)-N(3)-C(6)	73.9(6)
C(6)#3-N(3)-C(6)	107.4(11)
C(6)#7-N(3)-C(6)	69.5(6)
C(6)#5-N(3)-C(6)	69.5(6)
N(3)-C(6)-C(8)	108.6(6)
N(3)-C(6)-C(6)#7	55.3(3)
C(8)-C(6)-C(6)#7	125.3(2)
N(3)-C(6)-C(6)#5	55.3(3)
C(8)-C(6)-C(6)#5	125.3(2)
C(6)#7-C(6)-C(6)#5	90.001(1)
N(3)-C(6)-C(7)	52.8(4)
C(8)-C(6)-C(7)	55.8(4)
C(6)#7-C(6)-C(7)	89.4(3)
C(6)#5-C(6)-C(7)	89.4(3)
N(3)-C(7)-C(8)	109.5(6)
N(3)-C(7)-C(7)#7	55.9(2)
C(8)-C(7)-C(7)#7	126.4(2)
N(3)-C(7)-C(7)#5	55.9(2)
C(8)-C(7)-C(7)#5	126.4(2)
C(7)#7-C(7)-C(7)#5	90.000(1)
N(3)-C(7)-C(6)	53.3(5)
C(8)-C(7)-C(6)	56.2(5)
C(7)#7-C(7)-C(6)	90.6(3)
C(7)#5-C(7)-C(6)	90.6(3)
C(7)-C(8)-C(6)	68.0(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -y,x,-z #3 -x,-y,z #4 x,y,-z

#5 -y,x,z #6 y,-x,-z #7 y,-x,z #8 -x,-y+1,z

#9 -x,-y+1,-z #10 x,-y+1,z #11 -x,y,-z

Table 40. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for HoSCN. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ho(1)	26(1)	26(1)	30(1)	0	0	0
S(1)	77(1)	77(1)	61(1)	-6(1)	-6(1)	-31(1)
C(1)	57(2)	57(2)	60(2)	-7(1)	-7(1)	-14(2)
N(1)	67(2)	67(2)	89(4)	-16(2)	-16(2)	-15(3)
N(2)	177(18)	39(4)	92(8)	0	0	0
C(2)	186(18)	55(5)	151(13)	52(8)	0	0
C(3)	171(14)	175(14)	102(7)	0	0	0
C(4)	186(18)	55(5)	151(13)	52(8)	0	0
C(5)	171(14)	175(14)	102(7)	0	0	0
N(3)	59(3)	59(3)	40(3)	0	0	0
C(6)	146(13)	48(5)	57(5)	0	51(7)	0
C(7)	47(4)	57(4)	45(3)	0	-8(3)	0
C(8)	62(4)	77(4)	135(6)	0	17(5)	0

Table 41. Crystal data and structure refinement for ErSCN.

Identification code	i4mmm	
Empirical formula	C39 H0 Er N11 O0 S7	
Formula weight	1014.18	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	I4/mmm	
Unit cell dimensions	a = 11.4093(6) Å	α= 90°.
	b = 11.4093(6) Å	β= 90°.
	c = 22.5770(11) Å	γ = 90°.
Volume	2938.9(3) $Å^3$	
Z	2	
Density (calculated)	1.146 Mg/m^3	
Absorption coefficient	1.707 mm^{-1}	
F(000)	982	
Crystal size	0.160 x 0.074 x 0.070 mm^3	
Theta range for data collection	1.804 to 30.552°.	
Index ranges	-16<=h<=16, -16<=k<=16, -31<=l<=32	
Reflections collected	21183	
Independent reflections	1317 [R(int) = 0.0193]	
Completeness to theta = 25.242°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1317 / 12 / 57	
Goodness-of-fit on F^2	1.095	
Final R indices [I>2sigma(I)]	R1 = 0.0397, wR2 = 0.1143	
R indices (all data)	R1 = 0.0398, wR2 = 0.1145	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.944 and -0.868 $e.Å^{-3}$	

Table 42. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ErSCN. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Er(1)	0	0	0	27(1)
S(1)	2555(1)	2555(1)	1319(1)	72(1)
C(1)	1769(4)	1769(4)	914(3)	60(1)
N(1)	1202(4)	1202(4)	613(3)	75(2)
N(2)	0	5000	0	108(6)
C(2)	0	5811(12)	-524(8)	129(6)
C(3)	0	5000	-1117(8)	144(6)
C(4)	-1050(16)	5819(13)	0	129(6)
C(5)	-2220(20)	5000	0	160(9)
N(3)	0	0	2539(4)	54(2)
C(6)	1073(10)	0	2131(4)	61(2)
C(7)	1052(10)	0	2952(4)	61(2)
C(8)	2252(7)	0	2552(5)	90(2)

Table 43. Bond lengths [Å] and angles [°] for ErSCN.

Er(1)-N(1)	2.384(6)
Er(1)-N(1)#1	2.384(6)
Er(1)-N(1)#2	2.384(6)
Er(1)-N(1)#3	2.384(6)
Er(1)-N(1)#4	2.384(6)
Er(1)-N(1)#5	2.384(6)
Er(1)-N(1)#6	2.384(6)
Er(1)-N(1)#7	2.384(6)
S(1)-C(1)	1.564(6)
C(1)-N(1)	1.139(8)
N(2)-C(2)#4	1.503(12)
N(2)-C(2)#8	1.503(12)
N(2)-C(2)#9	1.503(12)
N(2)-C(2)	1.503(12)
N(2)-C(4)#10	1.519(14)
N(2)-C(4)#11	1.519(14)
N(2)-C(4)#9	1.519(14)
N(2)-C(4)	1.519(14)
C(2)-C(3)	1.628(15)
C(2)-C(4)#11	1.684(19)
C(2)-C(4)	1.684(19)
C(2)-C(2)#8	1.85(3)
C(3)-C(2)#8	1.628(15)
C(4)-C(5)	1.631(16)
C(4)-C(2)#4	1.684(19)
C(4)-C(4)#10	1.87(3)
C(5)-C(4)#10	1.631(16)
N(3)-C(7)#5	1.520(11)
N(3)-C(7)#7	1.520(11)
N(3)-C(7)#3	1.520(11)
N(3)-C(7)	1.520(11)
N(3)-C(6)#3	1.531(10)
N(3)-C(6)#7	1.531(10)
N(3)-C(6)#5	1.531(10)

N(3)-C(6)	1.531(10)
C(6)-C(8)	1.647(12)
C(6)-C(6)#7	1.731(16)
C(6)-C(6)#5	1.731(16)
C(6)-C(7)	1.853(12)
C(7)-C(8)	1.640(12)
C(7)-C(7)#7	1.697(16)
C(7)-C(7)#5	1.697(16)

N(1)-Er(1)-N(1)#1	180.0
N(1)-Er(1)-N(1)#2	109.73(17)
N(1)#1-Er(1)-N(1)#2	70.27(17)
N(1)-Er(1)-N(1)#3	109.0(3)
N(1)#1-Er(1)-N(1)#3	71.0(3)
N(1)#2-Er(1)-N(1)#3	109.73(17)
N(1)-Er(1)-N(1)#4	71.0(3)
N(1)#1-Er(1)-N(1)#4	109.0(3)
N(1)#2-Er(1)-N(1)#4	70.27(17)
N(1)#3-Er(1)-N(1)#4	180.0(4)
N(1)-Er(1)-N(1)#5	70.27(17)
N(1)#1-Er(1)-N(1)#5	109.73(17)
N(1)#2-Er(1)-N(1)#5	71.0(3)
N(1)#3-Er(1)-N(1)#5	70.27(17)
N(1)#4-Er(1)-N(1)#5	109.73(17)
N(1)-Er(1)-N(1)#6	109.73(17)
N(1)#1-Er(1)-N(1)#6	70.27(17)
N(1)#2-Er(1)-N(1)#6	109.0(3)
N(1)#3-Er(1)-N(1)#6	109.73(17)
N(1)#4-Er(1)-N(1)#6	70.27(17)
N(1)#5-Er(1)-N(1)#6	180.0(3)
N(1)-Er(1)-N(1)#7	70.27(17)
N(1)#1-Er(1)-N(1)#7	109.73(17)
N(1)#2-Er(1)-N(1)#7	180.0(4)
N(1)#3-Er(1)-N(1)#7	70.27(17)
N(1)#4-Er(1)-N(1)#7	109.73(17)
N(1)#5-Er(1)-N(1)#7	109.0(3)

N(1)#6-Er(1)-N(1)#7	71.0(3)
N(1)-C(1)-S(1)	179.2(7)
C(1)-N(1)-Er(1)	178.9(6)
C(2)#4-N(2)-C(2)#8	180.0(9)
C(2)#4-N(2)-C(2)#9	76.0(14)
C(2)#8-N(2)-C(2)#9	104.0(14)
C(2)#4-N(2)-C(2)	104.0(14)
C(2)#8-N(2)-C(2)	76.0(14)
C(2)#9-N(2)-C(2)	180.0
C(2)#4-N(2)-C(4)#10	112.3(5)
C(2)#8-N(2)-C(4)#10	67.7(5)
C(2)#9-N(2)-C(4)#10	67.7(5)
C(2)-N(2)-C(4)#10	112.3(5)
C(2)#4-N(2)-C(4)#11	67.7(5)
C(2)#8-N(2)-C(4)#11	112.3(5)
C(2)#9-N(2)-C(4)#11	112.3(5)
C(2)-N(2)-C(4)#11	67.7(5)
C(4)#10-N(2)-C(4)#11	180.0(9)
C(2)#4-N(2)-C(4)#9	112.3(5)
C(2)#8-N(2)-C(4)#9	67.7(5)
C(2)#9-N(2)-C(4)#9	67.7(5)
C(2)-N(2)-C(4)#9	112.3(5)
C(4)#10-N(2)-C(4)#9	104.1(14)
C(4)#11-N(2)-C(4)#9	75.9(14)
C(2)#4-N(2)-C(4)	67.7(5)
C(2)#8-N(2)-C(4)	112.3(5)
C(2)#9-N(2)-C(4)	112.3(5)
C(2)-N(2)-C(4)	67.7(5)
C(4)#10-N(2)-C(4)	75.9(14)
C(4)#11-N(2)-C(4)	104.1(14)
C(4)#9-N(2)-C(4)	180.0
N(2)-C(2)-C(3)	107.3(11)
N(2)-C(2)-C(4)#11	56.6(5)
C(3)-C(2)-C(4)#11	125.5(9)
N(2)-C(2)-C(4)	56.6(5)
C(3)-C(2)-C(4)	125.5(9)

C(4)#11-C(2)-C(4)	90.7(11)
N(2)-C(2)-C(2)#8	52.0(7)
C(3)-C(2)-C(2)#8	55.3(5)
C(4)#11-C(2)-C(2)#8	90.3(7)
C(4)-C(2)-C(2)#8	90.3(7)
C(2)#8-C(3)-C(2)	69.3(11)
N(2)-C(4)-C(5)	107.1(12)
N(2)-C(4)-C(2)	55.7(5)
C(5)-C(4)-C(2)	125.5(10)
N(2)-C(4)-C(2)#4	55.7(5)
C(5)-C(4)-C(2)#4	125.5(10)
C(2)-C(4)-C(2)#4	89.3(11)
N(2)-C(4)-C(4)#10	52.1(7)
C(5)-C(4)-C(4)#10	55.1(7)
C(2)-C(4)-C(4)#10	89.7(7)
C(2)#4-C(4)-C(4)#10	89.7(7)
C(4)-C(5)-C(4)#10	69.9(13)
C(7)#5-N(3)-C(7)#7	104.3(9)
C(7)#5-N(3)-C(7)#3	67.9(5)
C(7)#7-N(3)-C(7)#3	67.9(5)
C(7)#5-N(3)-C(7)	67.9(5)
C(7)#7-N(3)-C(7)	67.9(5)
C(7)#3-N(3)-C(7)	104.3(9)
C(7)#5-N(3)-C(6)#3	111.6(3)
C(7)#7-N(3)-C(6)#3	111.6(3)
C(7)#3-N(3)-C(6)#3	74.8(5)
C(7)-N(3)-C(6)#3	179.1(8)
C(7)#5-N(3)-C(6)#7	179.1(8)
C(7)#7-N(3)-C(6)#7	74.8(5)
C(7)#3-N(3)-C(6)#7	111.6(3)
C(7)-N(3)-C(6)#7	111.6(3)
C(6)#3-N(3)-C(6)#7	68.9(5)
C(7)#5-N(3)-C(6)#5	74.8(5)
C(7)#7-N(3)-C(6)#5	179.1(8)
C(7)#3-N(3)-C(6)#5	111.6(3)
C(7)-N(3)-C(6)#5	111.6(3)

C(6)#3-N(3)-C(6)#5	68.9(5)
C(6)#7-N(3)-C(6)#5	106.2(10)
C(7)#5-N(3)-C(6)	111.6(3)
C(7)#7-N(3)-C(6)	111.6(3)
C(7)#3-N(3)-C(6)	179.1(8)
C(7)-N(3)-C(6)	74.8(5)
C(6)#3-N(3)-C(6)	106.2(10)
C(6)#7-N(3)-C(6)	68.8(5)
C(6)#5-N(3)-C(6)	68.8(5)
N(3)-C(6)-C(8)	107.9(6)
N(3)-C(6)-C(6)#7	55.6(3)
C(8)-C(6)-C(6)#7	125.3(2)
N(3)-C(6)-C(6)#5	55.6(3)
C(8)-C(6)-C(6)#5	125.3(2)
C(6)#7-C(6)-C(6)#5	90.000(1)
N(3)-C(6)-C(7)	52.3(4)
C(8)-C(6)-C(7)	55.5(5)
C(6)#7-C(6)-C(7)	89.5(3)
C(6)#5-C(6)-C(7)	89.5(3)
N(3)-C(7)-C(8)	108.8(6)
N(3)-C(7)-C(7)#7	56.1(2)
C(8)-C(7)-C(7)#7	126.2(3)
N(3)-C(7)-C(7)#5	56.1(2)
C(8)-C(7)-C(7)#5	126.2(3)
C(7)#7-C(7)-C(7)#5	90.001(1)
N(3)-C(7)-C(6)	52.9(5)
C(8)-C(7)-C(6)	55.9(5)
C(7)#7-C(7)-C(6)	90.5(3)
C(7)#5-C(7)-C(6)	90.5(3)
C(7)-C(8)-C(6)	68.6(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -y,x,-z #3 -x,-y,z #4 x,y,-z

#5 -y,x,z #6 y,-x,-z #7 y,-x,z #8 -x,-y+1,z

#9 -x,-y+1,-z #10 x,-y+1,z #11 -x,y,-z

Table 44. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for ErSCN. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Er(1)	26(1)	26(1)	30(1)	0	0	0
S(1)	77(1)	77(1)	63(1)	-6(1)	-6(1)	-29(1)
C(1)	59(2)	59(2)	61(3)	-7(2)	-7(2)	-14(3)
N(1)	71(2)	71(2)	82(4)	-15(2)	-15(2)	-18(3)
N(2)	183(19)	31(5)	109(11)	0	0	0
C(2)	172(18)	58(6)	156(15)	52(10)	0	0
C(3)	160(20)	150(20)	122(12)	0	0	0
C(4)	172(18)	58(6)	156(15)	52(10)	0	0
C(5)	180(20)	200(20)	96(10)	0	0	0
N(3)	58(3)	58(3)	45(4)	0	0	0
C(6)	74(5)	63(4)	46(3)	0	8(3)	0
C(7)	74(5)	63(4)	46(3)	0	8(3)	0
C(8)	63(4)	75(4)	132(7)	0	15(5)	0

Table 45. Crystal data and structure refinement for TmSCN.

Identification code	i4mmm	
Empirical formula	C39 H0 N11 O0 S7 Tm	
Formula weight	1015.85	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	I4/mmm	
Unit cell dimensions	a = 11.3875(10) Å	α= 90°.
	b = 11.3875(10) Å	β= 90°.
	c = 22.478(2) Å	γ = 90°.
Volume	2914.9(6) $Å^3$	
Z	2	
Density (calculated)	1.157 Mg/m^3	
Absorption coefficient	1.804 mm^{-1}	
F(000)	984	
Crystal size	0.130 x 0.128 x 0.065 mm^3	
Theta range for data collection	1.812 to 33.060°.	
Index ranges	-17<=h<=17, -17<=k<=17, -34<=l<=34	
Reflections collected	25512	
Independent reflections	1582 [R(int) = 0.0248]	
Completeness to theta = 25.242°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1582 / 12 / 59	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I)]	R1 = 0.0390, wR2 = 0.1132	
R indices (all data)	R1 = 0.0391, wR2 = 0.1134	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.966 and -0.912 $e.Å^{-3}$	

Table 46. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for TmSCN. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Tm(1)	0	0	0	26(1)
S(1)	2559(1)	2559(1)	1316(1)	70(1)
C(1)	1773(4)	1773(4)	913(3)	59(1)
N(1)	1202(4)	1202(4)	603(3)	76(2)
N(2)	0	5000	0	103(6)
C(2)	0	5795(12)	-528(7)	126(6)
C(3)	0	5000	-1132(7)	150(6)
C(4)	-1046(15)	5814(12)	0	126(6)
C(5)	-2223(19)	5000	0	150(6)
N(3)	0	0	2536(4)	50(2)
C(6)	1076(12)	0	2131(4)	80(5)
C(7)	1053(7)	0	2948(4)	48(2)
C(8)	2256(7)	0	2552(5)	89(2)

Table 47. Bond lengths [Å] and angles [°] for TmSCN.

Tm(1)-N(1)#1	2.364(6)
Tm(1)-N(1)#2	2.364(6)
Tm(1)-N(1)#3	2.364(6)
Tm(1)-N(1)#4	2.364(6)
Tm(1)-N(1)#5	2.364(6)
Tm(1)-N(1)#6	2.364(6)
Tm(1)-N(1)#7	2.364(6)
Tm(1)-N(1)	2.364(6)
S(1)-C(1)	1.557(6)
C(1)-N(1)	1.152(7)
N(2)-C(2)	1.493(12)
N(2)-C(2)#5	1.493(12)
N(2)-C(2)#8	1.493(12)
N(2)-C(2)#9	1.493(12)
N(2)-C(4)	1.509(14)
N(2)-C(4)#10	1.509(14)
N(2)-C(4)#11	1.509(14)
N(2)-C(4)#9	1.509(14)
C(2)-C(3)	1.631(15)
C(2)-C(4)#11	1.682(18)
C(2)-C(4)	1.682(18)
C(2)-C(2)#8	1.81(3)
C(3)-C(2)#8	1.631(15)
C(4)-C(5)	1.629(16)
C(4)-C(2)#5	1.682(18)
C(4)-C(4)#10	1.85(3)
C(5)-C(4)#10	1.629(16)
N(3)-C(7)	1.516(8)
N(3)-C(7)#6	1.516(8)
N(3)-C(7)#3	1.516(8)
N(3)-C(7)#4	1.516(8)
N(3)-C(6)#4	1.527(10)
N(3)-C(6)#3	1.527(10)
N(3)-C(6)#6	1.527(10)

N(3)-C(6)	1.527(10)
C(6)-C(8)	1.644(14)
C(6)-C(6)#3	1.733(19)
C(6)-C(6)#6	1.733(19)
C(6)-C(7)	1.837(12)
C(7)-C(8)	1.634(10)
C(7)-C(7)#3	1.697(12)
C(7)-C(7)#6	1.697(12)

N(1)#1-Tm(1)-N(1)#2	70.79(18)
N(1)#1-Tm(1)-N(1)#3	109.21(18)
N(1)#2-Tm(1)-N(1)#3	180.0(4)
N(1)#1-Tm(1)-N(1)#4	70.0(4)
N(1)#2-Tm(1)-N(1)#4	109.21(18)
N(1)#3-Tm(1)-N(1)#4	70.79(18)
N(1)#1-Tm(1)-N(1)#5	110.0(4)
N(1)#2-Tm(1)-N(1)#5	70.79(18)
N(1)#3-Tm(1)-N(1)#5	109.21(18)
N(1)#4-Tm(1)-N(1)#5	180.0(3)
N(1)#1-Tm(1)-N(1)#6	109.21(18)
N(1)#2-Tm(1)-N(1)#6	70.0(4)
N(1)#3-Tm(1)-N(1)#6	110.0(4)
N(1)#4-Tm(1)-N(1)#6	70.79(18)
N(1)#5-Tm(1)-N(1)#6	109.21(18)
N(1)#1-Tm(1)-N(1)#7	70.79(18)
N(1)#2-Tm(1)-N(1)#7	110.0(4)
N(1)#3-Tm(1)-N(1)#7	70.0(4)
N(1)#4-Tm(1)-N(1)#7	109.21(18)
N(1)#5-Tm(1)-N(1)#7	70.79(18)
N(1)#6-Tm(1)-N(1)#7	180.0(3)
N(1)#1-Tm(1)-N(1)	180.0
N(1)#2-Tm(1)-N(1)	109.21(18)
N(1)#3-Tm(1)-N(1)	70.79(18)
N(1)#4-Tm(1)-N(1)	110.0(4)
N(1)#5-Tm(1)-N(1)	70.0(4)
N(1)#6-Tm(1)-N(1)	70.79(18)

N(1)#7-Tm(1)-N(1)	109.21(18)
N(1)-C(1)-S(1)	178.5(7)
C(1)-N(1)-Tm(1)	177.8(6)
C(2)-N(2)-C(2)#5	105.4(13)
C(2)-N(2)-C(2)#8	74.6(13)
C(2)#5-N(2)-C(2)#8	180.0(8)
C(2)-N(2)-C(2)#9	180.0
C(2)#5-N(2)-C(2)#9	74.6(13)
C(2)#8-N(2)-C(2)#9	105.4(13)
C(2)-N(2)-C(4)	68.1(5)
C(2)#5-N(2)-C(4)	68.1(5)
C(2)#8-N(2)-C(4)	111.9(5)
C(2)#9-N(2)-C(4)	111.9(5)
C(2)-N(2)-C(4)#10	111.9(5)
C(2)#5-N(2)-C(4)#10	111.9(5)
C(2)#8-N(2)-C(4)#10	68.1(5)
C(2)#9-N(2)-C(4)#10	68.1(5)
C(4)-N(2)-C(4)#10	75.8(13)
C(2)-N(2)-C(4)#11	68.1(5)
C(2)#5-N(2)-C(4)#11	68.1(5)
C(2)#8-N(2)-C(4)#11	111.9(5)
C(2)#9-N(2)-C(4)#11	111.9(5)
C(4)-N(2)-C(4)#11	104.2(13)
C(4)#10-N(2)-C(4)#11	180.0(8)
C(2)-N(2)-C(4)#9	111.9(5)
C(2)#5-N(2)-C(4)#9	111.9(5)
C(2)#8-N(2)-C(4)#9	68.1(5)
C(2)#9-N(2)-C(4)#9	68.1(5)
C(4)-N(2)-C(4)#9	180.0
C(4)#10-N(2)-C(4)#9	104.2(13)
C(4)#11-N(2)-C(4)#9	75.8(13)
N(2)-C(2)-C(3)	109.0(10)
N(2)-C(2)-C(4)#11	56.4(5)
C(3)-C(2)-C(4)#11	126.5(8)
N(2)-C(2)-C(4)	56.4(5)
C(3)-C(2)-C(4)	126.5(8)

C(4)#11-C(2)-C(4)	90.1(10)
N(2)-C(2)-C(2)#8	52.7(6)
C(3)-C(2)-C(2)#8	56.3(5)
C(4)#11-C(2)-C(2)#8	90.7(6)
C(4)-C(2)-C(2)#8	90.7(6)
C(2)#8-C(3)-C(2)	67.4(10)
N(2)-C(4)-C(5)	107.5(11)
N(2)-C(4)-C(2)	55.5(5)
C(5)-C(4)-C(2)	125.1(9)
N(2)-C(4)-C(2)#5	55.5(5)
C(5)-C(4)-C(2)#5	125.1(9)
C(2)-C(4)-C(2)#5	89.8(10)
N(2)-C(4)-C(4)#10	52.1(6)
C(5)-C(4)-C(4)#10	55.3(6)
C(2)-C(4)-C(4)#10	89.3(6)
C(2)#5-C(4)-C(4)#10	89.3(6)
C(4)-C(5)-C(4)#10	69.3(12)
C(7)-N(3)-C(7)#6	68.1(4)
C(7)-N(3)-C(7)#3	68.1(4)
C(7)#6-N(3)-C(7)#3	104.6(8)
C(7)-N(3)-C(7)#4	104.6(8)
C(7)#6-N(3)-C(7)#4	68.1(4)
C(7)#3-N(3)-C(7)#4	68.1(4)
C(7)-N(3)-C(6)#4	178.9(8)
C(7)#6-N(3)-C(6)#4	111.4(3)
C(7)#3-N(3)-C(6)#4	111.4(3)
C(7)#4-N(3)-C(6)#4	74.3(6)
C(7)-N(3)-C(6)#3	111.4(3)
C(7)#6-N(3)-C(6)#3	178.9(8)
C(7)#3-N(3)-C(6)#3	74.3(6)
C(7)#4-N(3)-C(6)#3	111.4(3)
C(6)#4-N(3)-C(6)#3	69.2(6)
C(7)-N(3)-C(6)#6	111.4(3)
C(7)#6-N(3)-C(6)#6	74.3(6)
C(7)#3-N(3)-C(6)#6	178.9(8)
C(7)#4-N(3)-C(6)#6	111.4(3)

C(6)#4-N(3)-C(6)#6	69.2(6)
C(6)#3-N(3)-C(6)#6	106.8(11)
C(7)-N(3)-C(6)	74.3(6)
C(7)#6-N(3)-C(6)	111.4(3)
C(7)#3-N(3)-C(6)	111.4(3)
C(7)#4-N(3)-C(6)	178.9(8)
C(6)#4-N(3)-C(6)	106.8(11)
C(6)#3-N(3)-C(6)	69.2(6)
C(6)#6-N(3)-C(6)	69.2(6)
N(3)-C(6)-C(8)	108.2(6)
N(3)-C(6)-C(6)#3	55.4(3)
C(8)-C(6)-C(6)#3	125.3(2)
N(3)-C(6)-C(6)#6	55.4(3)
C(8)-C(6)-C(6)#6	125.3(2)
C(6)#3-C(6)-C(6)#6	89.999(1)
N(3)-C(6)-C(7)	52.6(4)
C(8)-C(6)-C(7)	55.6(5)
C(6)#3-C(6)-C(7)	89.4(3)
C(6)#6-C(6)-C(7)	89.4(3)
N(3)-C(7)-C(8)	109.3(6)
N(3)-C(7)-C(7)#3	56.0(2)
C(8)-C(7)-C(7)#3	126.4(2)
N(3)-C(7)-C(7)#6	56.0(2)
C(8)-C(7)-C(7)#6	126.4(2)
C(7)#3-C(7)-C(7)#6	90.000(1)
N(3)-C(7)-C(6)	53.1(5)
C(8)-C(7)-C(6)	56.2(5)
C(7)#3-C(7)-C(6)	90.6(3)
C(7)#6-C(7)-C(6)	90.6(3)
C(7)-C(8)-C(6)	68.2(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -y,x,-z #3 y,-x,z #4 -x,-y,z

#5 x,y,-z #6 -y,x,z #7 y,-x,-z #8 -x,-y+1,z

#9 -x,-y+1,-z #10 x,-y+1,z #11 -x,y,-z

Table 48. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for TmSCN. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Tm(1)	25(1)	25(1)	28(1)	0	0	0
S(1)	76(1)	76(1)	59(1)	-6(1)	-6(1)	-33(1)
C(1)	57(2)	57(2)	63(3)	-7(2)	-7(2)	-13(2)
N(1)	66(2)	66(2)	98(4)	-18(2)	-18(2)	-15(3)
N(2)	186(19)	36(4)	87(8)	0	0	0
C(2)	189(19)	52(5)	136(12)	45(8)	0	0
C(3)	179(16)	183(16)	90(6)	0	0	0
C(4)	189(19)	52(5)	136(12)	45(8)	0	0
C(5)	179(16)	183(16)	90(6)	0	0	0
N(3)	55(3)	55(3)	41(3)	0	0	0
C(6)	137(13)	43(4)	61(5)	0	50(7)	0
C(7)	44(4)	57(5)	43(3)	0	-10(3)	0
C(8)	60(4)	76(4)	132(6)	0	17(5)	0

Table 49. Crystal data and structure refinement for YbSCN.

Identification code	i4mmm	
Empirical formula	C39 H0 N11 O0 S7 Yb	
Formula weight	1019.96	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	I4/mmm	
Unit cell dimensions	a = 11.3736(4) Å	α= 90°.
	b = 11.3736(4) Å	β= 90°.
	c = 22.4950(8) Å	γ = 90°.
Volume	2909.9(2) $Å^3$	
Z	2	
Density (calculated)	1.164 Mg/m^3	
Absorption coefficient	1.889 mm^{-1}	
F(000)	986	
Crystal size	0.202 x 0.139 x 0.081 mm^3	
Theta range for data collection	1.811 to 33.115°.	
Index ranges	-17<=h<=17, -16<=k<=16, -33<=l<=33	
Reflections collected	25655	
Independent reflections	1600 [R(int) = 0.0192]	
Completeness to theta = 25.242°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1600 / 12 / 56	
Goodness-of-fit on F^2	1.110	
Final R indices [I>2sigma(I)]	R1 = 0.0446, wR2 = 0.1261	
R indices (all data)	R1 = 0.0446, wR2 = 0.1261	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.921 and -1.630 $e.Å^{-3}$	

Table 50. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for YbSCN. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Yb(1)	0	0	0	26(1)
S(1)	2573(1)	2573(1)	1318(1)	67(1)
C(1)	1785(4)	1785(4)	914(3)	54(1)
N(1)	1214(4)	1214(4)	603(3)	71(2)
N(2)	0	5000	0	78(3)
C(2)	0	5806(12)	-527(8)	124(7)
C(3)	0	5000	-1120(8)	164(7)
C(4)	-1027(17)	5835(13)	0	124(7)
C(5)	-2170(20)	5000	0	164(7)
N(3)	0	0	2524(5)	78(3)
C(6)	1085(12)	0	2119(5)	76(5)
C(7)	1056(8)	0	2936(3)	44(2)
C(8)	2261(7)	0	2541(6)	84(2)

Table 51. Bond lengths [Å] and angles [°] for YbSCN.

Yb(1)-N(1)	2.378(6)
Yb(1)-N(1)#1	2.378(6)
Yb(1)-N(1)#2	2.378(6)
Yb(1)-N(1)#3	2.378(6)
Yb(1)-N(1)#4	2.378(6)
Yb(1)-N(1)#5	2.378(6)
Yb(1)-N(1)#6	2.378(6)
Yb(1)-N(1)#7	2.378(6)
S(1)-C(1)	1.558(6)
C(1)-N(1)	1.156(8)
N(2)-C(2)#4	1.498(12)
N(2)-C(2)#8	1.498(12)
N(2)-C(2)#9	1.498(12)
N(2)-C(2)	1.498(12)
N(2)-C(4)	1.505(15)
N(2)-C(4)#10	1.505(15)
N(2)-C(4)#11	1.505(15)
N(2)-C(4)#9	1.505(15)
C(2)-C(3)	1.620(15)
C(2)-C(4)	1.66(2)
C(2)-C(4)#11	1.66(2)
C(2)-C(2)#8	1.83(3)
C(3)-C(2)#8	1.620(15)
C(4)-C(5)	1.612(17)
C(4)-C(2)#4	1.66(2)
C(4)-C(4)#10	1.90(3)
C(5)-C(4)#10	1.612(17)
N(3)-C(7)#5	1.516(9)
N(3)-C(7)#7	1.516(9)
N(3)-C(7)#3	1.516(9)
N(3)-C(7)	1.517(9)
N(3)-C(6)#3	1.533(11)
N(3)-C(6)#7	1.533(11)
N(3)-C(6)#5	1.533(11)

N(3)-C(6)	1.533(11)
C(6)-C(8)	1.640(14)
C(6)-C(6)#7	1.74(2)
C(6)-C(6)#5	1.74(2)
C(6)-C(7)	1.836(12)
C(7)-C(8)	1.633(11)
C(7)-C(7)#7	1.698(12)
C(7)-C(7)#5	1.698(12)

N(1)-Yb(1)-N(1)#1	180.0
N(1)-Yb(1)-N(1)#2	109.01(19)
N(1)#1-Yb(1)-N(1)#2	70.99(19)
N(1)-Yb(1)-N(1)#3	110.4(4)
N(1)#1-Yb(1)-N(1)#3	69.6(4)
N(1)#2-Yb(1)-N(1)#3	109.01(19)
N(1)-Yb(1)-N(1)#4	69.6(4)
N(1)#1-Yb(1)-N(1)#4	110.4(4)
N(1)#2-Yb(1)-N(1)#4	70.99(19)
N(1)#3-Yb(1)-N(1)#4	180.0(4)
N(1)-Yb(1)-N(1)#5	70.99(19)
N(1)#1-Yb(1)-N(1)#5	109.01(19)
N(1)#2-Yb(1)-N(1)#5	69.6(4)
N(1)#3-Yb(1)-N(1)#5	70.99(19)
N(1)#4-Yb(1)-N(1)#5	109.01(19)
N(1)-Yb(1)-N(1)#6	109.01(19)
N(1)#1-Yb(1)-N(1)#6	70.99(19)
N(1)#2-Yb(1)-N(1)#6	110.4(4)
N(1)#3-Yb(1)-N(1)#6	109.01(19)
N(1)#4-Yb(1)-N(1)#6	70.99(19)
N(1)#5-Yb(1)-N(1)#6	180.0(3)
N(1)-Yb(1)-N(1)#7	70.99(19)
N(1)#1-Yb(1)-N(1)#7	109.01(19)
N(1)#2-Yb(1)-N(1)#7	180.0(4)
N(1)#3-Yb(1)-N(1)#7	70.99(19)
N(1)#4-Yb(1)-N(1)#7	109.01(19)
N(1)#5-Yb(1)-N(1)#7	110.4(4)

N(1)#6-Yb(1)-N(1)#7	69.6(4)
N(1)-C(1)-S(1)	178.3(7)
C(1)-N(1)-Yb(1)	177.5(7)
C(2)#4-N(2)-C(2)#8	180.0(9)
C(2)#4-N(2)-C(2)#9	75.5(14)
C(2)#8-N(2)-C(2)#9	104.5(14)
C(2)#4-N(2)-C(2)	104.5(14)
C(2)#8-N(2)-C(2)	75.5(14)
C(2)#9-N(2)-C(2)	180.0
C(2)#4-N(2)-C(4)	67.3(6)
C(2)#8-N(2)-C(4)	112.7(6)
C(2)#9-N(2)-C(4)	112.7(6)
C(2)-N(2)-C(4)	67.3(6)
C(2)#4-N(2)-C(4)#10	112.7(6)
C(2)#8-N(2)-C(4)#10	67.3(6)
C(2)#9-N(2)-C(4)#10	67.3(6)
C(2)-N(2)-C(4)#10	112.7(6)
C(4)-N(2)-C(4)#10	78.3(15)
C(2)#4-N(2)-C(4)#11	67.3(6)
C(2)#8-N(2)-C(4)#11	112.7(6)
C(2)#9-N(2)-C(4)#11	112.7(6)
C(2)-N(2)-C(4)#11	67.3(6)
C(4)-N(2)-C(4)#11	101.7(15)
C(4)#10-N(2)-C(4)#11	180.0(8)
C(2)#4-N(2)-C(4)#9	112.7(6)
C(2)#8-N(2)-C(4)#9	67.3(5)
C(2)#9-N(2)-C(4)#9	67.3(5)
C(2)-N(2)-C(4)#9	112.7(6)
C(4)-N(2)-C(4)#9	180.0
C(4)#10-N(2)-C(4)#9	101.7(15)
C(4)#11-N(2)-C(4)#9	78.3(15)
N(2)-C(2)-C(3)	107.8(11)
N(2)-C(2)-C(4)	56.6(5)
C(3)-C(2)-C(4)	126.7(9)
N(2)-C(2)-C(4)#11	56.6(5)
C(3)-C(2)-C(4)#11	126.7(9)

C(4)-C(2)-C(4)#11	89.1(11)
N(2)-C(2)-C(2)#8	52.3(7)
C(3)-C(2)-C(2)#8	55.5(5)
C(4)-C(2)-C(2)#8	91.1(7)
C(4)#11-C(2)-C(2)#8	91.1(7)
C(2)-C(3)-C(2)#8	69.0(11)
N(2)-C(4)-C(5)	104.8(12)
N(2)-C(4)-C(2)#4	56.2(6)
C(5)-C(4)-C(2)#4	123.7(10)
N(2)-C(4)-C(2)	56.2(6)
C(5)-C(4)-C(2)	123.7(10)
C(2)#4-C(4)-C(2)	90.8(11)
N(2)-C(4)-C(4)#10	50.9(7)
C(5)-C(4)-C(4)#10	53.9(7)
C(2)#4-C(4)-C(4)#10	88.9(7)
C(2)-C(4)-C(4)#10	88.9(7)
C(4)#10-C(5)-C(4)	72.2(14)
C(7)#5-N(3)-C(7)#7	104.7(10)
C(7)#5-N(3)-C(7)#3	68.1(5)
C(7)#7-N(3)-C(7)#3	68.1(5)
C(7)#5-N(3)-C(7)	68.1(5)
C(7)#7-N(3)-C(7)	68.1(5)
C(7)#3-N(3)-C(7)	104.7(10)
C(7)#5-N(3)-C(6)#3	111.3(3)
C(7)#7-N(3)-C(6)#3	111.3(3)
C(7)#3-N(3)-C(6)#3	74.0(6)
C(7)-N(3)-C(6)#3	178.8(10)
C(7)#5-N(3)-C(6)#7	178.8(10)
C(7)#7-N(3)-C(6)#7	74.0(6)
C(7)#3-N(3)-C(6)#7	111.3(3)
C(7)-N(3)-C(6)#7	111.3(3)
C(6)#3-N(3)-C(6)#7	69.4(7)
C(7)#5-N(3)-C(6)#5	74.0(6)
C(7)#7-N(3)-C(6)#5	178.8(10)
C(7)#3-N(3)-C(6)#5	111.3(3)
C(7)-N(3)-C(6)#5	111.3(3)

C(6)#3-N(3)-C(6)#5	69.4(7)
C(6)#7-N(3)-C(6)#5	107.2(13)
C(7)#5-N(3)-C(6)	111.3(3)
C(7)#7-N(3)-C(6)	111.3(3)
C(7)#3-N(3)-C(6)	178.8(10)
C(7)-N(3)-C(6)	74.0(6)
C(6)#3-N(3)-C(6)	107.2(13)
C(6)#7-N(3)-C(6)	69.4(7)
C(6)#5-N(3)-C(6)	69.4(7)
N(3)-C(6)-C(8)	108.2(7)
N(3)-C(6)-C(6)#7	55.3(3)
C(8)-C(6)-C(6)#7	125.2(2)
N(3)-C(6)-C(6)#5	55.3(3)
C(8)-C(6)-C(6)#5	125.2(2)
C(6)#7-C(6)-C(6)#5	90.000(1)
N(3)-C(6)-C(7)	52.6(5)
C(8)-C(6)-C(7)	55.7(5)
C(6)#7-C(6)-C(7)	89.3(4)
C(6)#5-C(6)-C(7)	89.3(4)
N(3)-C(7)-C(8)	109.5(6)
N(3)-C(7)-C(7)#7	55.9(3)
C(8)-C(7)-C(7)#7	126.4(2)
N(3)-C(7)-C(7)#5	55.9(3)
C(8)-C(7)-C(7)#5	126.4(2)
C(7)#7-C(7)-C(7)#5	90.000(1)
N(3)-C(7)-C(6)	53.4(5)
C(8)-C(7)-C(6)	56.1(5)
C(7)#7-C(7)-C(6)	90.7(4)
C(7)#5-C(7)-C(6)	90.7(4)
C(7)-C(8)-C(6)	68.3(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -y,x,-z #3 -x,-y,z #4 x,y,-z

#5 -y,x,z #6 y,-x,-z #7 y,-x,z #8 -x,-y+1,z

#9 -x,-y+1,-z #10 x,-y+1,z #11 -x,y,-z

Table 52. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for YbSCN. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Yb(1)	24(1)	24(1)	29(1)	0	0	0
S(1)	76(1)	76(1)	50(1)	-5(1)	-5(1)	-35(1)
C(1)	52(2)	52(2)	59(3)	-7(2)	-7(2)	-13(2)
N(1)	60(2)	60(2)	94(5)	-17(2)	-17(2)	-13(3)
N(2)	154(11)	29(3)	52(3)	0	0	0
C(2)	190(20)	49(6)	128(12)	44(8)	0	0
C(3)	200(20)	200(20)	87(7)	0	0	0
C(4)	190(20)	49(6)	128(12)	44(8)	0	0
C(5)	200(20)	200(20)	87(7)	0	0	0
N(3)	154(11)	29(3)	52(3)	0	0	0
C(6)	132(13)	42(5)	54(5)	0	47(7)	0
C(7)	40(4)	53(4)	38(3)	0	-6(3)	0
C(8)	57(4)	68(4)	127(6)	0	16(5)	0

Table 53. Crystal data and structure refinement for LuSCN.

Identification code	i4mmm	
Empirical formula	C39 H0 Lu N11 O0 S7	
Formula weight	1021.89	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	I4/mmm	
Unit cell dimensions	a = 11.3929(17) Å	α= 90°.
	b = 11.3929(17) Å	β= 90°.
	c = 22.386(3) Å	γ = 90°.
Volume	2905.7(10) $Å^3$	
Z	2	
Density (calculated)	1.168 Mg/m^3	
Absorption coefficient	1.982 mm^{-1}	
F(000)	988	
Crystal size	0.154 x 0.081 x 0.038 mm^3	
Theta range for data collection	1.819 to 30.501°.	
Index ranges	-15<=h<=16, -16<=k<=15, -30<=l<=30	
Reflections collected	20870	
Independent reflections	1296 [R(int) = 0.0212]	
Completeness to theta = 25.242°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1296 / 12 / 59	
Goodness-of-fit on F^2	1.141	
Final R indices [I>2sigma(I)]	R1 = 0.0374, wR2 = 0.1088	
R indices (all data)	R1 = 0.0374, wR2 = 0.1088	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.978 and -0.801 $e.Å^{-3}$	

Table 54. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for LuSCN. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Lu(1)	0	0	0	28(1)
S(1)	2552(1)	2552(1)	1314(1)	73(1)
C(1)	1759(4)	1759(4)	905(3)	64(2)
N(1)	1195(4)	1195(4)	598(4)	83(2)
N(2)	0	5000	0	106(6)
C(2)	0	5806(13)	-530(7)	132(7)
C(3)	0	5000	-1137(8)	152(6)
C(4)	-1039(16)	5817(13)	0	132(7)
C(5)	-2220(20)	5000	0	152(6)
N(3)	0	0	2543(4)	55(2)
C(6)	1069(13)	0	2134(5)	84(5)
C(7)	1057(8)	0	2956(4)	54(2)
C(8)	2255(7)	0	2553(5)	94(2)

Table 55. Bond lengths [Å] and angles [°] for LuSCN.

Lu(1)-N(1)#1	2.345(6)
Lu(1)-N(1)#2	2.345(6)
Lu(1)-N(1)#3	2.345(6)
Lu(1)-N(1)#4	2.345(6)
Lu(1)-N(1)#5	2.345(6)
Lu(1)-N(1)#6	2.345(6)
Lu(1)-N(1)#7	2.345(6)
Lu(1)-N(1)	2.345(6)
S(1)-C(1)	1.572(7)
C(1)-N(1)	1.140(9)
N(2)-C(2)#2	1.500(12)
N(2)-C(2)#8	1.500(12)
N(2)-C(2)#9	1.500(12)
N(2)-C(2)	1.500(12)
N(2)-C(4)#10	1.506(14)
N(2)-C(4)#11	1.506(14)
N(2)-C(4)#9	1.506(14)
N(2)-C(4)	1.506(14)
C(2)-C(3)	1.640(16)
C(2)-C(4)#11	1.676(19)
C(2)-C(4)	1.676(19)
C(2)-C(2)#8	1.84(3)
C(3)-C(2)#8	1.640(16)
C(4)-C(5)	1.636(16)
C(4)-C(2)#2	1.676(19)
C(4)-C(4)#10	1.86(3)
C(5)-C(4)#10	1.636(16)
N(3)-C(7)#6	1.519(9)
N(3)-C(7)#5	1.519(9)
N(3)-C(7)#3	1.519(9)
N(3)-C(7)	1.519(9)
N(3)-C(6)#3	1.523(11)
N(3)-C(6)#5	1.523(11)
N(3)-C(6)#6	1.523(11)

N(3)-C(6)	1.523(11)
C(6)-C(8)	1.645(14)
C(6)-C(6)#5	1.72(2)
C(6)-C(6)#6	1.72(2)
C(6)-C(7)	1.841(14)
C(7)-C(8)	1.637(11)
C(7)-C(7)#5	1.703(13)
C(7)-C(7)#6	1.703(13)

N(1)#1-Lu(1)-N(1)#2	110.3(4)
N(1)#1-Lu(1)-N(1)#3	69.7(4)
N(1)#2-Lu(1)-N(1)#3	180.0(4)
N(1)#1-Lu(1)-N(1)#4	71.0(2)
N(1)#2-Lu(1)-N(1)#4	71.0(2)
N(1)#3-Lu(1)-N(1)#4	109.0(2)
N(1)#1-Lu(1)-N(1)#5	109.0(2)
N(1)#2-Lu(1)-N(1)#5	109.0(2)
N(1)#3-Lu(1)-N(1)#5	71.0(2)
N(1)#4-Lu(1)-N(1)#5	180.0(4)
N(1)#1-Lu(1)-N(1)#6	109.0(2)
N(1)#2-Lu(1)-N(1)#6	109.0(2)
N(1)#3-Lu(1)-N(1)#6	71.0(2)
N(1)#4-Lu(1)-N(1)#6	69.7(4)
N(1)#5-Lu(1)-N(1)#6	110.3(4)
N(1)#1-Lu(1)-N(1)#7	71.0(2)
N(1)#2-Lu(1)-N(1)#7	71.0(2)
N(1)#3-Lu(1)-N(1)#7	109.0(2)
N(1)#4-Lu(1)-N(1)#7	110.3(4)
N(1)#5-Lu(1)-N(1)#7	69.7(4)
N(1)#6-Lu(1)-N(1)#7	180.0(3)
N(1)#1-Lu(1)-N(1)	180.0
N(1)#2-Lu(1)-N(1)	69.7(4)
N(1)#3-Lu(1)-N(1)	110.3(4)
N(1)#4-Lu(1)-N(1)	109.0(2)
N(1)#5-Lu(1)-N(1)	71.0(2)
N(1)#6-Lu(1)-N(1)	71.0(2)

N(1)#7-Lu(1)-N(1)	109.0(2)
N(1)-C(1)-S(1)	178.6(8)
C(1)-N(1)-Lu(1)	177.8(7)
C(2)#2-N(2)-C(2)#8	180.0(9)
C(2)#2-N(2)-C(2)#9	75.5(14)
C(2)#8-N(2)-C(2)#9	104.5(14)
C(2)#2-N(2)-C(2)	104.5(14)
C(2)#8-N(2)-C(2)	75.5(14)
C(2)#9-N(2)-C(2)	180.0
C(2)#2-N(2)-C(4)#10	112.2(5)
C(2)#8-N(2)-C(4)#10	67.8(5)
C(2)#9-N(2)-C(4)#10	67.8(5)
C(2)-N(2)-C(4)#10	112.2(5)
C(2)#2-N(2)-C(4)#11	67.8(5)
C(2)#8-N(2)-C(4)#11	112.2(5)
C(2)#9-N(2)-C(4)#11	112.2(5)
C(2)-N(2)-C(4)#11	67.8(5)
C(4)#10-N(2)-C(4)#11	180.0(9)
C(2)#2-N(2)-C(4)#9	112.2(5)
C(2)#8-N(2)-C(4)#9	67.8(5)
C(2)#9-N(2)-C(4)#9	67.8(5)
C(2)-N(2)-C(4)#9	112.2(5)
C(4)#10-N(2)-C(4)#9	103.7(14)
C(4)#11-N(2)-C(4)#9	76.3(14)
C(2)#2-N(2)-C(4)	67.8(5)
C(2)#8-N(2)-C(4)	112.2(5)
C(2)#9-N(2)-C(4)	112.2(5)
C(2)-N(2)-C(4)	67.8(5)
C(4)#10-N(2)-C(4)	76.3(14)
C(4)#11-N(2)-C(4)	103.7(14)
C(4)#9-N(2)-C(4)	180.0
N(2)-C(2)-C(3)	108.2(11)
N(2)-C(2)-C(4)#11	56.3(5)
C(3)-C(2)-C(4)#11	126.2(9)
N(2)-C(2)-C(4)	56.3(5)
C(3)-C(2)-C(4)	126.2(9)

C(4)#11-C(2)-C(4)	89.9(11)
N(2)-C(2)-C(2)#8	52.2(7)
C(3)-C(2)-C(2)#8	55.9(5)
C(4)#11-C(2)-C(2)#8	90.4(7)
C(4)-C(2)-C(2)#8	90.4(7)
C(2)#8-C(3)-C(2)	68.1(11)
N(2)-C(4)-C(5)	107.2(12)
N(2)-C(4)-C(2)#2	55.9(6)
C(5)-C(4)-C(2)#2	125.2(10)
N(2)-C(4)-C(2)	55.9(6)
C(5)-C(4)-C(2)	125.2(10)
C(2)#2-C(4)-C(2)	90.1(11)
N(2)-C(4)-C(4)#10	51.8(7)
C(5)-C(4)-C(4)#10	55.3(7)
C(2)#2-C(4)-C(4)#10	89.6(7)
C(2)-C(4)-C(4)#10	89.6(7)
C(4)#10-C(5)-C(4)	69.3(13)
C(7)#6-N(3)-C(7)#5	104.8(9)
C(7)#6-N(3)-C(7)#3	68.2(5)
C(7)#5-N(3)-C(7)#3	68.2(5)
C(7)#6-N(3)-C(7)	68.2(5)
C(7)#5-N(3)-C(7)	68.2(5)
C(7)#3-N(3)-C(7)	104.8(9)
C(7)#6-N(3)-C(6)#3	111.5(3)
C(7)#5-N(3)-C(6)#3	111.5(3)
C(7)#3-N(3)-C(6)#3	74.5(6)
C(7)-N(3)-C(6)#3	179.3(9)
C(7)#6-N(3)-C(6)#5	179.3(9)
C(7)#5-N(3)-C(6)#5	74.5(6)
C(7)#3-N(3)-C(6)#5	111.5(3)
C(7)-N(3)-C(6)#5	111.5(3)
C(6)#3-N(3)-C(6)#5	68.8(6)
C(7)#6-N(3)-C(6)#6	74.5(6)
C(7)#5-N(3)-C(6)#6	179.3(9)
C(7)#3-N(3)-C(6)#6	111.5(3)
C(7)-N(3)-C(6)#6	111.5(3)

C(6)#3-N(3)-C(6)#6	68.8(6)
C(6)#5-N(3)-C(6)#6	106.1(13)
C(7)#6-N(3)-C(6)	111.5(3)
C(7)#5-N(3)-C(6)	111.5(3)
C(7)#3-N(3)-C(6)	179.3(9)
C(7)-N(3)-C(6)	74.5(6)
C(6)#3-N(3)-C(6)	106.1(13)
C(6)#5-N(3)-C(6)	68.8(6)
C(6)#6-N(3)-C(6)	68.8(6)
N(3)-C(6)-C(8)	108.3(7)
N(3)-C(6)-C(6)#5	55.6(3)
C(8)-C(6)-C(6)#5	125.5(3)
N(3)-C(6)-C(6)#6	55.6(3)
C(8)-C(6)-C(6)#6	125.5(3)
C(6)#5-C(6)-C(6)#6	89.999(1)
N(3)-C(6)-C(7)	52.7(4)
C(8)-C(6)-C(7)	55.7(5)
C(6)#5-C(6)-C(7)	89.7(4)
C(6)#6-C(6)-C(7)	89.7(4)
N(3)-C(7)-C(8)	108.9(6)
N(3)-C(7)-C(7)#5	55.9(2)
C(8)-C(7)-C(7)#5	126.1(2)
N(3)-C(7)-C(7)#6	55.9(2)
C(8)-C(7)-C(7)#6	126.1(2)
C(7)#5-C(7)-C(7)#6	90.000(1)
N(3)-C(7)-C(6)	52.8(5)
C(8)-C(7)-C(6)	56.1(5)
C(7)#5-C(7)-C(6)	90.3(4)
C(7)#6-C(7)-C(6)	90.3(4)
C(7)-C(8)-C(6)	68.3(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 x,y,-z #3 -x,-y,z #4 -y,x,-z

#5 y,-x,z #6 -y,x,z #7 y,-x,-z #8 -x,-y+1,z

#9 -x,-y+1,-z #10 x,-y+1,z #11 -x,y,-z

Table 56. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for LuSCN. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Lu(1)	27(1)	27(1)	32(1)	0	0	0
S(1)	79(1)	79(1)	63(1)	-6(1)	-6(1)	-33(1)
C(1)	60(2)	60(2)	71(4)	-8(2)	-8(2)	-15(3)
N(1)	71(3)	71(3)	108(5)	-20(3)	-20(3)	-15(3)
N(2)	200(20)	31(4)	88(9)	0	0	0
C(2)	200(20)	60(6)	140(13)	54(9)	0	0
C(3)	179(16)	184(16)	94(7)	0	0	0
C(4)	200(20)	60(6)	140(13)	54(9)	0	0
C(5)	179(16)	184(16)	94(7)	0	0	0
N(3)	58(3)	58(3)	47(4)	0	0	0
C(6)	138(14)	53(6)	61(6)	0	47(8)	0
C(7)	44(4)	68(6)	48(4)	0	-9(4)	0
C(8)	66(4)	81(5)	133(7)	0	18(5)	0

Table 57. Crystal data and structure refinement for AmSCN.

Identification code	rew	
Empirical formula	C39 Am N11 S7	
Formula weight	1089.92	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Cubic	
Space group	Pm-3m	
Unit cell dimensions	a = 11.3641(18) Å	α= 90°.
	b = 11.3641(18) Å	β= 90°.
	c = 11.3641(18) Å	γ = 90°.
Volume	1467.6(7) $Å^3$	
Z	1	
Density (calculated)	1.233 Mg/m^3	
Absorption coefficient	1.587 mm^{-1}	
F(000)	518	
Crystal size	0.100 x 0.075 x 0.050 mm^3	
Theta range for data collection	1.792 to 33.101°.	
Index ranges	-16<=h<=16, -16<=k<=16, -17<=l<=17	
Reflections collected	25900	
Independent reflections	609 [R(int) = 0.0633]	
Completeness to theta = 25.242°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	609 / 1 / 28	
Goodness-of-fit on F^2	1.224	
Final R indices [I>2sigma(I)]	R1 = 0.0431, wR2 = 0.1104	
R indices (all data)	R1 = 0.0442, wR2 = 0.1108	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.462 and -2.889 $e.Å^{-3}$	

Table 58. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for AmSCN. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Am(1)	0	0	0	26(1)
N(2)	0	0	5000	145(15)
C(2)	0	1060(30)	4170(30)	171(10)
N(3)	5000	5000	5000	40(4)
C(3)	0	2283(19)	5000	171(10)
C(4)	4047(15)	4047(15)	5000	64(7)
C(5)	2909(17)	5000	5000	91(7)
S(1)	2620(2)	2620(2)	2620(2)	112(2)
C(1)	1829(7)	1829(7)	1829(7)	73(4)
N(1)	1262(6)	1262(6)	1262(6)	86(4)

Table 59. Bond lengths [Å] and angles [°] for AmSCN.

Am(1)-N(1)	2.484(13)
Am(1)-N(1)#1	2.485(13)
Am(1)-N(1)#2	2.485(13)
Am(1)-N(1)#3	2.485(13)
Am(1)-N(1)#4	2.485(13)
Am(1)-N(1)#5	2.485(13)
Am(1)-N(1)#6	2.485(13)
Am(1)-N(1)#7	2.485(13)
Am(1)-C(1)#1	3.601(13)
Am(1)-C(1)#2	3.601(13)
Am(1)-C(1)#7	3.601(13)
Am(1)-C(1)#3	3.601(13)
N(2)-C(2)	1.53(3)
N(2)-C(2)#8	1.53(3)
N(2)-C(2)#9	1.53(3)
N(2)-C(2)#3	1.53(3)
N(2)-C(2)#10	1.53(3)
N(2)-C(2)#11	1.53(3)
N(2)-C(2)#12	1.53(3)
N(2)-C(2)#13	1.53(3)
C(2)-C(2)#8	1.70(4)
C(2)-C(2)#11	1.70(4)
C(2)-C(3)	1.68(4)
C(2)-C(2)#10	1.88(6)
N(3)-C(4)#14	1.53(2)
N(3)-C(4)	1.53(2)
N(3)-C(4)#15	1.53(2)
N(3)-C(4)#16	1.53(2)
N(3)-C(4)#17	1.53(2)
N(3)-C(4)#18	1.53(2)
N(3)-C(4)#19	1.53(2)
N(3)-C(4)#20	1.53(2)
N(3)-C(4)#21	1.53(2)
N(3)-C(4)#22	1.53(2)

N(3)-C(4)#23	1.53(2)
N(3)-C(4)#24	1.53(2)
C(3)-C(2)#10	1.68(4)
C(4)-C(4)#24	1.53(2)
C(4)-C(4)#21	1.53(2)
C(4)-C(4)#16	1.53(2)
C(4)-C(4)#18	1.53(2)
C(4)-C(5)#18	1.684(15)
C(4)-C(5)	1.688(15)
C(5)-C(4)#24	1.684(15)
C(5)-C(4)#22	1.688(15)
C(5)-C(4)#16	1.684(15)
S(1)-C(1)	1.557(14)
C(1)-N(1)	1.116(18)

N(1)-Am(1)-N(1)#1	180.0(6)
N(1)-Am(1)-N(1)#2	70.5
N(1)#1-Am(1)-N(1)#2	109.5
N(1)-Am(1)-N(1)#3	109.5
N(1)#1-Am(1)-N(1)#3	70.5
N(1)#2-Am(1)-N(1)#3	180.0(6)
N(1)-Am(1)-N(1)#4	70.522(1)
N(1)#1-Am(1)-N(1)#4	109.478(1)
N(1)#2-Am(1)-N(1)#4	109.5
N(1)#3-Am(1)-N(1)#4	70.5
N(1)-Am(1)-N(1)#5	109.478(1)
N(1)#1-Am(1)-N(1)#5	70.522(1)
N(1)#2-Am(1)-N(1)#5	70.5
N(1)#3-Am(1)-N(1)#5	109.5
N(1)#4-Am(1)-N(1)#5	180.0
N(1)-Am(1)-N(1)#6	70.5
N(1)#1-Am(1)-N(1)#6	109.5
N(1)#2-Am(1)-N(1)#6	109.5
N(1)#3-Am(1)-N(1)#6	70.5
N(1)#4-Am(1)-N(1)#6	109.5
N(1)#5-Am(1)-N(1)#6	70.5

N(1)-Am(1)-N(1)#7	109.5
N(1)#1-Am(1)-N(1)#7	70.5
N(1)#2-Am(1)-N(1)#7	70.5
N(1)#3-Am(1)-N(1)#7	109.5
N(1)#4-Am(1)-N(1)#7	70.5
N(1)#5-Am(1)-N(1)#7	109.5
N(1)#6-Am(1)-N(1)#7	180.0(3)
N(1)-Am(1)-C(1)#1	180.00(15)
N(1)#1-Am(1)-C(1)#1	0.00(15)
N(1)#2-Am(1)-C(1)#1	109.5
N(1)#3-Am(1)-C(1)#1	70.5
N(1)#4-Am(1)-C(1)#1	109.5
N(1)#5-Am(1)-C(1)#1	70.5
N(1)#6-Am(1)-C(1)#1	109.5
N(1)#7-Am(1)-C(1)#1	70.5
N(1)-Am(1)-C(1)#2	70.5
N(1)#1-Am(1)-C(1)#2	109.5
N(1)#2-Am(1)-C(1)#2	0.00(15)
N(1)#3-Am(1)-C(1)#2	180.00(15)
N(1)#4-Am(1)-C(1)#2	109.5
N(1)#5-Am(1)-C(1)#2	70.5
N(1)#6-Am(1)-C(1)#2	109.5
N(1)#7-Am(1)-C(1)#2	70.5
C(1)#1-Am(1)-C(1)#2	109.5
N(1)-Am(1)-C(1)#7	109.5
N(1)#1-Am(1)-C(1)#7	70.5
N(1)#2-Am(1)-C(1)#7	70.5
N(1)#3-Am(1)-C(1)#7	109.5
N(1)#4-Am(1)-C(1)#7	70.5
N(1)#5-Am(1)-C(1)#7	109.5
N(1)#6-Am(1)-C(1)#7	180.00(15)
N(1)#7-Am(1)-C(1)#7	0.00(15)
C(1)#1-Am(1)-C(1)#7	70.5
C(1)#2-Am(1)-C(1)#7	70.5
N(1)-Am(1)-C(1)#3	109.5
N(1)#1-Am(1)-C(1)#3	70.5

N(1)#2-Am(1)-C(1)#3	180.00(15)
N(1)#3-Am(1)-C(1)#3	0.00(15)
N(1)#4-Am(1)-C(1)#3	70.5
N(1)#5-Am(1)-C(1)#3	109.5
N(1)#6-Am(1)-C(1)#3	70.5
N(1)#7-Am(1)-C(1)#3	109.5
C(1)#1-Am(1)-C(1)#3	70.5
C(1)#2-Am(1)-C(1)#3	180.0(4)
C(1)#7-Am(1)-C(1)#3	109.5
C(2)-N(2)-C(2)#8	67.8(13)
C(2)-N(2)-C(2)#9	112.2(13)
C(2)#8-N(2)-C(2)#9	180.0(17)
C(2)-N(2)-C(2)#3	104(3)
C(2)#8-N(2)-C(2)#3	67.8(13)
C(2)#9-N(2)-C(2)#3	112.2(13)
C(2)-N(2)-C(2)#10	76(3)
C(2)#8-N(2)-C(2)#10	112.2(13)
C(2)#9-N(2)-C(2)#10	67.8(13)
C(2)#3-N(2)-C(2)#10	180.0(17)
C(2)-N(2)-C(2)#11	67.8(13)
C(2)#8-N(2)-C(2)#11	104(3)
C(2)#9-N(2)-C(2)#11	76(3)
C(2)#3-N(2)-C(2)#11	67.8(13)
C(2)#10-N(2)-C(2)#11	112.2(13)
C(2)-N(2)-C(2)#12	180.0
C(2)#8-N(2)-C(2)#12	112.2(13)
C(2)#9-N(2)-C(2)#12	67.8(13)
C(2)#3-N(2)-C(2)#12	76(3)
C(2)#10-N(2)-C(2)#12	104(3)
C(2)#11-N(2)-C(2)#12	112.2(13)
C(2)-N(2)-C(2)#13	112.2(13)
C(2)#8-N(2)-C(2)#13	76(3)
C(2)#9-N(2)-C(2)#13	104(3)
C(2)#3-N(2)-C(2)#13	112.2(13)
C(2)#10-N(2)-C(2)#13	67.8(13)
C(2)#11-N(2)-C(2)#13	180.0

C(2)#12-N(2)-C(2)#13	67.8(13)
N(2)-C(2)-C(2)#8	56.1(7)
N(2)-C(2)-C(2)#11	56.1(7)
C(2)#8-C(2)-C(2)#11	90.000(1)
N(2)-C(2)-C(3)	108.0(19)
C(2)#8-C(2)-C(3)	125.9(6)
C(2)#11-C(2)-C(3)	125.9(6)
N(2)-C(2)-C(2)#10	52.1(13)
C(2)#8-C(2)-C(2)#10	90.000(3)
C(2)#11-C(2)-C(2)#10	90.000(1)
C(3)-C(2)-C(2)#10	55.9(12)
C(4)#14-N(3)-C(4)	120.000(2)
C(4)#14-N(3)-C(4)#15	60.000(2)
C(4)-N(3)-C(4)#15	180.0
C(4)#14-N(3)-C(4)#16	180.0
C(4)-N(3)-C(4)#16	60.000(2)
C(4)#15-N(3)-C(4)#16	120.0
C(4)#14-N(3)-C(4)#17	60.000(1)
C(4)-N(3)-C(4)#17	120.000(1)
C(4)#15-N(3)-C(4)#17	60.0
C(4)#16-N(3)-C(4)#17	120.0
C(4)#14-N(3)-C(4)#18	120.000(2)
C(4)-N(3)-C(4)#18	60.000(1)
C(4)#15-N(3)-C(4)#18	120.000(2)
C(4)#16-N(3)-C(4)#18	60.000(2)
C(4)#17-N(3)-C(4)#18	180.0
C(4)#14-N(3)-C(4)#19	89.852(5)
C(4)-N(3)-C(4)#19	120.0
C(4)#15-N(3)-C(4)#19	60.000(1)
C(4)#16-N(3)-C(4)#19	90.148(1)
C(4)#17-N(3)-C(4)#19	120.000(2)
C(4)#18-N(3)-C(4)#19	60.000(1)
C(4)#14-N(3)-C(4)#20	120.000(1)
C(4)-N(3)-C(4)#20	120.000(2)
C(4)#15-N(3)-C(4)#20	60.0
C(4)#16-N(3)-C(4)#20	60.0

C(4)#17-N(3)-C(4)#20	90.1
C(4)#18-N(3)-C(4)#20	89.852(3)
C(4)#19-N(3)-C(4)#20	60.000(1)
C(4)#14-N(3)-C(4)#21	60.0
C(4)-N(3)-C(4)#21	60.0
C(4)#15-N(3)-C(4)#21	120.000(1)
C(4)#16-N(3)-C(4)#21	120.000(1)
C(4)#17-N(3)-C(4)#21	89.852(1)
C(4)#18-N(3)-C(4)#21	90.148(5)
C(4)#19-N(3)-C(4)#21	120.000(1)
C(4)#20-N(3)-C(4)#21	180.0
C(4)#14-N(3)-C(4)#22	120.000(1)
C(4)-N(3)-C(4)#22	90.148(5)
C(4)#15-N(3)-C(4)#22	89.852(3)
C(4)#16-N(3)-C(4)#22	60.000(1)
C(4)#17-N(3)-C(4)#22	60.000(1)
C(4)#18-N(3)-C(4)#22	120.000(1)
C(4)#19-N(3)-C(4)#22	120.000(1)
C(4)#20-N(3)-C(4)#22	60.000(1)
C(4)#21-N(3)-C(4)#22	120.000(1)
C(4)#14-N(3)-C(4)#23	60.000(1)
C(4)-N(3)-C(4)#23	89.852(2)
C(4)#15-N(3)-C(4)#23	90.1
C(4)#16-N(3)-C(4)#23	120.000(1)
C(4)#17-N(3)-C(4)#23	120.000(2)
C(4)#18-N(3)-C(4)#23	60.000(1)
C(4)#19-N(3)-C(4)#23	60.000(1)
C(4)#20-N(3)-C(4)#23	120.000(2)
C(4)#21-N(3)-C(4)#23	60.000(1)
C(4)#22-N(3)-C(4)#23	180.0
C(4)#14-N(3)-C(4)#24	90.148(3)
C(4)-N(3)-C(4)#24	60.000(2)
C(4)#15-N(3)-C(4)#24	120.0
C(4)#16-N(3)-C(4)#24	89.9
C(4)#17-N(3)-C(4)#24	60.000(1)
C(4)#18-N(3)-C(4)#24	120.000(2)

C(4)#19-N(3)-C(4)#24	180.0
C(4)#20-N(3)-C(4)#24	120.000(2)
C(4)#21-N(3)-C(4)#24	60.000(2)
C(4)#22-N(3)-C(4)#24	60.000(2)
C(4)#23-N(3)-C(4)#24	120.000(2)
C(2)-C(3)-C(2)#10	68(2)
C(4)#24-C(4)-N(3)	60.000(4)
C(4)#24-C(4)-C(4)#21	60.000(1)
N(3)-C(4)-C(4)#21	60.000(3)
C(4)#24-C(4)-C(4)#16	89.852(4)
N(3)-C(4)-C(4)#16	60.000(2)
C(4)#21-C(4)-C(4)#16	120.000(12)
C(4)#24-C(4)-C(4)#18	120.000(13)
N(3)-C(4)-C(4)#18	60.000(3)
C(4)#21-C(4)-C(4)#18	90.148(5)
C(4)#16-C(4)-C(4)#18	60.0
C(4)#24-C(4)-C(5)#18	122.9(5)
N(3)-C(4)-C(5)#18	95.1(9)
C(4)#21-C(4)-C(5)#18	63.1(6)
C(4)#16-C(4)-C(5)#18	122.9(5)
C(4)#18-C(4)-C(5)#18	63.1(6)
C(4)#24-C(4)-C(5)	62.8(6)
N(3)-C(4)-C(5)	94.9(9)
C(4)#21-C(4)-C(5)	122.7(5)
C(4)#16-C(4)-C(5)	62.8(6)
C(4)#18-C(4)-C(5)	122.7(5)
C(5)#18-C(4)-C(5)	170.1(18)
C(4)#24-C(5)-C(4)#22	54.1(11)
C(4)#24-C(5)-C(4)	54.1(11)
C(4)#22-C(5)-C(4)	80.1(18)
C(4)#24-C(5)-C(4)#16	80.0(18)
C(4)#22-C(5)-C(4)#16	54.1(11)
C(4)-C(5)-C(4)#16	54.1(11)
N(1)-C(1)-S(1)	180.0(6)
N(1)-C(1)-Am(1)	0.0(3)
S(1)-C(1)-Am(1)	180.0(3)

C(1)-N(1)-Am(1) 180.0(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 x,y,-z #3 -x,-y,z #4 -x,y,z

#5 x,-y,-z #6 x,-y,z #7 -x,y,-z #8 -y,-x,z

#9 y,x,-z+1 #10 x,y,-z+1 #11 y,x,z #12 -x,-y,-z+1

#13 -y,-x,-z+1 #14 -y+1,-z+1,-x+1 #15 -x+1,-y+1,-z+1

#16 y,z,x #17 -z+1,-x+1,-y+1 #18 z,x,y #19 -y+1,z,x

#20 -z+1,-x+1,y #21 z,x,-y+1 #22 x,-y+1,z

#23 -x+1,y,-z+1 #24 y,-z+1,-x+1

Table 60. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for AmSCN. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Am(1)	26(1)	26(1)	26(1)	0	0	0
N(2)	190(20)	190(20)	52(12)	0	0	0
C(2)	144(13)	230(30)	136(18)	99(19)	0	0
N(3)	40(4)	40(4)	40(4)	0	0	0
C(3)	144(13)	230(30)	136(18)	99(19)	0	0
C(4)	78(12)	78(12)	38(9)	0	0	-33(14)
C(5)	79(14)	97(12)	97(12)	0	0	0
S(1)	112(2)	112(2)	112(2)	-36(1)	-36(1)	-36(1)
C(1)	73(4)	73(4)	73(4)	-16(3)	-16(3)	-16(3)
N(1)	86(4)	86(4)	86(4)	-20(4)	-20(4)	-20(4)

Table 61. Crystal data and structure refinement for CmSCN.

Identification code	rew	
Empirical formula	C39 H0 Cm N11 O3 S7	
Formula weight	1142.92	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Cubic	
Space group	Pm-3m	
Unit cell dimensions	a = 11.3752(11) Å	α= 90°.
	b = 11.3752(11) Å	β= 90°.
	c = 11.3752(11) Å	γ = 90°.
Volume	1471.9(4) $Å^3$	
Z	1	
Density (calculated)	1.289 Mg/m^3	
Absorption coefficient	1.670 mm^{-1}	
F(000)	543	
Crystal size	0.350 x 0.175 x 0.125 mm^3	
Theta range for data collection	1.790 to 30.631°.	
Index ranges	-15<=h<=15, -16<=k<=16, -15<=l<=15	
Reflections collected	19756	
Independent reflections	513 [R(int) = 0.0554]	
Completeness to theta = 25.242°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	513 / 20 / 33	
Goodness-of-fit on F^2	1.476	
Final R indices [I>2sigma(I)]	R1 = 0.0435, wR2 = 0.1500	
R indices (all data)	R1 = 0.0435, wR2 = 0.1500	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.960 and -1.735 $e.Å^{-3}$	

Table 62. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for CmSCN. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cm(1)	0	0	0	16(1)
S(1)	2610(3)	2610(3)	2610(3)	90(3)
N(1)	1256(10)	1256(10)	1256(10)	78(7)
C(1)	1822(11)	1822(11)	1822(11)	70(7)
N(2)	5000	5000	5000	26(5)
C(2)	4090(20)	5000	4090(20)	43(8)
C(3)	5000	5000	2760(20)	60(8)
O(1)	5000	5000	0	72(8)
N(3)	0	0	5000	119(13)
C(4)	798(15)	0	4019(14)	132(13)
C(5)	1730(30)	0	5000	182(14)

Table 63. Bond lengths [Å] and angles [°] for CmSCN.

Cm(1)-N(1)#1	2.475(19)
Cm(1)-N(1)#2	2.475(19)
Cm(1)-N(1)#3	2.475(19)
Cm(1)-N(1)#4	2.475(19)
Cm(1)-N(1)#5	2.475(19)
Cm(1)-N(1)#6	2.475(19)
Cm(1)-N(1)#7	2.475(19)
Cm(1)-N(1)	2.475(19)
Cm(1)-C(1)	3.59(2)
Cm(1)-C(1)#1	3.59(2)
Cm(1)-C(1)#2	3.59(2)
Cm(1)-C(1)#3	3.59(2)
S(1)-C(1)	1.55(2)
N(1)-C(1)	1.12(3)
N(2)-C(2)	1.46(3)
N(2)-C(2)#8	1.46(3)
N(2)-C(2)#9	1.46(3)
N(2)-C(2)#10	1.46(3)
N(2)-C(2)#11	1.46(3)
N(2)-C(2)#12	1.46(3)
N(2)-C(2)#13	1.46(3)
N(2)-C(2)#14	1.46(3)
N(2)-C(2)#15	1.46(3)
N(2)-C(2)#16	1.46(3)
N(2)-C(2)#17	1.46(3)
N(2)-C(2)#18	1.46(3)
C(2)-C(2)#17	1.46(3)
C(2)-C(2)#13	1.46(3)
C(2)-C(2)#10	1.46(3)
C(2)-C(2)#12	1.46(3)
C(2)-C(3)	1.84(2)
C(2)-C(3)#19	1.84(2)
C(3)-C(2)#17	1.84(2)
C(3)-C(2)#14	1.84(2)

C(3)-C(2)#10	1.84(2)
N(3)-C(4)	1.439(10)
N(3)-C(4)#20	1.439(10)
N(3)-C(4)#16	1.439(10)
N(3)-C(4)#21	1.439(10)
N(3)-C(4)#4	1.439(10)
N(3)-C(4)#22	1.439(10)
N(3)-C(4)#23	1.439(10)
N(3)-C(4)#24	1.439(10)
C(4)-C(4)#20	1.28(2)
C(4)-C(4)#22	1.28(2)
C(4)-C(5)	1.543(10)
C(4)-C(4)#4	1.82(3)
C(5)-C(4)#21	1.543(10)

N(1)#1-Cm(1)-N(1)#2	70.5
N(1)#1-Cm(1)-N(1)#3	109.5
N(1)#2-Cm(1)-N(1)#3	180.0(8)
N(1)#1-Cm(1)-N(1)#4	109.5
N(1)#2-Cm(1)-N(1)#4	70.5
N(1)#3-Cm(1)-N(1)#4	109.5
N(1)#1-Cm(1)-N(1)#5	109.5
N(1)#2-Cm(1)-N(1)#5	70.529(1)
N(1)#3-Cm(1)-N(1)#5	109.471(1)
N(1)#4-Cm(1)-N(1)#5	109.5
N(1)#1-Cm(1)-N(1)#6	70.5
N(1)#2-Cm(1)-N(1)#6	109.471(1)
N(1)#3-Cm(1)-N(1)#6	70.529(1)
N(1)#4-Cm(1)-N(1)#6	70.5
N(1)#5-Cm(1)-N(1)#6	180.0(4)
N(1)#1-Cm(1)-N(1)#7	70.5
N(1)#2-Cm(1)-N(1)#7	109.5
N(1)#3-Cm(1)-N(1)#7	70.5
N(1)#4-Cm(1)-N(1)#7	180.0(4)
N(1)#5-Cm(1)-N(1)#7	70.5
N(1)#6-Cm(1)-N(1)#7	109.5

N(1)#1-Cm(1)-N(1)	180.0(8)
N(1)#2-Cm(1)-N(1)	109.5
N(1)#3-Cm(1)-N(1)	70.5
N(1)#4-Cm(1)-N(1)	70.5
N(1)#5-Cm(1)-N(1)	70.5
N(1)#6-Cm(1)-N(1)	109.5
N(1)#7-Cm(1)-N(1)	109.5
N(1)#1-Cm(1)-C(1)	180.0(8)
N(1)#2-Cm(1)-C(1)	109.5
N(1)#3-Cm(1)-C(1)	70.5
N(1)#4-Cm(1)-C(1)	70.5
N(1)#5-Cm(1)-C(1)	70.5
N(1)#6-Cm(1)-C(1)	109.5
N(1)#7-Cm(1)-C(1)	109.5
N(1)-Cm(1)-C(1)	0.0(2)
N(1)#1-Cm(1)-C(1)#1	0.0(8)
N(1)#2-Cm(1)-C(1)#1	70.5
N(1)#3-Cm(1)-C(1)#1	109.5
N(1)#4-Cm(1)-C(1)#1	109.5
N(1)#5-Cm(1)-C(1)#1	109.5
N(1)#6-Cm(1)-C(1)#1	70.5
N(1)#7-Cm(1)-C(1)#1	70.5
N(1)-Cm(1)-C(1)#1	180.0(5)
C(1)-Cm(1)-C(1)#1	180.0(6)
N(1)#1-Cm(1)-C(1)#2	70.5
N(1)#2-Cm(1)-C(1)#2	0.0(7)
N(1)#3-Cm(1)-C(1)#2	180.0(5)
N(1)#4-Cm(1)-C(1)#2	70.529(1)
N(1)#5-Cm(1)-C(1)#2	70.5
N(1)#6-Cm(1)-C(1)#2	109.5
N(1)#7-Cm(1)-C(1)#2	109.471(1)
N(1)-Cm(1)-C(1)#2	109.5
C(1)-Cm(1)-C(1)#2	109.471(1)
C(1)#1-Cm(1)-C(1)#2	70.5
N(1)#1-Cm(1)-C(1)#3	109.5
N(1)#2-Cm(1)-C(1)#3	180.0(5)

N(1)#3-Cm(1)-C(1)#3	0.0(3)
N(1)#4-Cm(1)-C(1)#3	109.471(1)
N(1)#5-Cm(1)-C(1)#3	109.5
N(1)#6-Cm(1)-C(1)#3	70.5
N(1)#7-Cm(1)-C(1)#3	70.529(1)
N(1)-Cm(1)-C(1)#3	70.5
C(1)-Cm(1)-C(1)#3	70.5
C(1)#1-Cm(1)-C(1)#3	109.471(1)
C(1)#2-Cm(1)-C(1)#3	180.0(6)
C(1)-N(1)-Cm(1)	180(2)
N(1)-C(1)-S(1)	180(3)
N(1)-C(1)-Cm(1)	0.0(17)
S(1)-C(1)-Cm(1)	180.0(16)
C(2)-N(2)-C(2)#8	120.000(1)
C(2)-N(2)-C(2)#9	180.0
C(2)#8-N(2)-C(2)#9	60.000(2)
C(2)-N(2)-C(2)#10	60.000(2)
C(2)#8-N(2)-C(2)#10	180.0
C(2)#9-N(2)-C(2)#10	120.000(2)
C(2)-N(2)-C(2)#11	120.000(2)
C(2)#8-N(2)-C(2)#11	60.000(2)
C(2)#9-N(2)-C(2)#11	60.000(2)
C(2)#10-N(2)-C(2)#11	120.000(2)
C(2)-N(2)-C(2)#12	60.000(2)
C(2)#8-N(2)-C(2)#12	120.000(2)
C(2)#9-N(2)-C(2)#12	120.000(2)
C(2)#10-N(2)-C(2)#12	60.000(2)
C(2)#11-N(2)-C(2)#12	180.0
C(2)-N(2)-C(2)#13	60.000(2)
C(2)#8-N(2)-C(2)#13	60.000(2)
C(2)#9-N(2)-C(2)#13	120.000(2)
C(2)#10-N(2)-C(2)#13	120.000(2)
C(2)#11-N(2)-C(2)#13	90.000(1)
C(2)#12-N(2)-C(2)#13	90.000(3)
C(2)-N(2)-C(2)#14	90.000(2)
C(2)#8-N(2)-C(2)#14	120.000(2)

C(2)#9-N(2)-C(2)#14	90.000(4)
C(2)#10-N(2)-C(2)#14	60.000(2)
C(2)#11-N(2)-C(2)#14	60.000(2)
C(2)#12-N(2)-C(2)#14	120.0
C(2)#13-N(2)-C(2)#14	120.000(2)
C(2)-N(2)-C(2)#15	90.000(3)
C(2)#8-N(2)-C(2)#15	60.000(2)
C(2)#9-N(2)-C(2)#15	90.000(2)
C(2)#10-N(2)-C(2)#15	120.000(2)
C(2)#11-N(2)-C(2)#15	120.0
C(2)#12-N(2)-C(2)#15	60.000(2)
C(2)#13-N(2)-C(2)#15	60.000(2)
C(2)#14-N(2)-C(2)#15	180.0
C(2)-N(2)-C(2)#16	120.000(2)
C(2)#8-N(2)-C(2)#16	90.000(2)
C(2)#9-N(2)-C(2)#16	60.0
C(2)#10-N(2)-C(2)#16	90.000(3)
C(2)#11-N(2)-C(2)#16	120.000(2)
C(2)#12-N(2)-C(2)#16	60.0
C(2)#13-N(2)-C(2)#16	120.000(2)
C(2)#14-N(2)-C(2)#16	120.000(2)
C(2)#15-N(2)-C(2)#16	60.000(2)
C(2)-N(2)-C(2)#17	60.0
C(2)#8-N(2)-C(2)#17	90.000(4)
C(2)#9-N(2)-C(2)#17	120.000(2)
C(2)#10-N(2)-C(2)#17	90.000(2)
C(2)#11-N(2)-C(2)#17	60.0
C(2)#12-N(2)-C(2)#17	120.000(2)
C(2)#13-N(2)-C(2)#17	60.000(1)
C(2)#14-N(2)-C(2)#17	60.000(1)
C(2)#15-N(2)-C(2)#17	120.000(1)
C(2)#16-N(2)-C(2)#17	180.0
C(2)-N(2)-C(2)#18	120.000(1)
C(2)#8-N(2)-C(2)#18	120.000(2)
C(2)#9-N(2)-C(2)#18	60.000(1)
C(2)#10-N(2)-C(2)#18	60.000(1)

C(2)#11-N(2)-C(2)#18	90.000(4)
C(2)#12-N(2)-C(2)#18	90.0
C(2)#13-N(2)-C(2)#18	180.0
C(2)#14-N(2)-C(2)#18	60.000(1)
C(2)#15-N(2)-C(2)#18	120.000(1)
C(2)#16-N(2)-C(2)#18	60.000(1)
C(2)#17-N(2)-C(2)#18	120.000(2)
N(2)-C(2)-C(2)#17	60.000(4)
N(2)-C(2)-C(2)#13	60.000(2)
C(2)#17-C(2)-C(2)#13	60.000(2)
N(2)-C(2)-C(2)#10	60.000(2)
C(2)#17-C(2)-C(2)#10	90.000(13)
C(2)#13-C(2)-C(2)#10	120.000(12)
N(2)-C(2)-C(2)#12	60.000(1)
C(2)#17-C(2)-C(2)#12	120.000(8)
C(2)#13-C(2)-C(2)#12	90.000(2)
C(2)#10-C(2)-C(2)#12	60.000(3)
N(2)-C(2)-C(3)	100.8(11)
C(2)#17-C(2)-C(3)	66.6(7)
C(2)#13-C(2)-C(3)	125.8(5)
C(2)#10-C(2)-C(3)	66.6(7)
C(2)#12-C(2)-C(3)	125.8(5)
N(2)-C(2)-C(3)#19	100.8(11)
C(2)#17-C(2)-C(3)#19	125.8(5)
C(2)#13-C(2)-C(3)#19	66.6(7)
C(2)#10-C(2)-C(3)#19	125.8(5)
C(2)#12-C(2)-C(3)#19	66.6(7)
C(3)-C(2)-C(3)#19	158(2)
C(2)#17-C(3)-C(2)#14	46.9(14)
C(2)#17-C(3)-C(2)#10	68(2)
C(2)#14-C(3)-C(2)#10	46.9(14)
C(2)#17-C(3)-C(2)	46.9(14)
C(2)#14-C(3)-C(2)	68(2)
C(2)#10-C(3)-C(2)	46.9(14)
C(4)-N(3)-C(4)#20	53.0(10)
C(4)-N(3)-C(4)#16	127.0(10)

C(4)#20-N(3)-C(4)#16	180.0
C(4)-N(3)-C(4)#21	101.8(17)
C(4)#20-N(3)-C(4)#21	127.0(10)
C(4)#16-N(3)-C(4)#21	53.0(10)
C(4)-N(3)-C(4)#4	78.2(17)
C(4)#20-N(3)-C(4)#4	53.0(10)
C(4)#16-N(3)-C(4)#4	127.0(10)
C(4)#21-N(3)-C(4)#4	180.0
C(4)-N(3)-C(4)#22	53.0(10)
C(4)#20-N(3)-C(4)#22	78.2(17)
C(4)#16-N(3)-C(4)#22	101.8(17)
C(4)#21-N(3)-C(4)#22	127.0(10)
C(4)#4-N(3)-C(4)#22	53.0(10)
C(4)-N(3)-C(4)#23	180.0
C(4)#20-N(3)-C(4)#23	127.0(10)
C(4)#16-N(3)-C(4)#23	53.0(10)
C(4)#21-N(3)-C(4)#23	78.2(17)
C(4)#4-N(3)-C(4)#23	101.8(17)
C(4)#22-N(3)-C(4)#23	127.0(10)
C(4)-N(3)-C(4)#24	127.0(10)
C(4)#20-N(3)-C(4)#24	101.8(17)
C(4)#16-N(3)-C(4)#24	78.2(17)
C(4)#21-N(3)-C(4)#24	53.0(10)
C(4)#4-N(3)-C(4)#24	127.0(10)
C(4)#22-N(3)-C(4)#24	180.0
C(4)#23-N(3)-C(4)#24	53.0(10)
C(4)#20-C(4)-C(4)#22	90.0
C(4)#20-C(4)-N(3)	63.5(5)
C(4)#22-C(4)-N(3)	63.5(5)
C(4)#20-C(4)-C(5)	119.2(5)
C(4)#22-C(4)-C(5)	119.2(5)
N(3)-C(4)-C(5)	82.8(16)
C(4)#20-C(4)-C(4)#4	45.000(1)
C(4)#22-C(4)-C(4)#4	45.000(2)
N(3)-C(4)-C(4)#4	50.9(8)
C(5)-C(4)-C(4)#4	133.7(8)

C(4)-C(5)-C(4)#21 92.7(17)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -x,-z,y #3 x,z,-y #4 -x,y,z

#5 x,-z,y #6 -x,z,-y #7 x,-y,-z #8 -y+1,-z+1,-x+1

#9 -x+1,-y+1,-z+1 #10 y,z,x #11 -x+1,-z+1,y

#12 x,z,-y+1 #13 x,-z+1,y #14 -x+1,y,z #15 x,-y+1,-z+1

#16 y,x,-z+1 #17 -y+1,-x+1,z #18 -x+1,z,-y+1

#19 z,y,-x+1 #20 -y,-x,z #21 x,-y,-z+1 #22 y,x,z

#23 -x,-y,-z+1 #24 -y,-x,-z+1

Table 64. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for CmSCN. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cm(1)	16(1)	16(1)	16(1)	0	0	0
S(1)	90(3)	90(3)	90(3)	-30(2)	-30(2)	-30(2)
N(1)	78(7)	78(7)	78(7)	-23(6)	-23(6)	-23(6)
C(1)	70(7)	70(7)	70(7)	-23(6)	-23(6)	-23(6)
N(2)	26(5)	26(5)	26(5)	0	0	0
C(2)	45(11)	40(16)	45(11)	0	-19(14)	0
C(3)	78(14)	78(14)	23(10)	0	0	0
O(1)	61(9)	61(9)	90(20)	0	0	0
N(3)	150(20)	150(20)	50(16)	0	0	0
C(4)	180(30)	140(20)	81(18)	0	-31(19)	0
C(5)	240(30)	150(20)	160(20)	0	0	0

Raman Spectroscopy

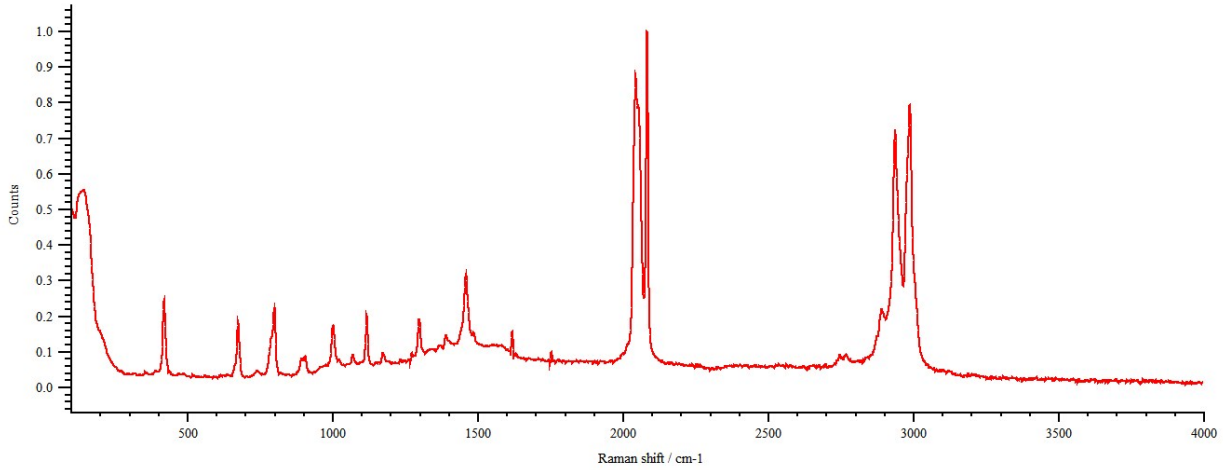

Figure 1. Representative full Raman spectrum of **La-NCS**.

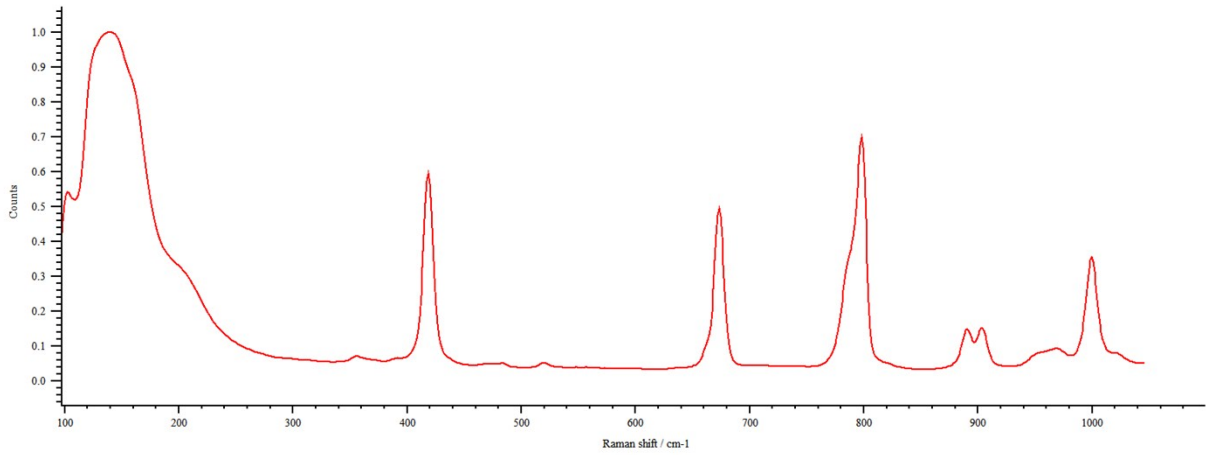

Figure 2. Raman spectrum of **La-NCS** in the low frequency region.

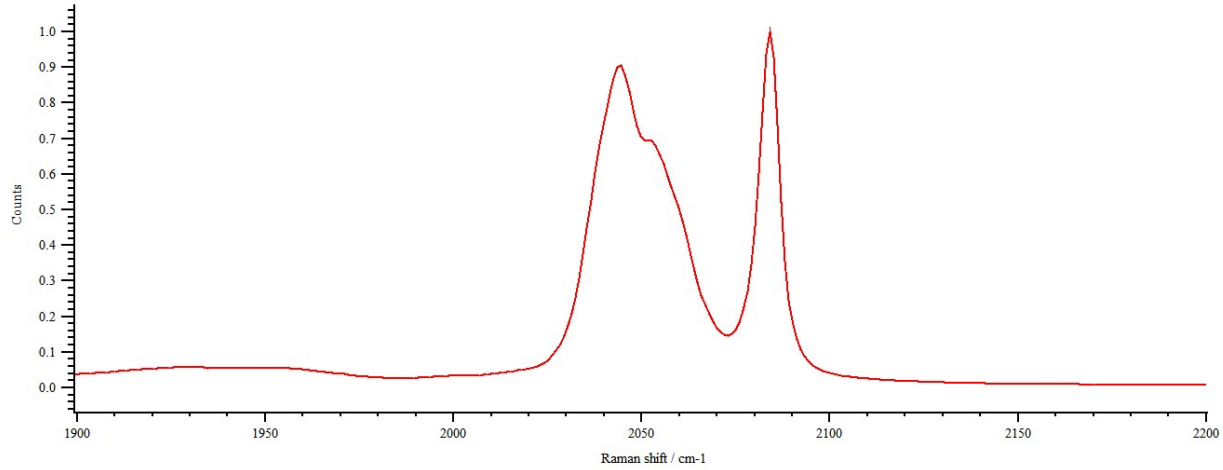

Figure 3. Raman spectrum of **La-NCS** in the C=N stretching region.

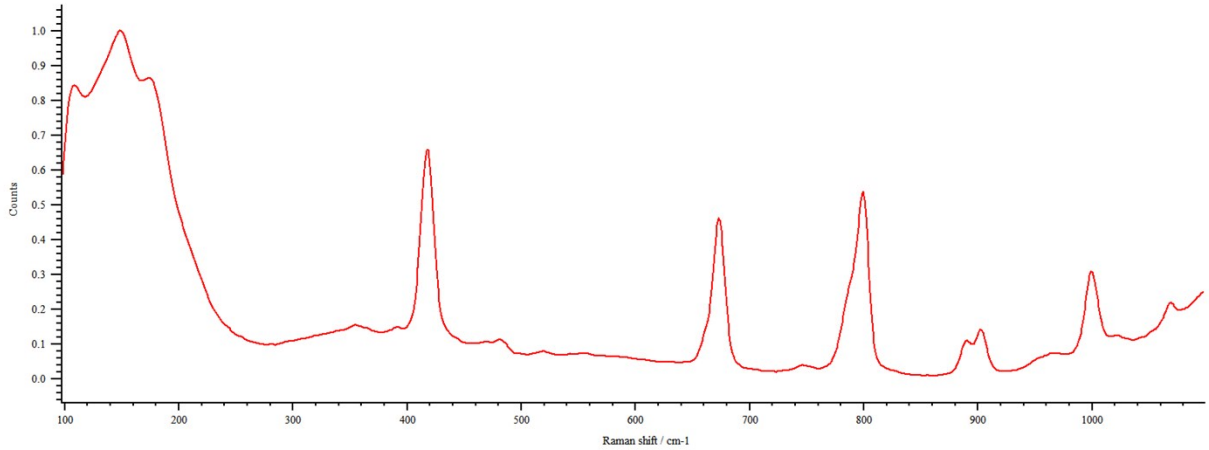

Figure 4. Raman spectrum of **Pr-NCS** in the low frequency region.

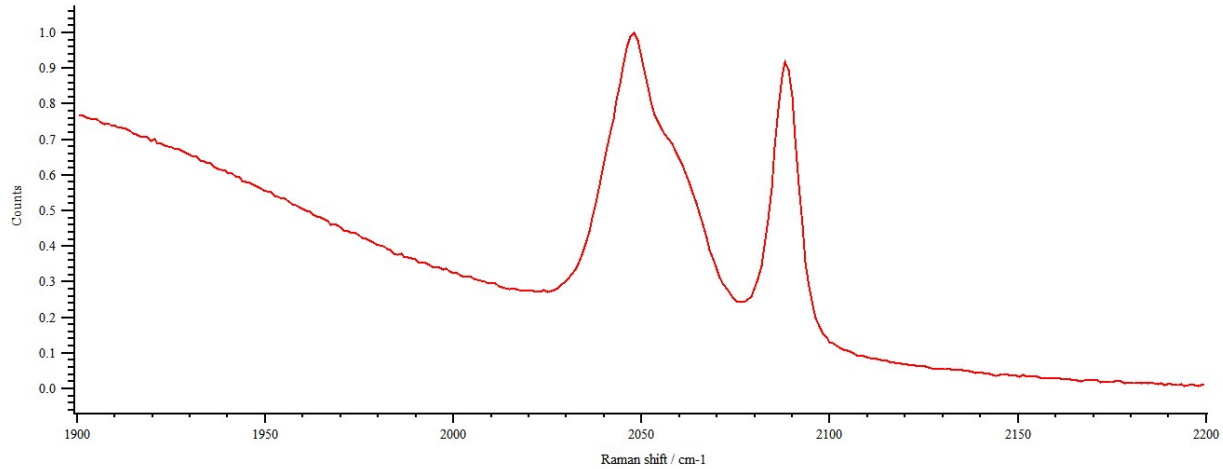

Figure 5. Raman spectrum of **Pr-NCS** in the C=N stretching region.

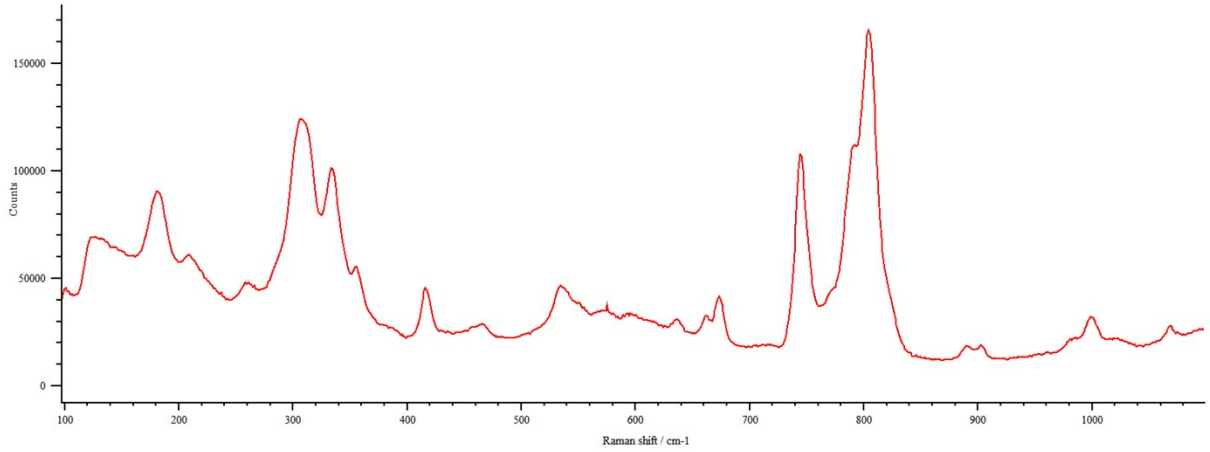

Figure 6. Raman spectrum of **Nd-NCS** in the low frequency region.

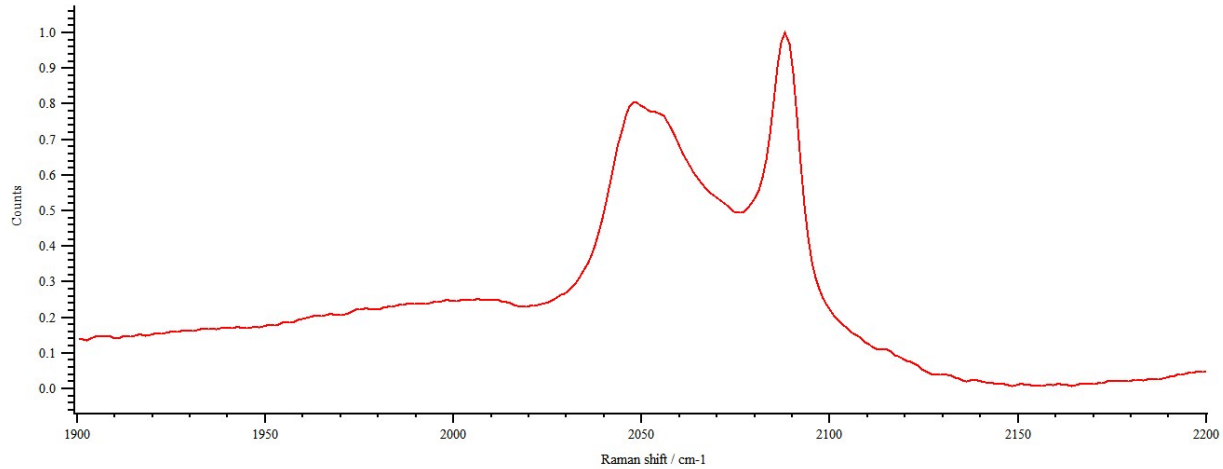

Figure 7. Raman spectrum of **Nd-NCS** in the C=N stretching region.

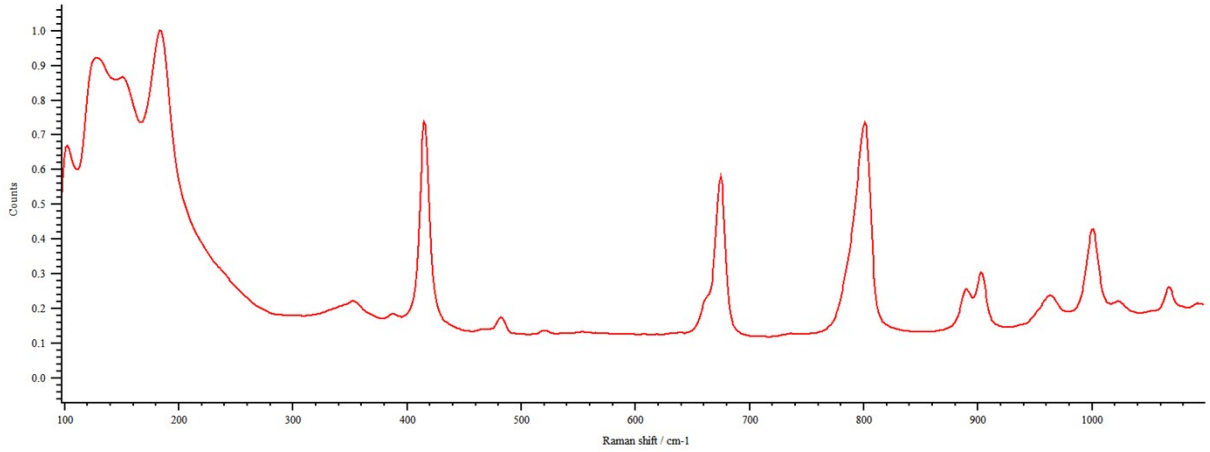

Figure 8. Raman spectrum of **Sm-NCS** in the low frequency region.

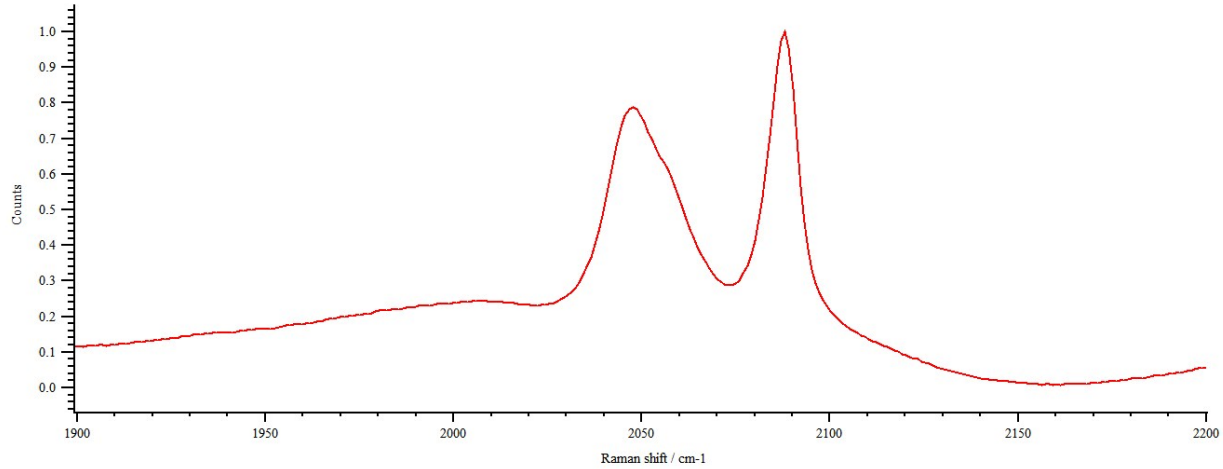

Figure 9. Raman spectrum of **Sm-NCS** in the C=N stretching region.

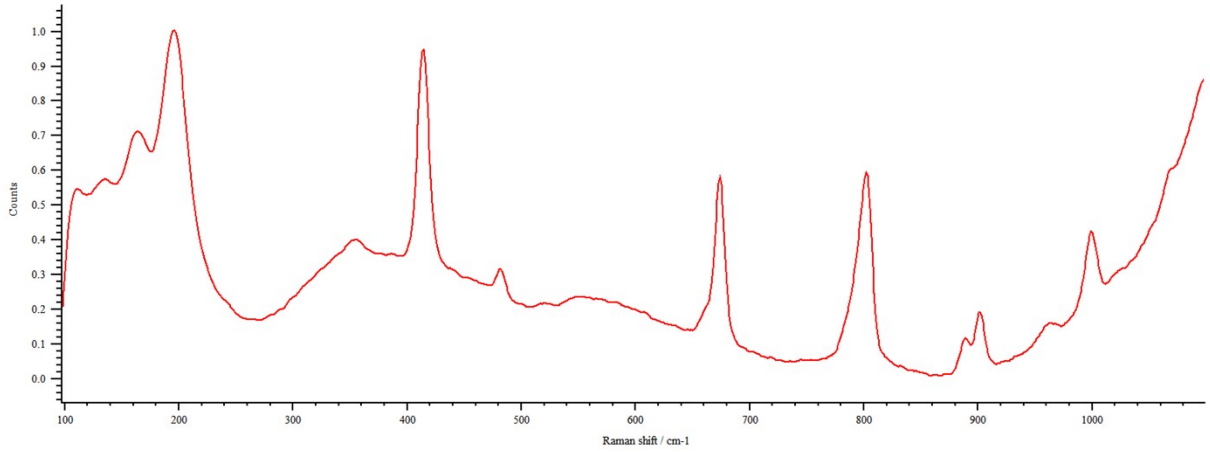

Figure 10. Raman spectrum of **Eu-NCS** in the low frequency region.

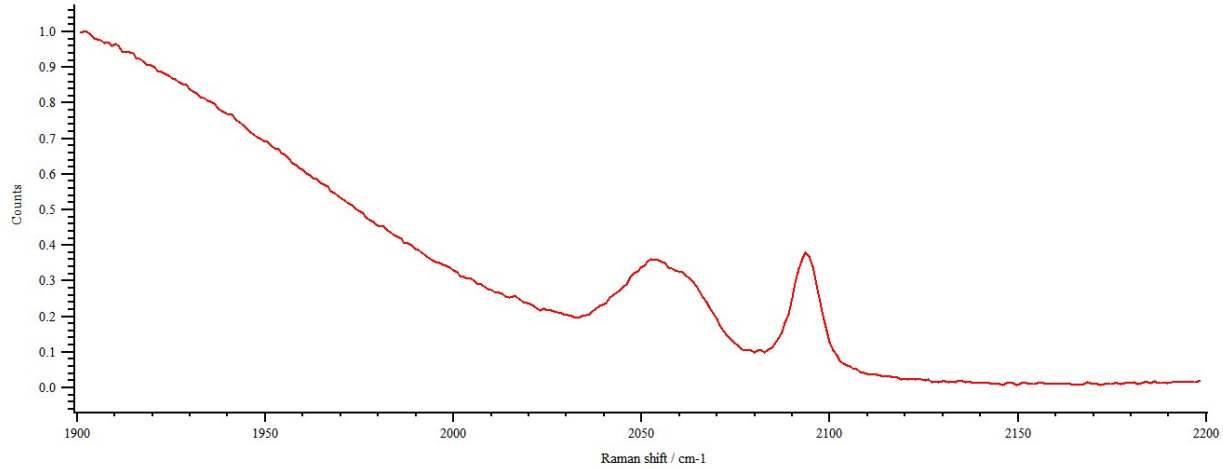

Figure 11 Raman spectrum of **Eu-NCS** in the C=N stretching region.

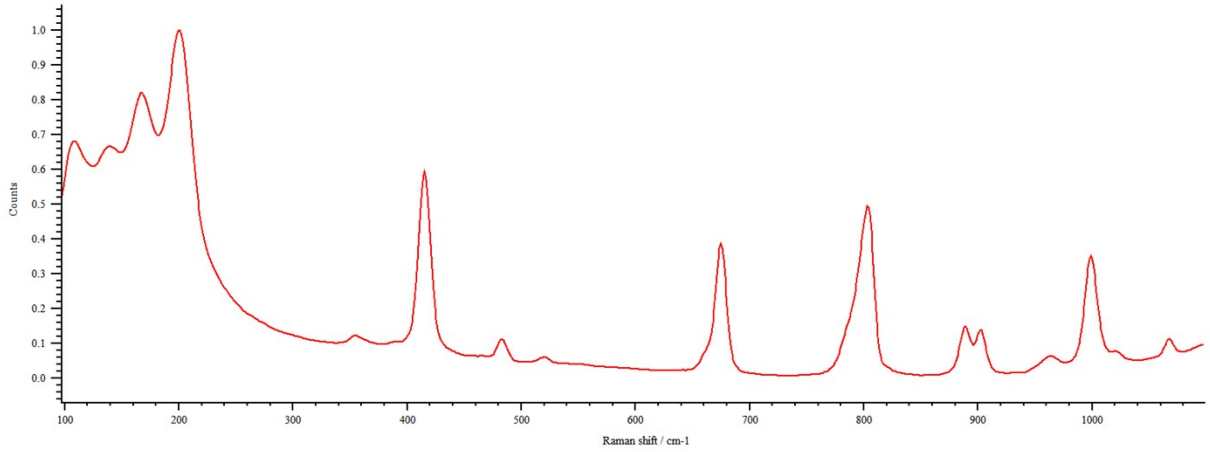

Figure 12. Raman spectrum of **Gd-NCS** in the low frequency region.

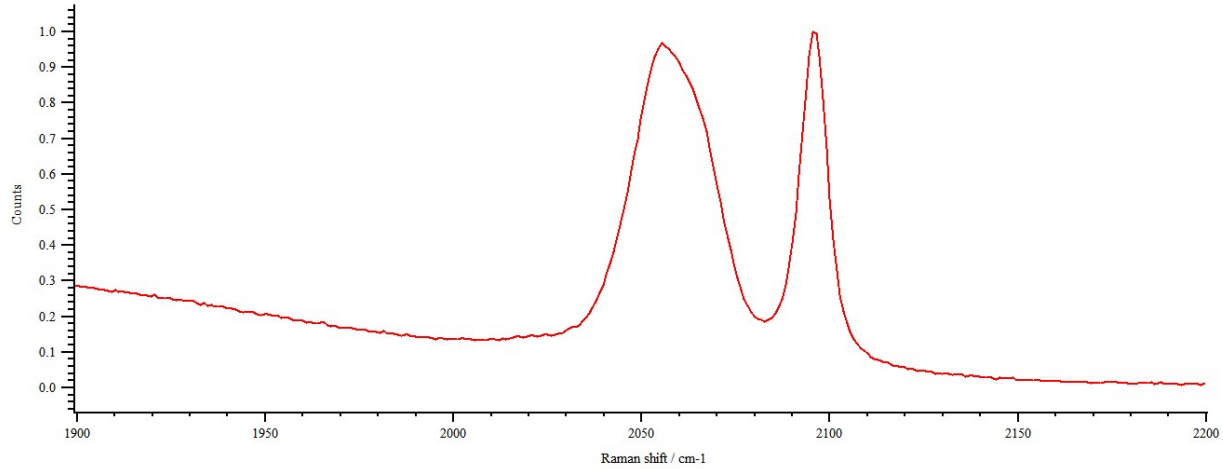

Figure 13. Raman spectrum of **Gd-NCS** in the C=N stretching region.

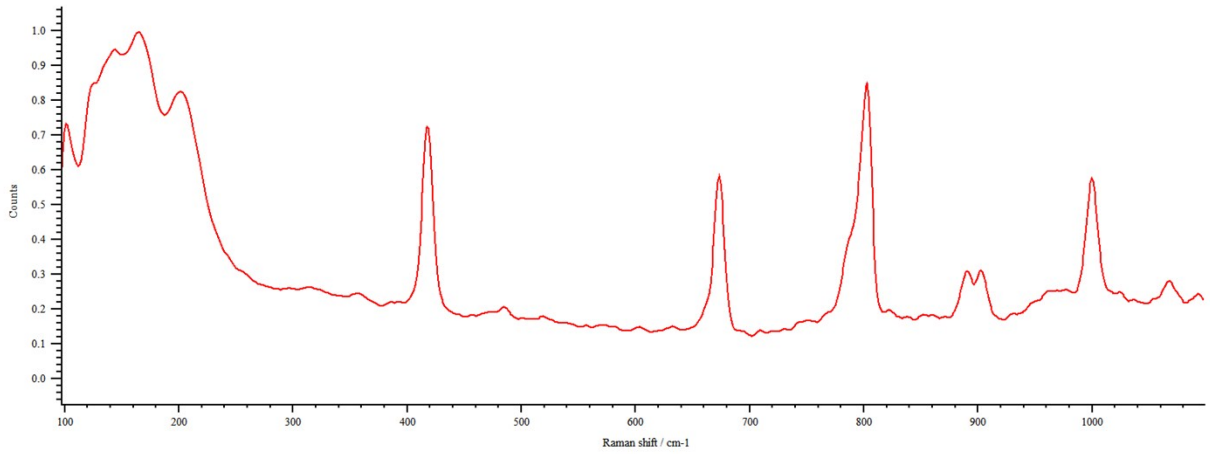

Figure 14. Raman spectrum of **Tb-NCS** in the low frequency region.

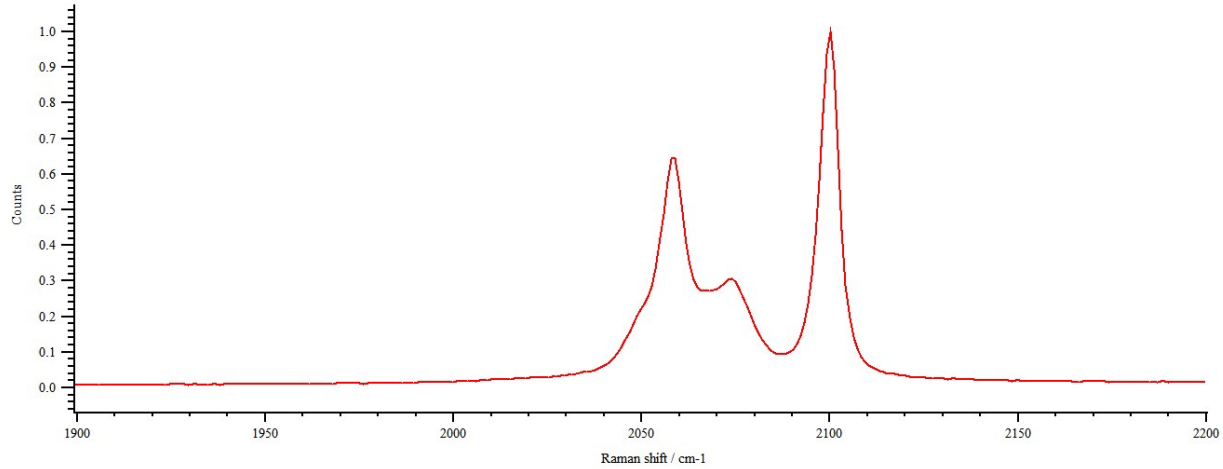

Figure 15. Raman spectrum of **Tb-NCS** in the C=N stretching region.

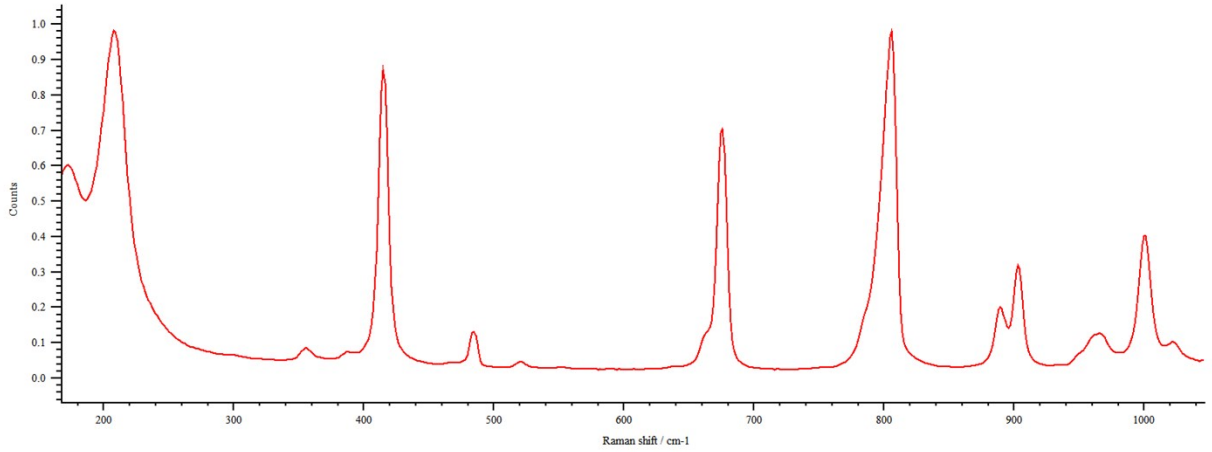

Figure16. Raman spectrum of **Dy-NCS** in the low frequency region.

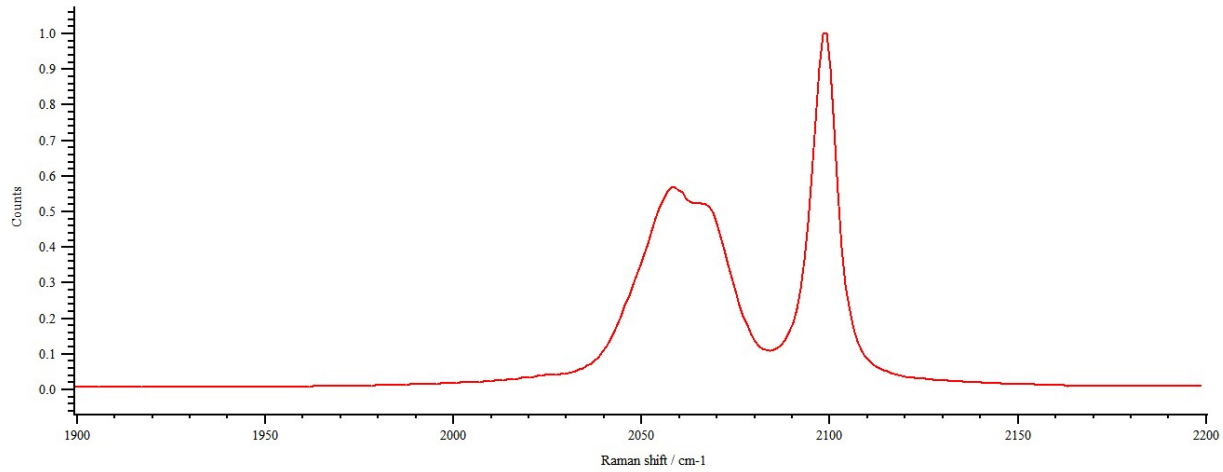

Figure 17. Raman spectrum of **Dy-NCS** in the C=N stretching region.

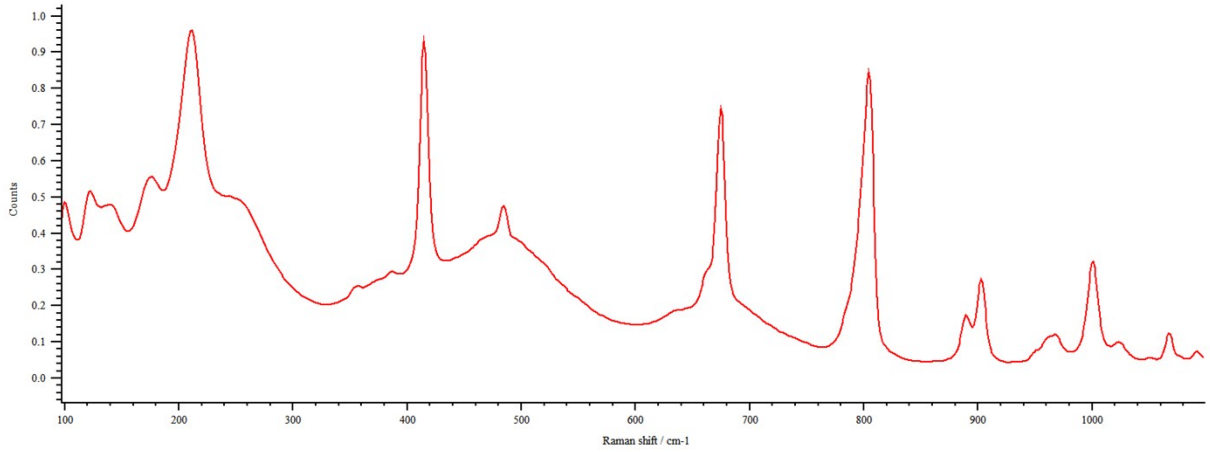

Figure 18. Raman spectrum of **Ho-NCS** in the low frequency region.

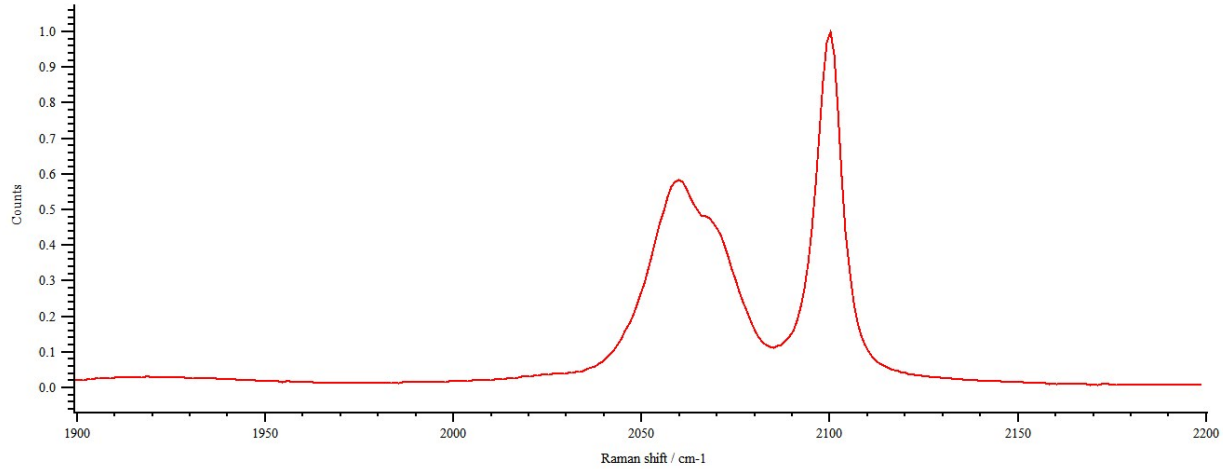

Figure 19. Raman spectrum of **Ho-NCS** in the C=N stretching region.

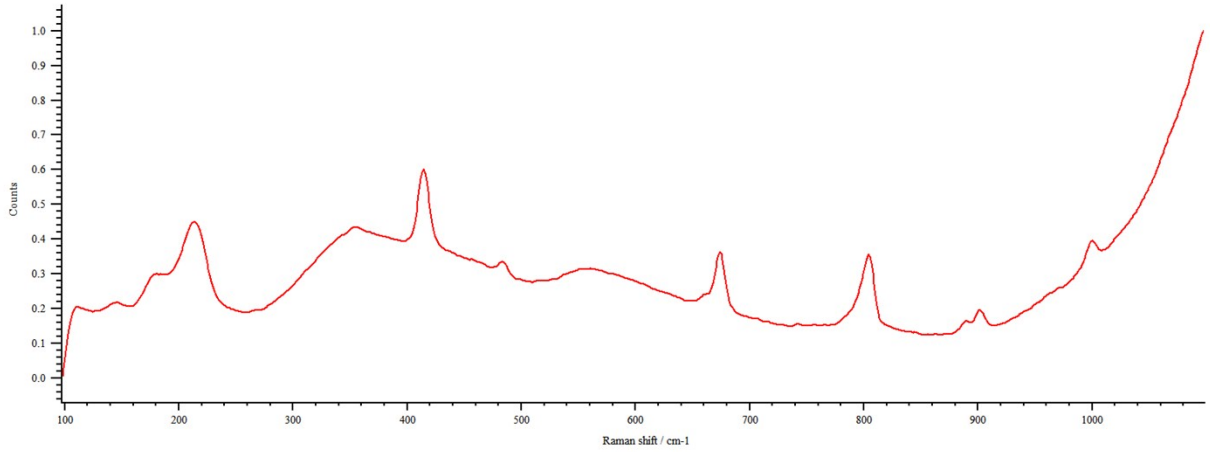

Figure 20. Raman spectrum of **Er-NCS** in the low frequency region.

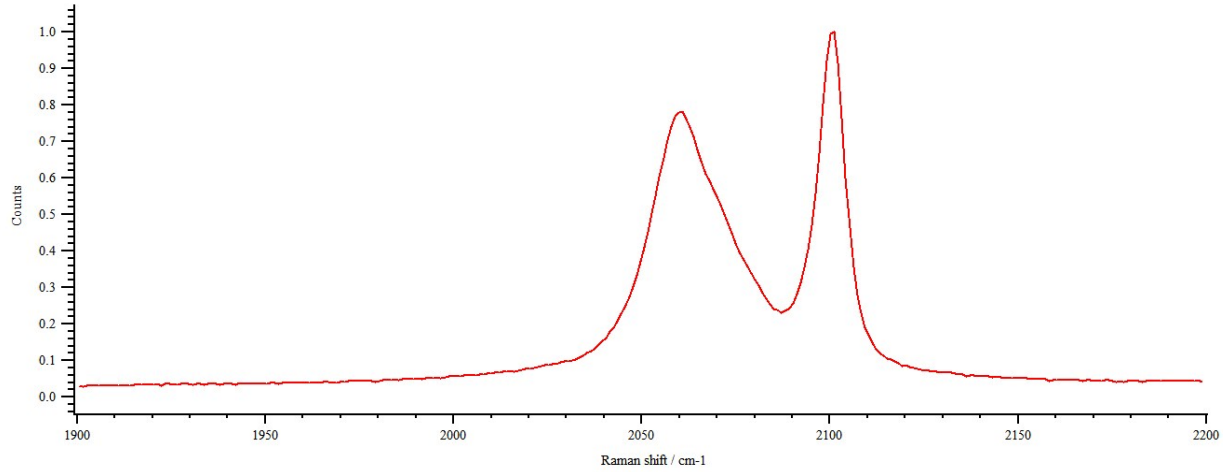

Figure 21. Raman spectrum of **Er-NCS** in the C=N stretching region.

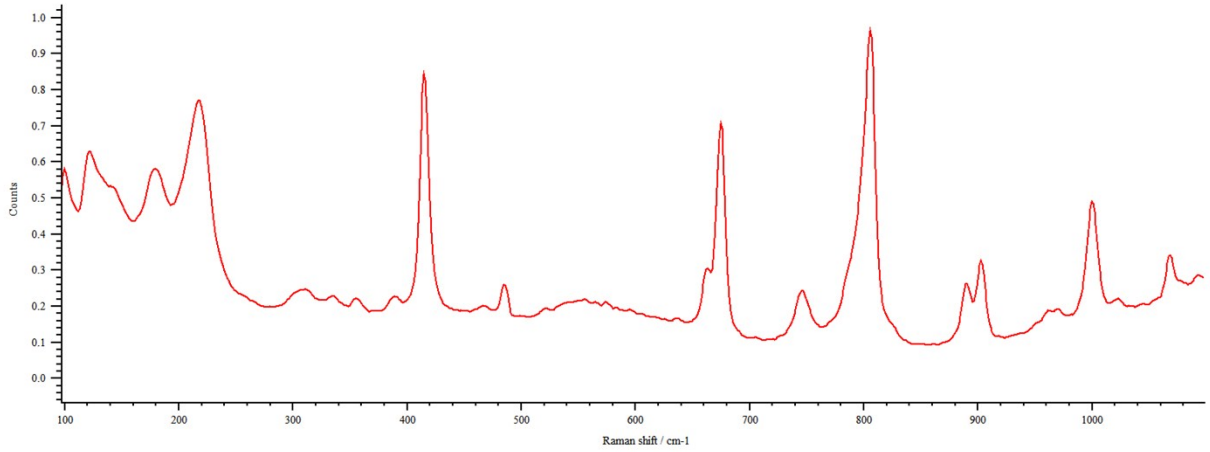

Figure 22. Raman spectrum of **Tm-NCS** in the low frequency region.

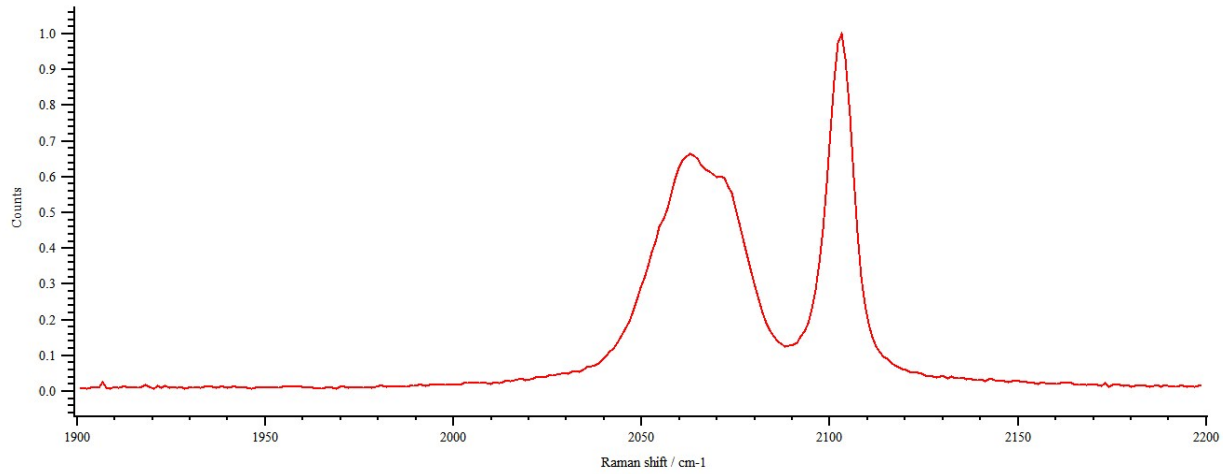

Figure 23. Raman spectrum of **Tm-NCS** in the C=N stretching region.

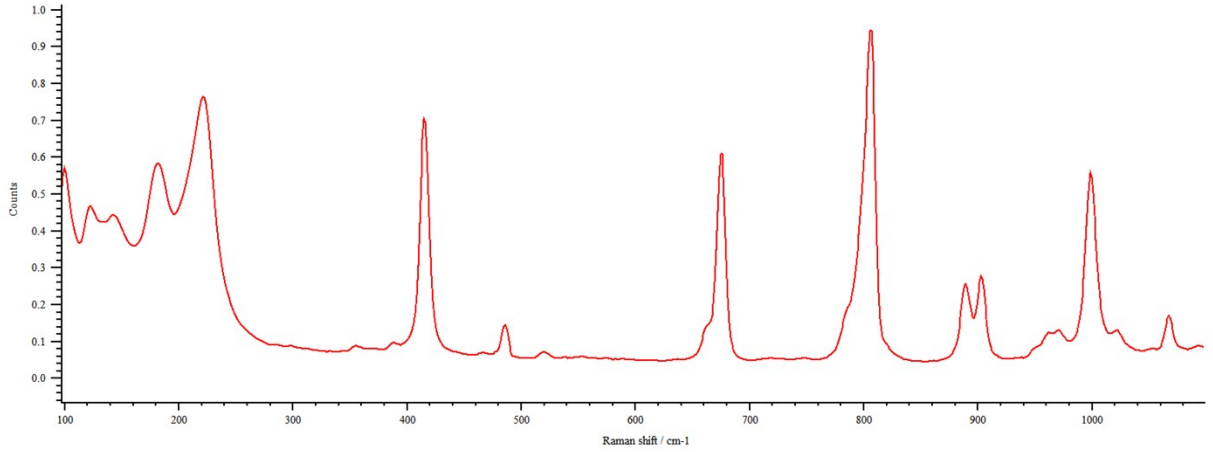

Figure 24. Raman spectrum of **Yb-NCS** in the low frequency region.

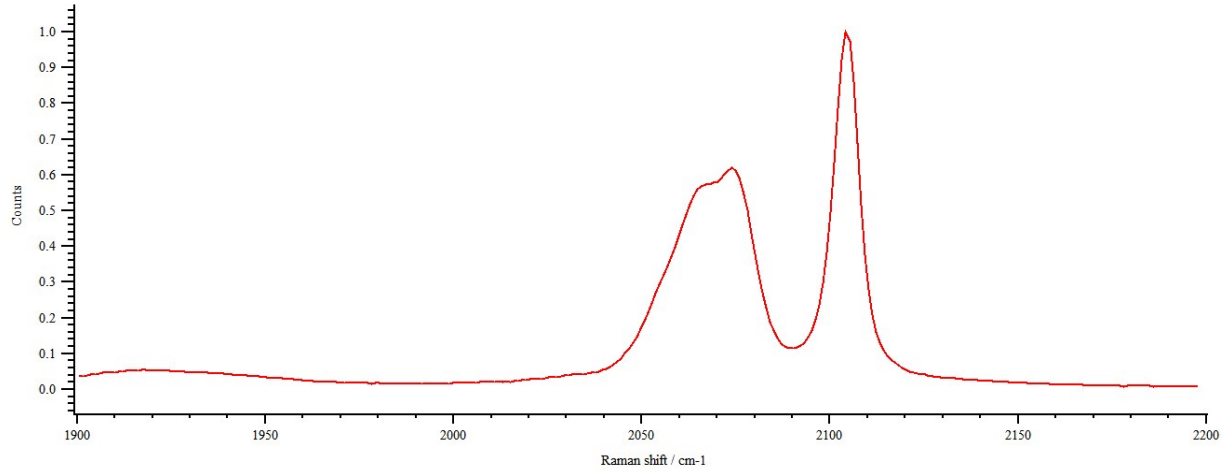

Figure 25. Raman spectrum of **Yb-NCS** in the C=N stretching region.

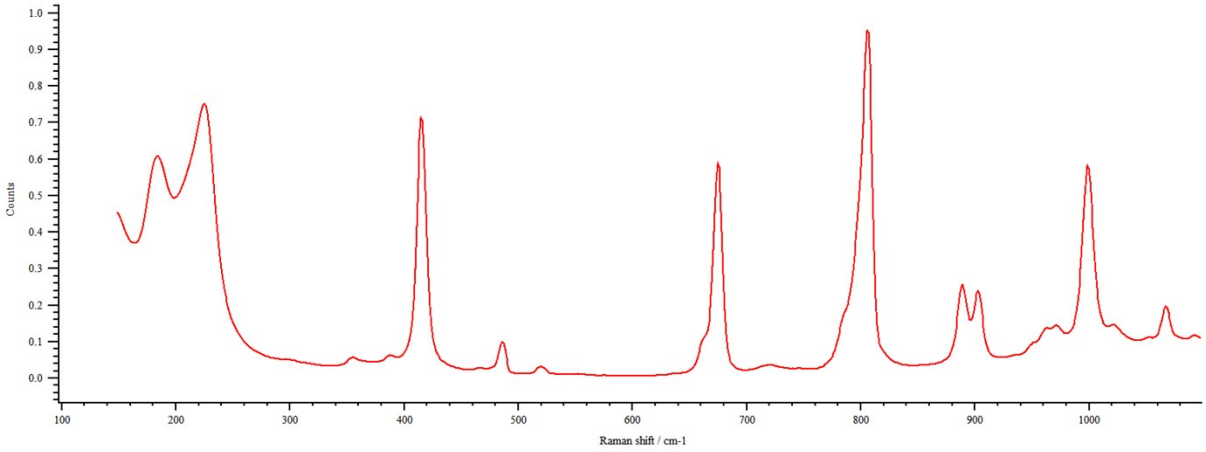

Figure 26 Raman spectrum of **Lu-NCS** in the low frequency region.

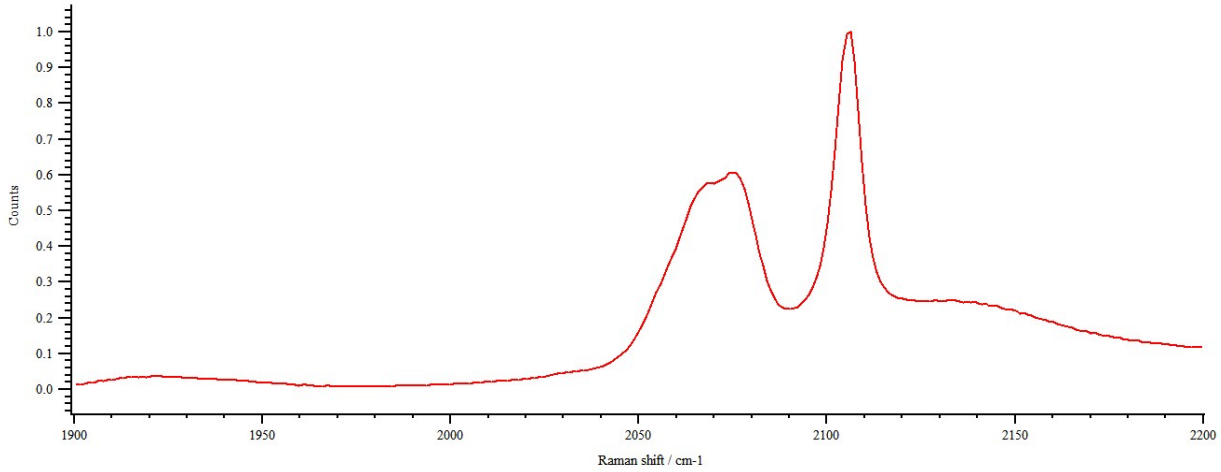

Figure 27 Raman spectrum of **Lu-NCS** in the C=N stretching region.

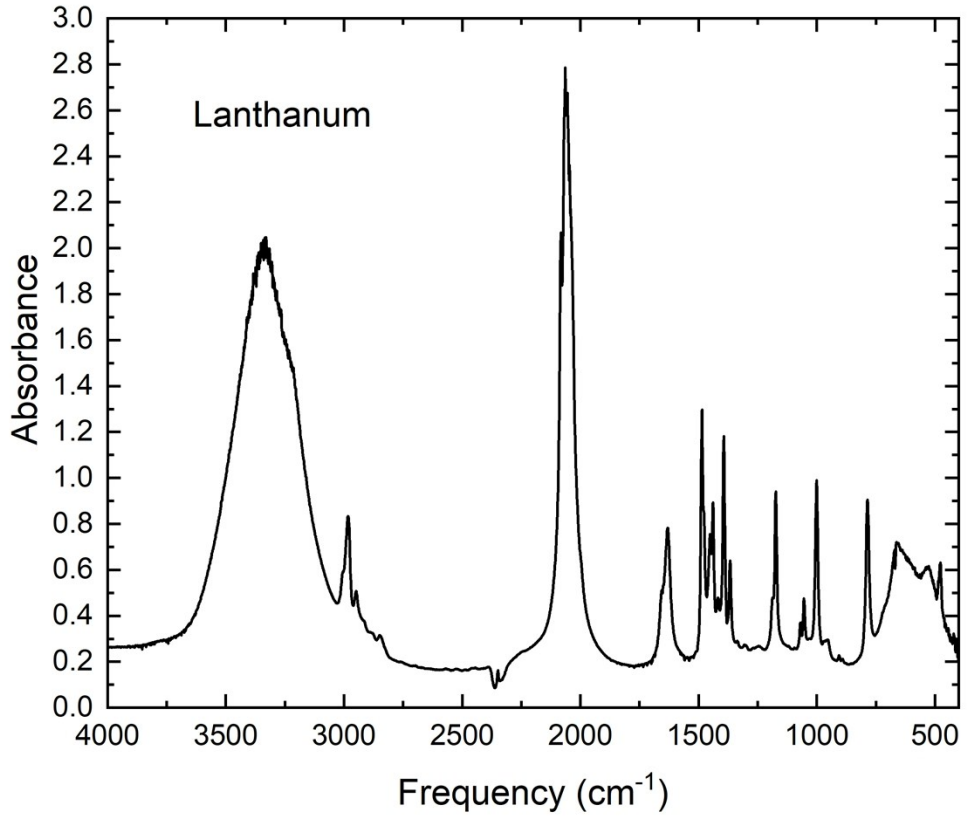

Figure 28. FT-IR of $[Et_4N]_4La(NCS)_7$

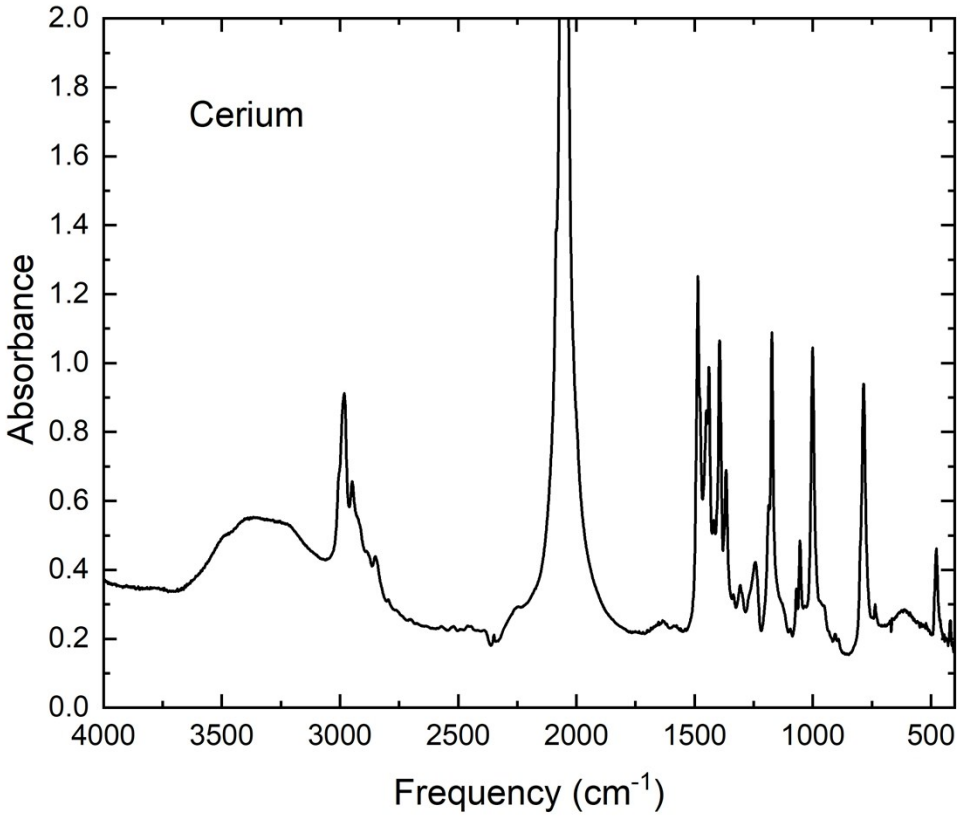

Figure 29. FT-IR of $[Et_4N]_4Ce(NCS)_7$

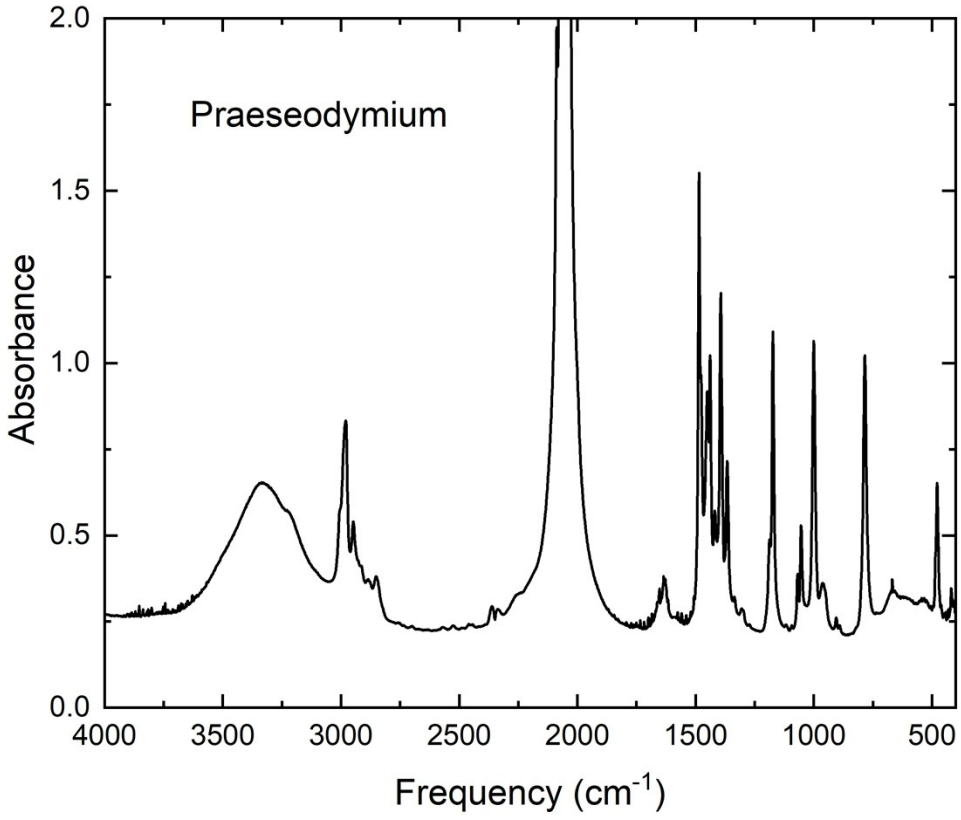

Figure 30. FT-IR of $[Et_4N]_4Pr(NCS)_7$

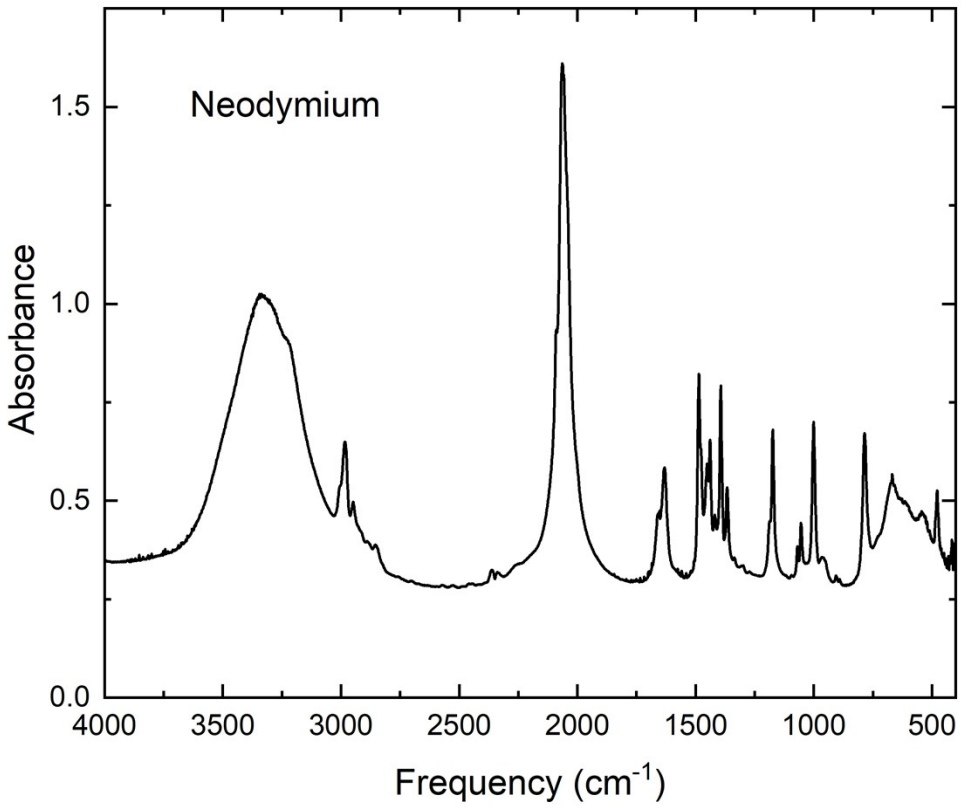

Figure 31. FT-IR of $[Et_4N]_4Nd(NCS)_7$

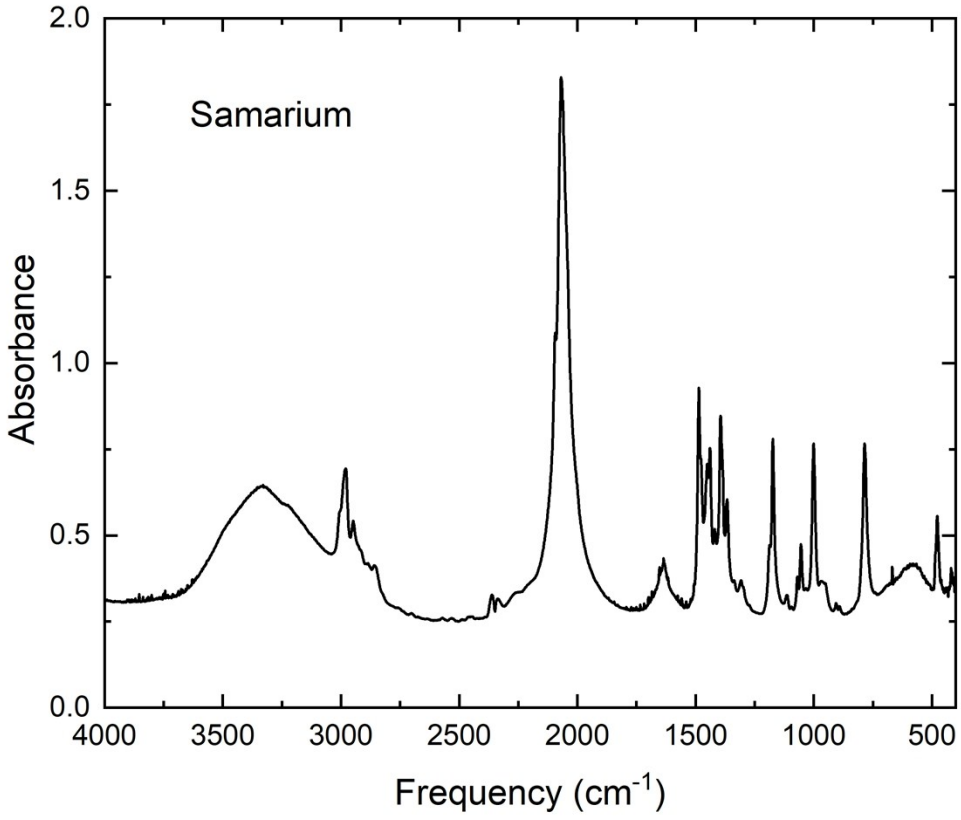

Figure 32. FT-IR of $[Et_4N]_4Sm(NCS)_7$

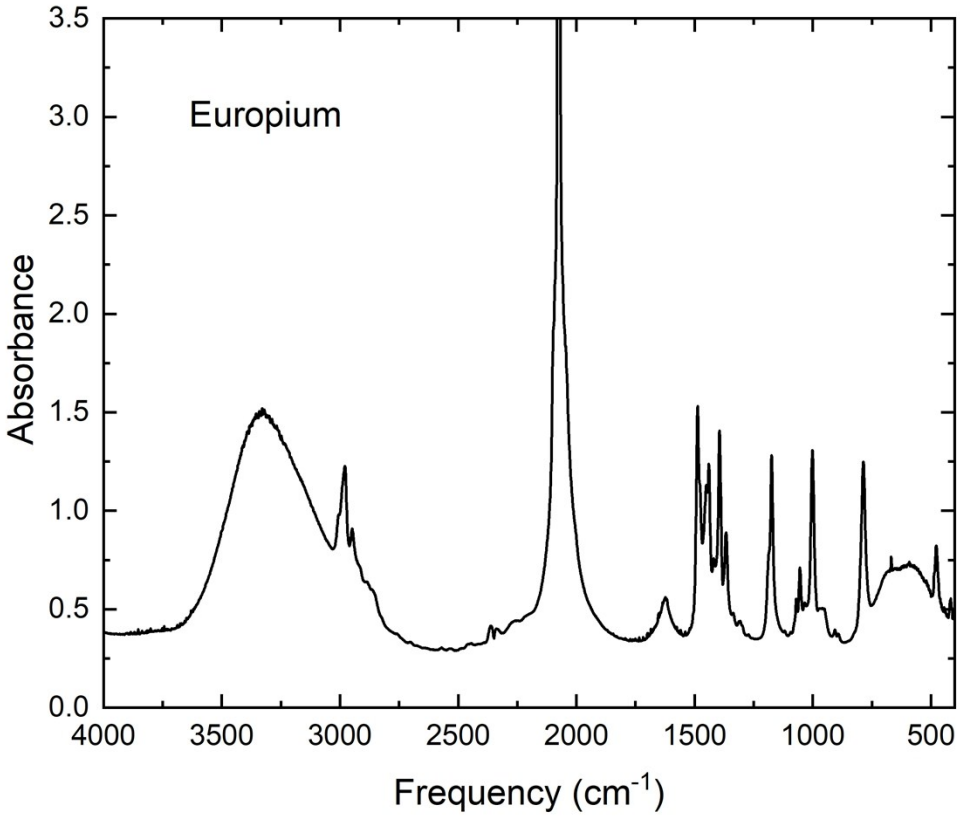

Figure 33. FT-IR of $[Et_4N]_4Eu(NCS)_7$

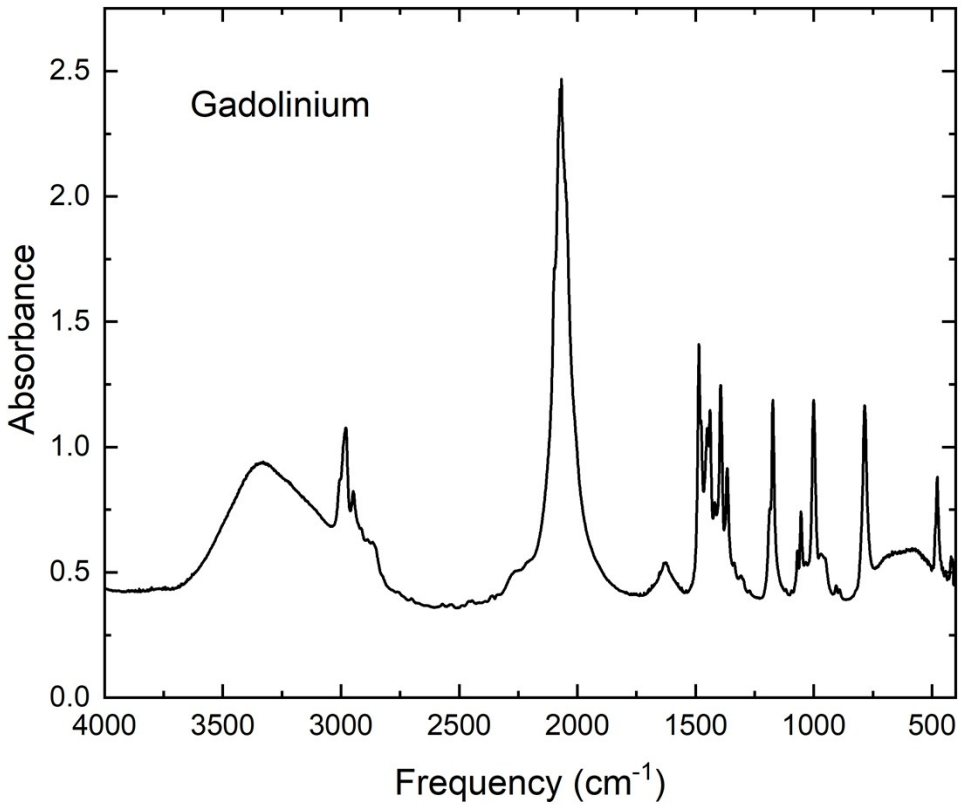

Figure 34. FT-IR of $[Et_4N]_4Gd(NCS)_7$

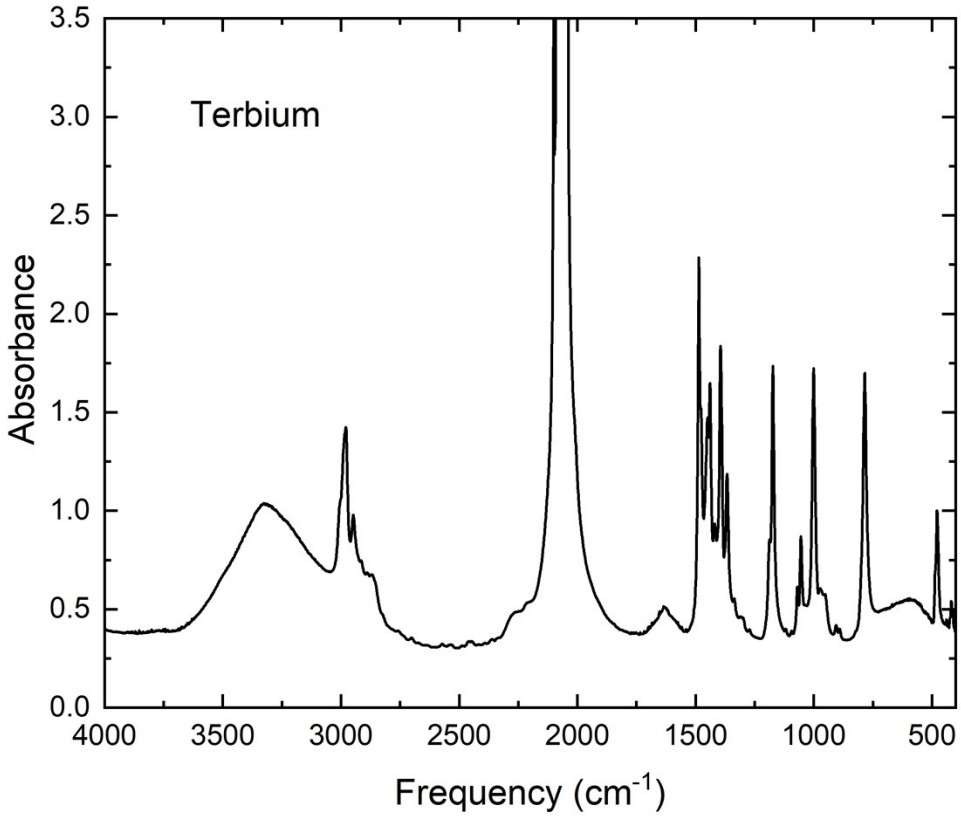

Figure 35. FT-IR of $[Et_4N]_4Tb(NCS)_7$

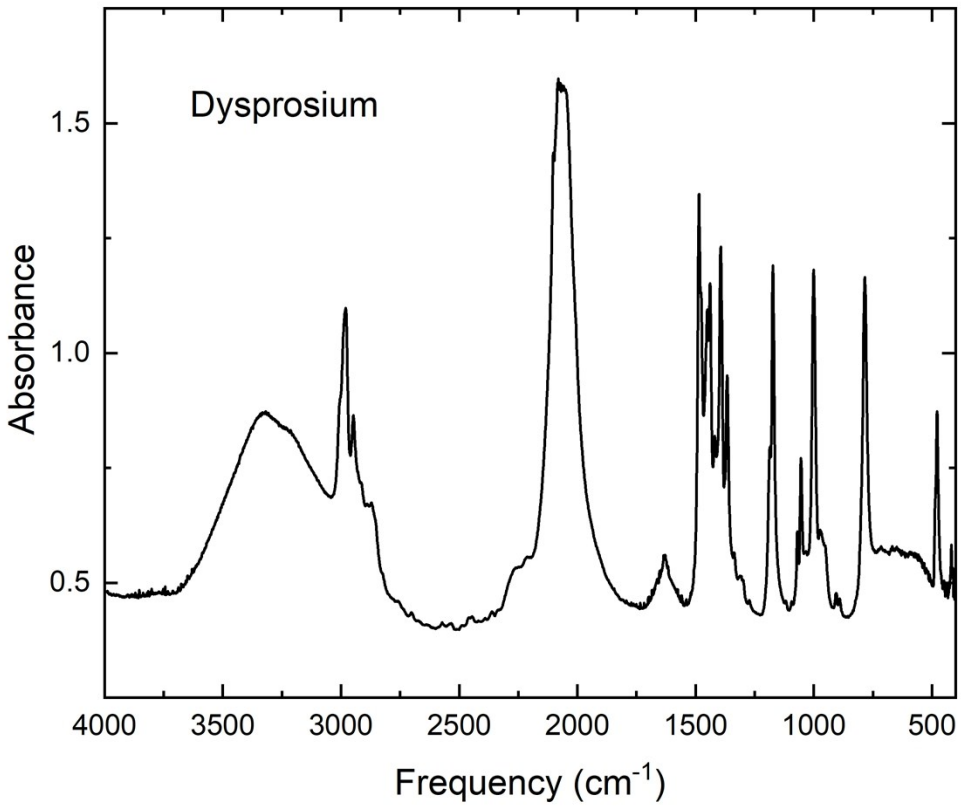

Figure 36. FT-IR of $[Et_4N]_4Dy(NCS)_7$

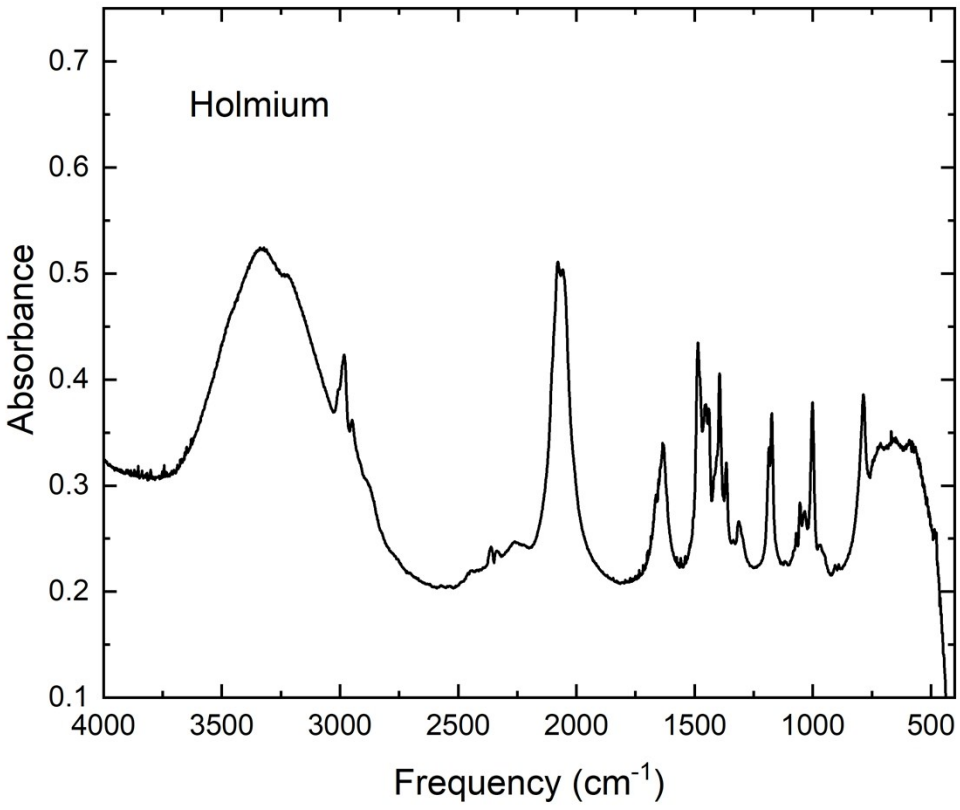

Figure 37. FT-IR of $[Et_4N]_4Ho(NCS)_7$

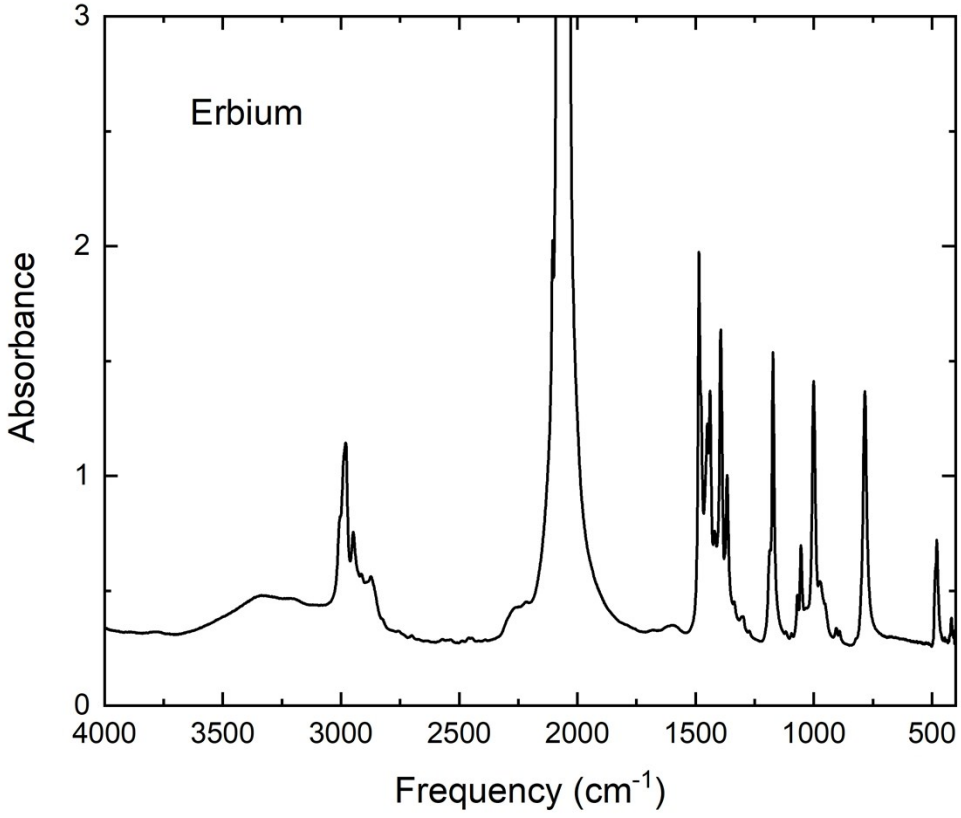

Figure 38. FT-IR of $[Et_4N]_4Er(NCS)_7$

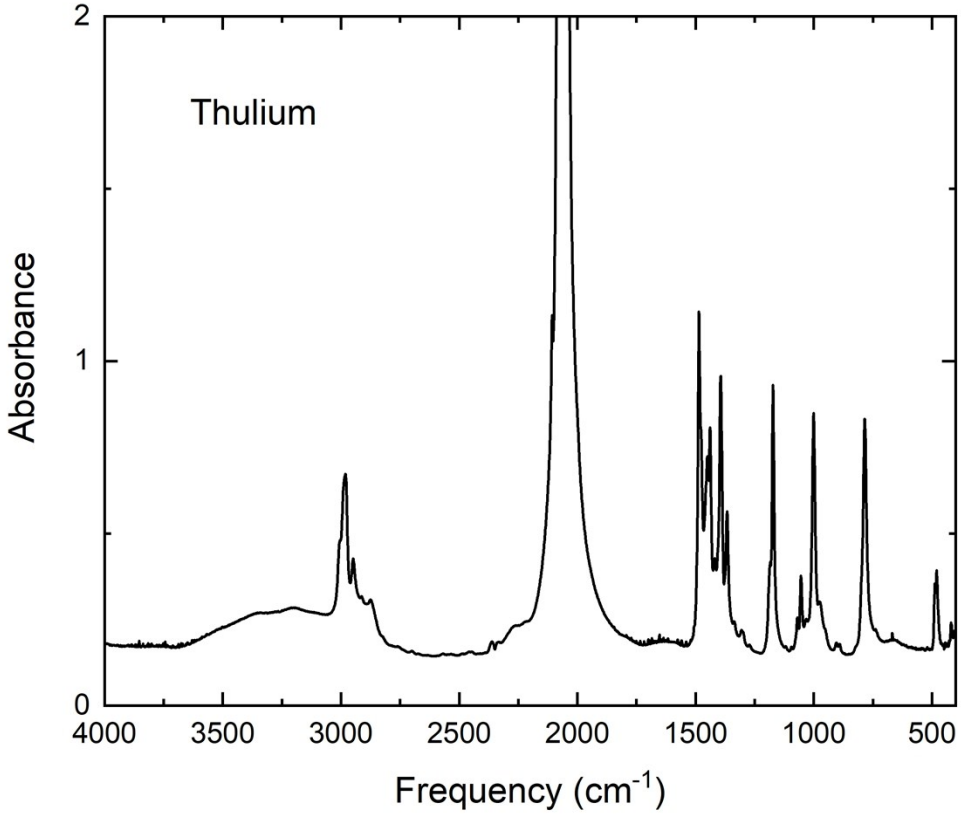

Figure 39. FT-IR of $[Et_4N]_4Tm(NCS)_7$

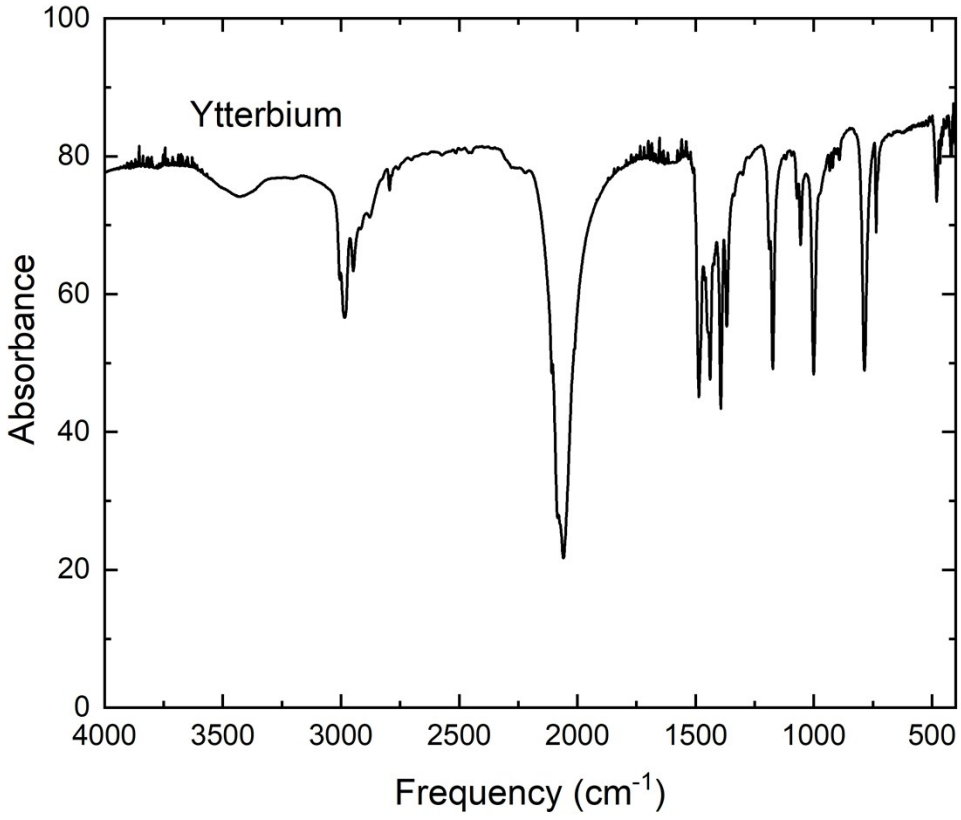

Figure 40. FT-IR of $[Et_4N]_4Yb(NCS)_7$

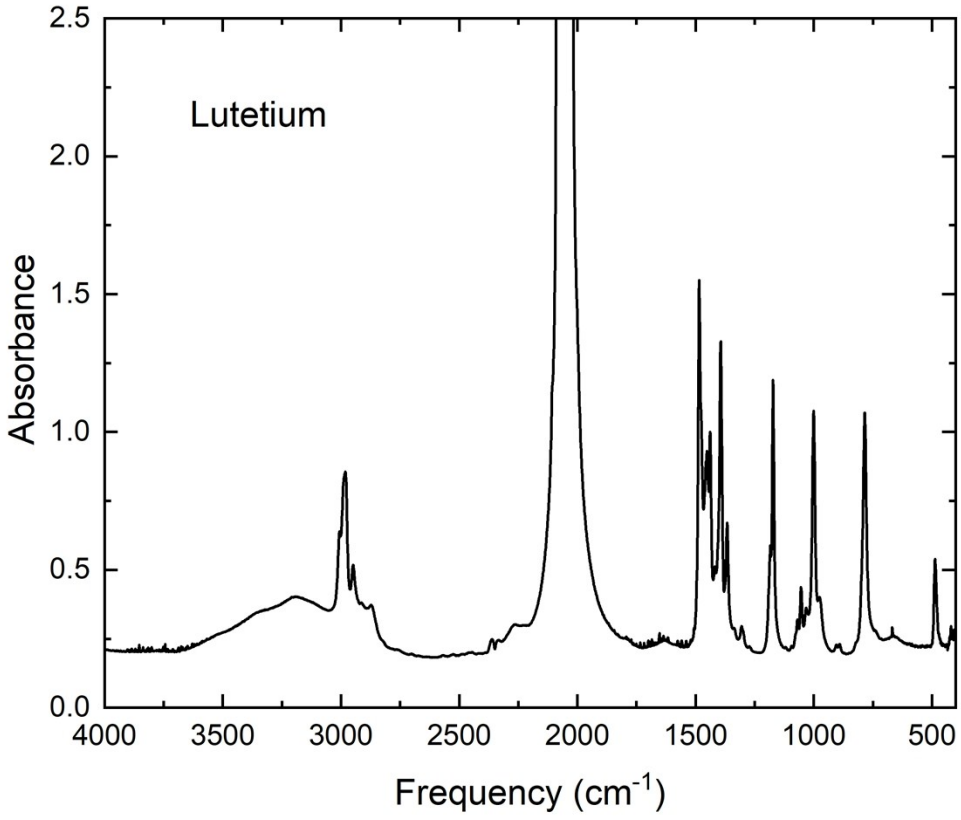

Figure 41. FT-IR of $[Et_4N]_4Lu(NCS)_7$

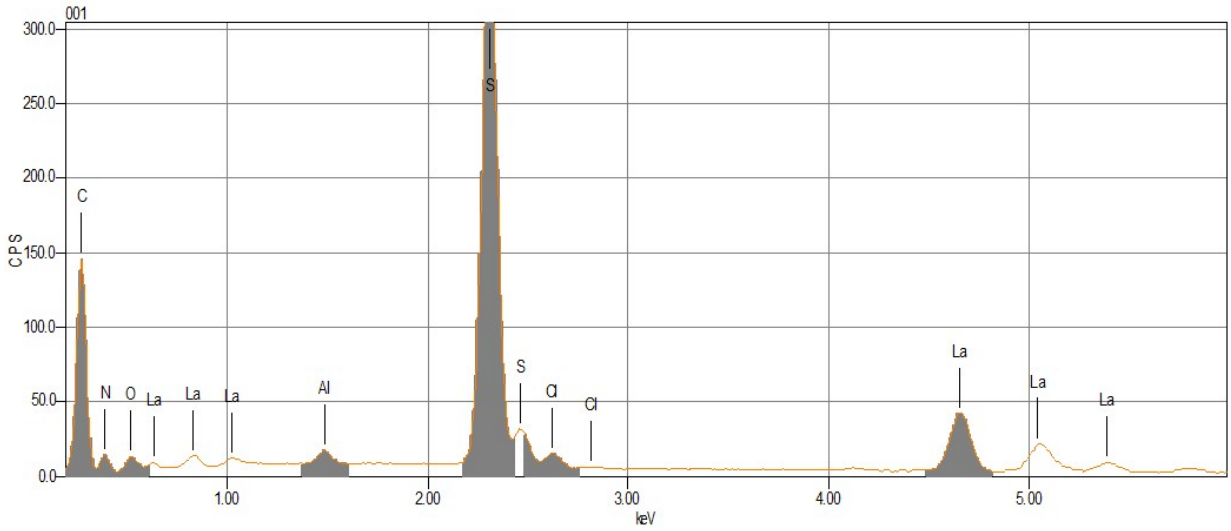

Figure 42. EDS of La-NCS, a small contaminant of Al and some residual chloride is noted. All other peaks consistent with the reported composition.

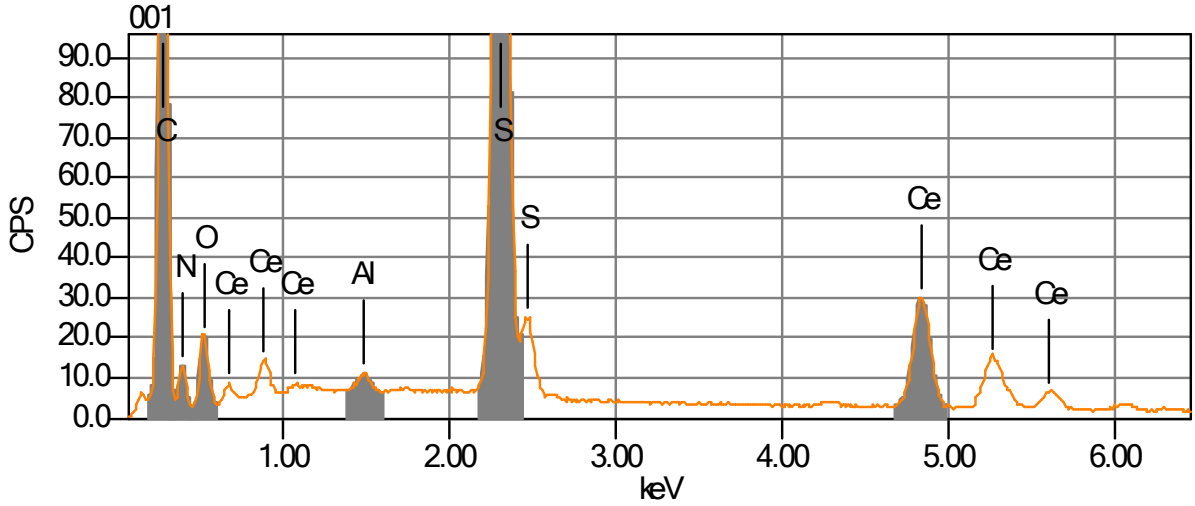

Figure 43: EDS of Ce-NCS. a small contaminant of Al is noted in the spectrum. All other peaks are consistent with the reported composition.

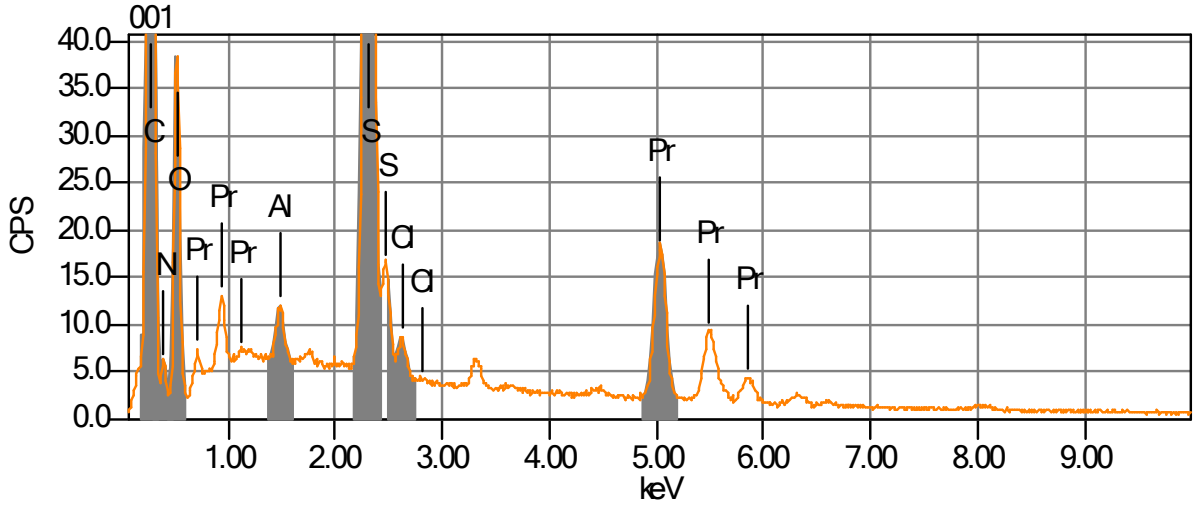

Figure 44. EDS of La-NCS, a small contaminant of Al and some residual chloride is noted. All other peaks consistent with the reported composition.

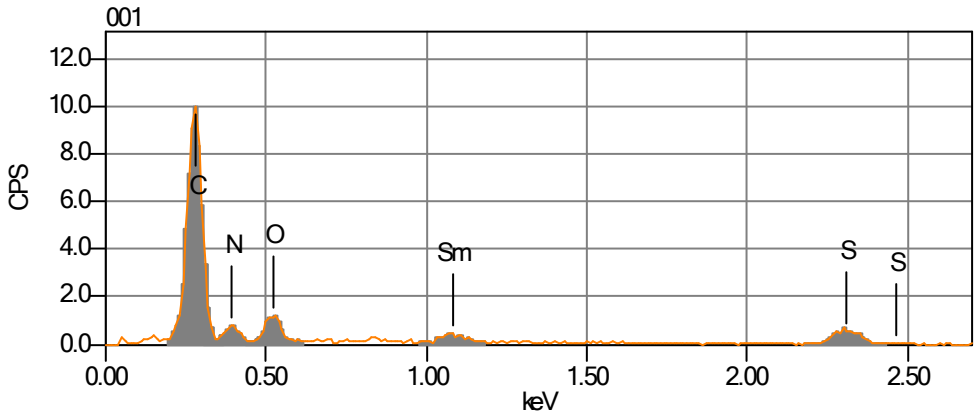

Figure 45. EDS of Sm-NCS. All peaks are consistent with the reported composition.

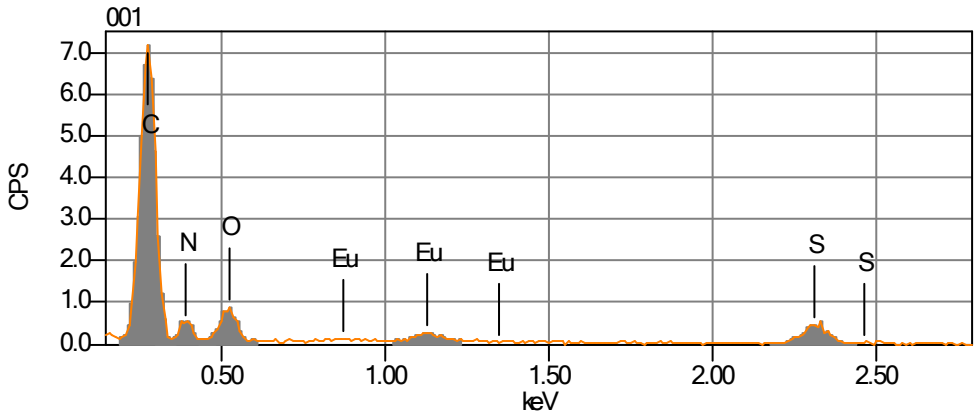

Figure 46. EDS of Eu-NCS.

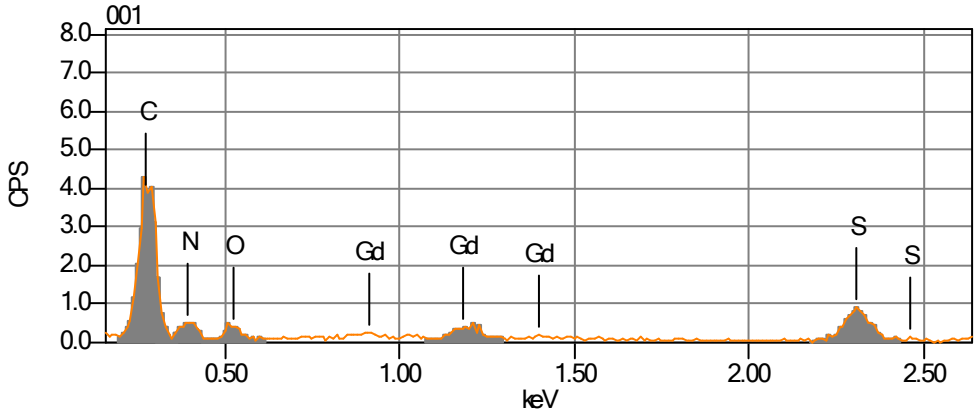

Figure 47. EDS of Gd-NCS

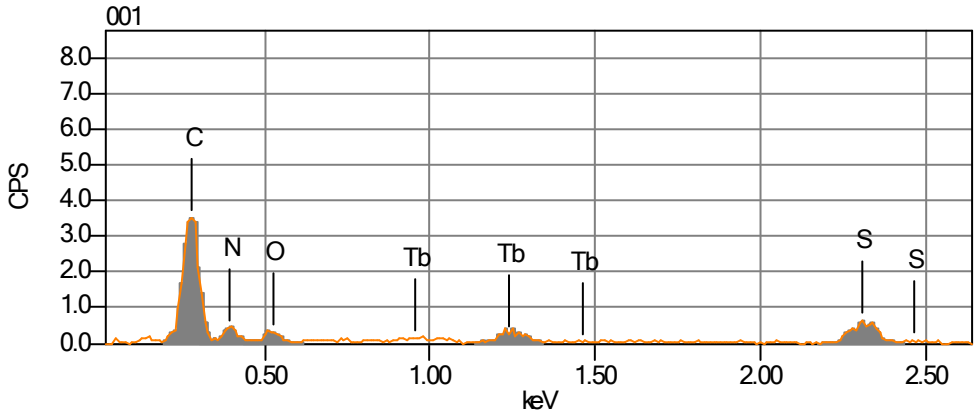

Figure 48. EDS of Tb-NCS

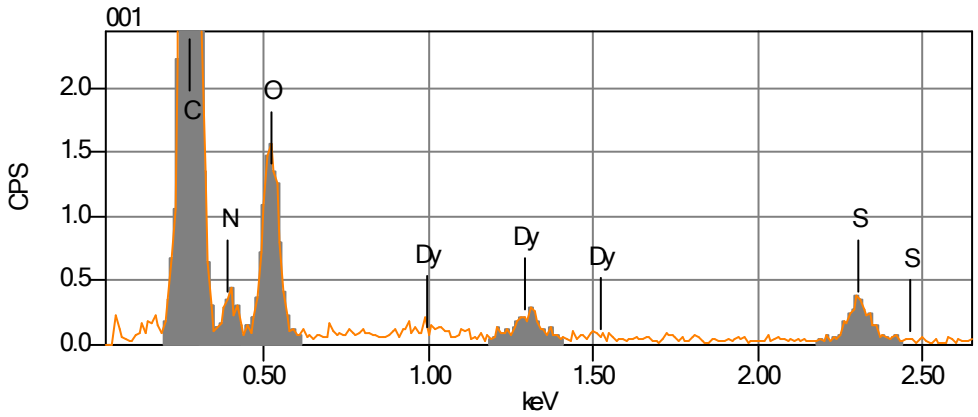

Figure 49. EDS of Dy-NCS

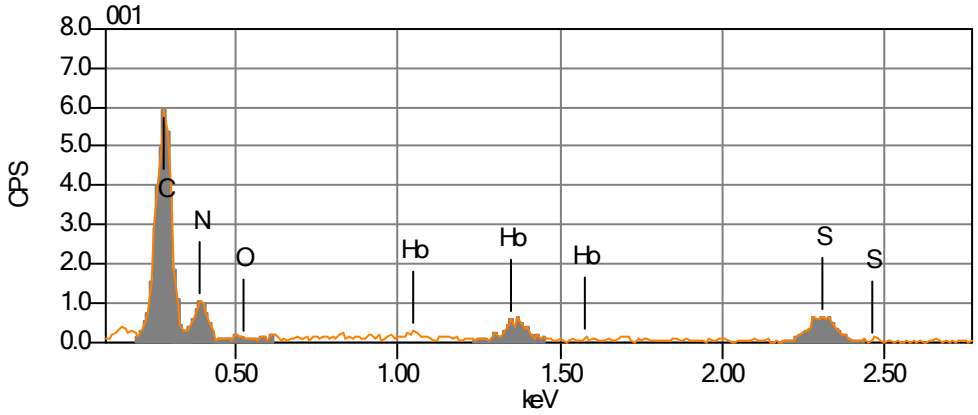

Figure 50. EDS of Ho-NCS

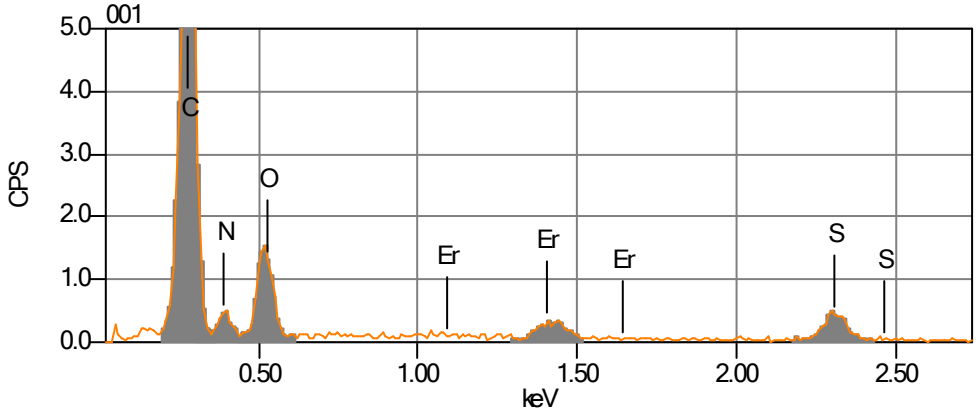

Figure 51. EDS of Er-NCS

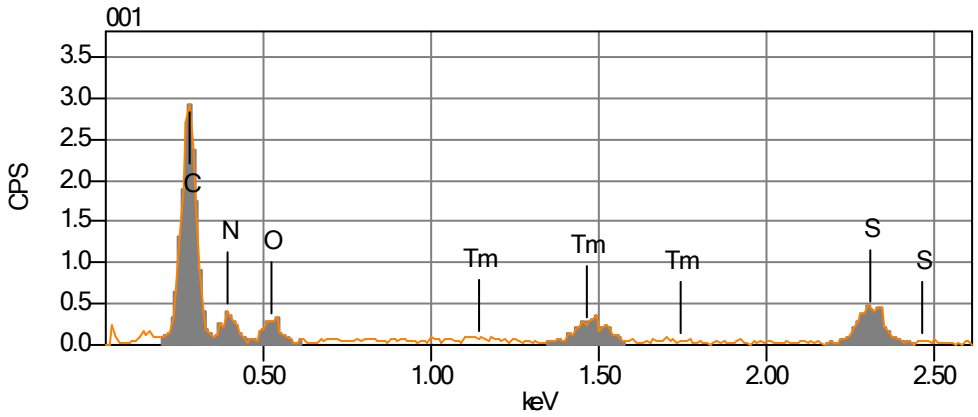

Figure 52. EDS of Tm-NCS

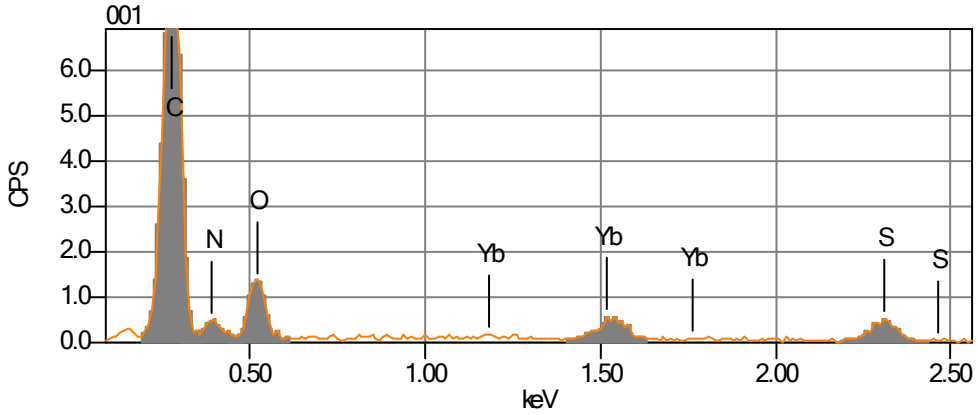

Figure 53. EDS of Yb-NCS

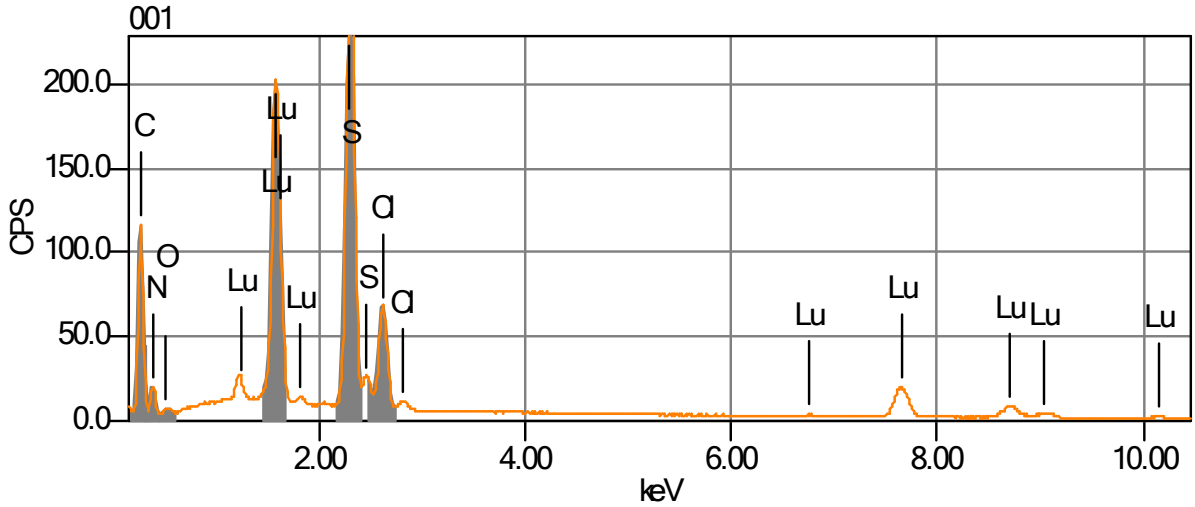

Figure 54. EDS of Lu-NCS. A small contaminant from chlorine is present in the spectrum. All of the remaining peaks are consistent with the reported composition.

Table 65. CHN Analysis of the bulk as synthesized salts.

$(Et_4N)_4Ln(NCS)_7$	expected C, H, N	result C, H, N
La	43.92, 7.56, 14.45	43.30, 8.89, 11.58
Ce	43.87, 7.55, 13.12	44.84, 8.92, 11.77
Pr	43.87, 7.55, 13.12	42.22, 8.31, 11.92
Nd	43.7, 7.52, 14.38	43.11, 7.27, 10.18
Sm	43.45, 7.48, 14.29	42.6, 8.34, 11.81
Eu	43.39, 7.47, 14.27	43.70, 8.48, 11.06
Gd	43.18, 7.43, 14.20	43.19, 8.35, 11.36
Tb	43.11, 7.42, 14.18	44.96, 8.71, 12.53
Dy	42.97, 7.4, 14.13	43.46, 8.66, 11.76
Ho	42.88, 7.38, 14.10	43.97, 8.38, 12.86
Er	42.78, 7.36, 14.07	42.19, 6.21, 12.10
Tm	42.72, 7.35, 14.05	40.59, 7.99, 10.26
Yb	42.56, 7.33, 14.00	44.27, 8.76, 11.70
Lu	42.48, 7.31, 13.97	41.22, 8.06, 10.82

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2. G. Sheldrick, *University of Göttingen, Germany*, 1996.
3. G. Sheldrick, *Acta Crystallographica Section A: Foundations of Crystallography*, 2008, **64**, 112-122.
4. T. J. Carter and R. E. Wilson, *Chem. - Eur. J.*, 2015, **21**, 15575-15582.