Dalton Transactions

Stabilization of molecular lanthanide polysulfides by bulky scorpionate ligands

Marcel Kühling,[a] Robert McDonald,[b] Phil Liebing,[a] Liane Hilfert,[a] Michael J. Ferguson,[b] Josef Takats,*[b] and Frank T. Edelmann*[a]

[a] *Chemisches Institut der Otto-von-Guericke-Universität, 39106 Magdeburg, Germany.*

[b] *Department of Chemistry, University of Alberta, Edmonton, Alberta, AB, Canada T6G 2G2.*

Supporting Information

STRUCTURE REPORT for Compound 3

XCL Code: TAK1506 **Date:** 1 May 2015

Compound: [{HB(3,5-^{i}Pr$_2$-pyrazolyl)$_3$}Sm(3,5-^{i}Pr$_2$-pyrazole)(S$_5$)]•THF

Formula: $C_{40}H_{70}BN_8OS_5Sm$ ($C_{36}H_{62}BN_8S_5Sm$•C_4H_8O)

Supervisor: J. Takats **Crystallographer:** M. J. Ferguson

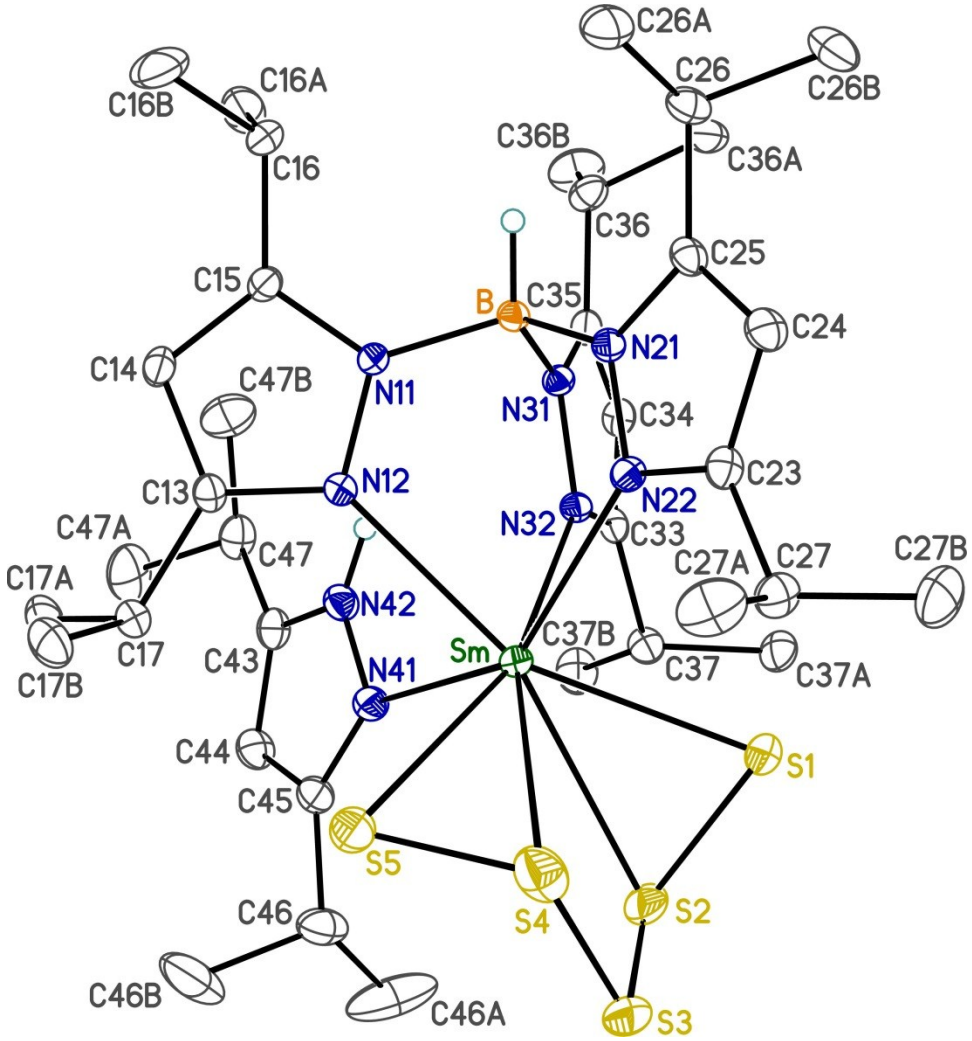
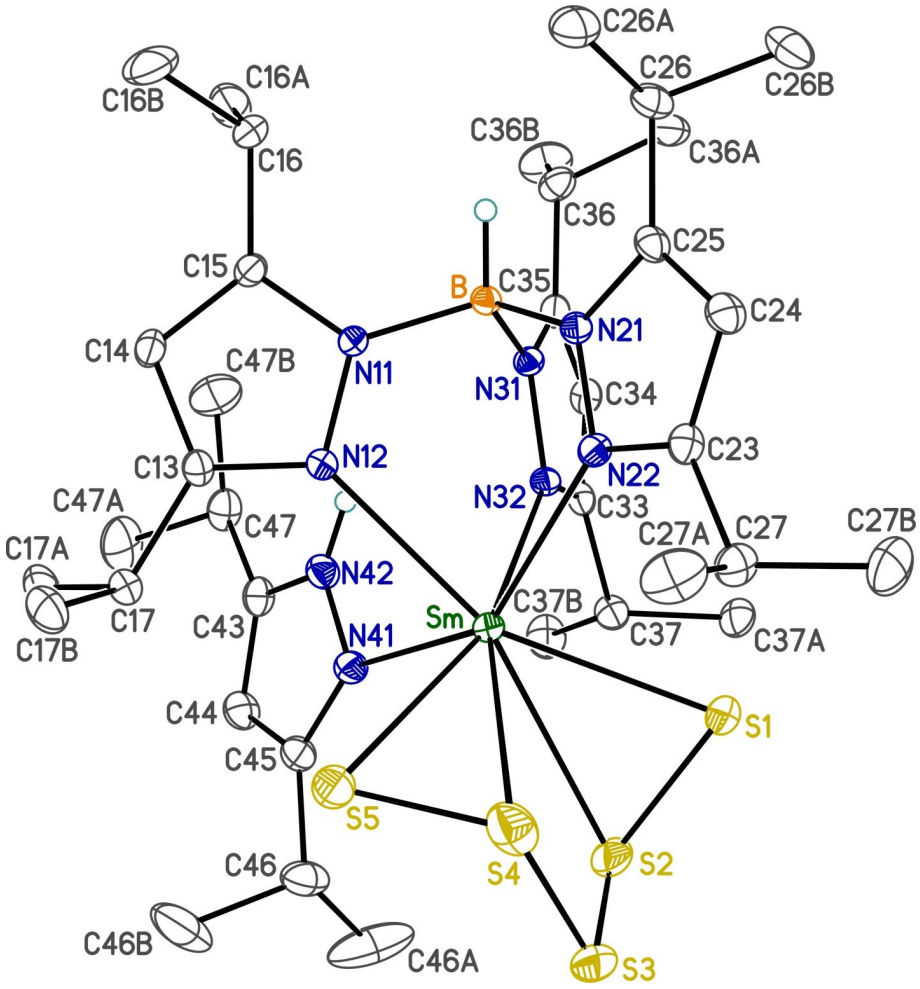


Figure Legends

Figure S1. Perspective view of the [{HB(3,5-^{i}Pr$_2$-pyrazolyl)$_3$}Sm(3,5-^{i}Pr$_2$-pyrazole)(S$_5$)] molecule showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 30% probability level. Hydrogen atoms are shown with arbitrarily small thermal parameters for the B–H and N–H groups; the remaining hydrogen atoms are not shown.

Figure S2. Alternate view of the molecule.

Figure S3. Alternate view of the molecule.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C26B
C16B
C16A
C16
C36B
C36A
C36
C25
C15
B
C35
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C14
C47B
N11
N31
C34
C23
C13
N12
N22
N32
C33
C47A
C47
C27A
C27
C27B
C17A
N42
C17
C43
Sm
C37B
C37
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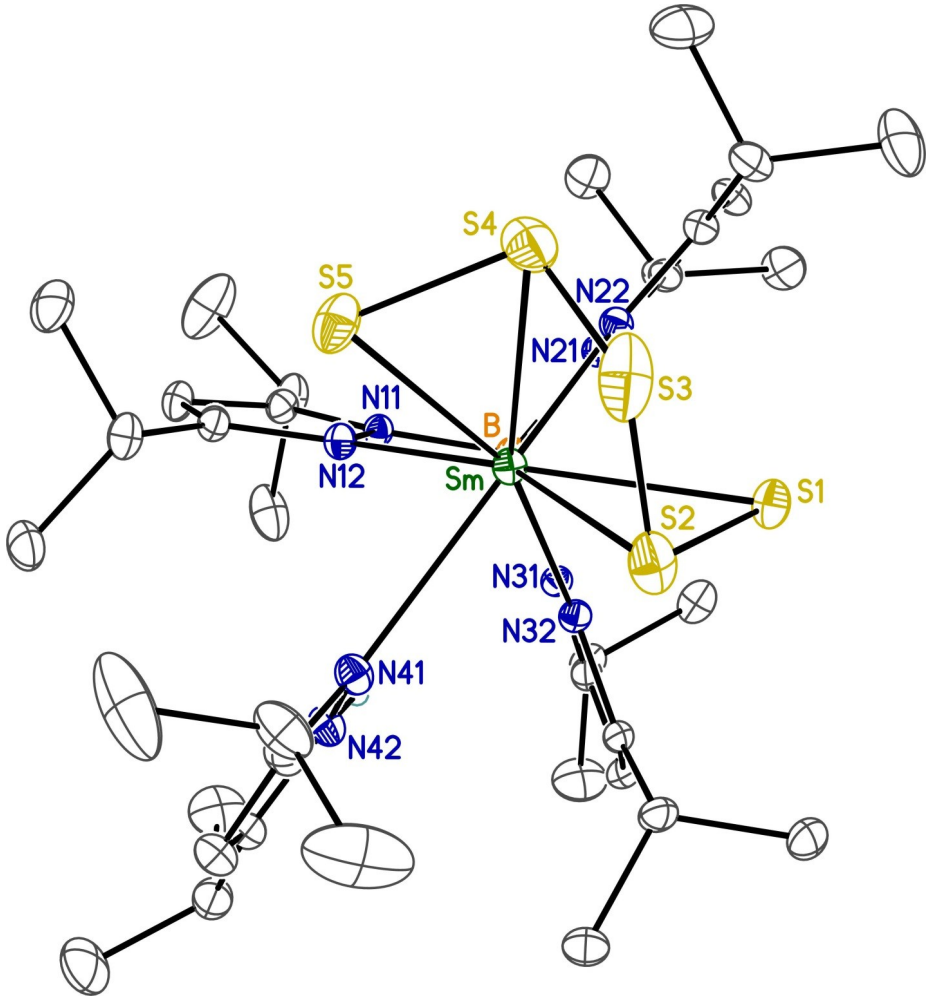
C17B
N41
C44
S1
C45
S5
S4
S2
C46
S3
C46B
C46A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N21
S3
N11
B
N12
Sm
S1
S2
N31
N32
N41
N42

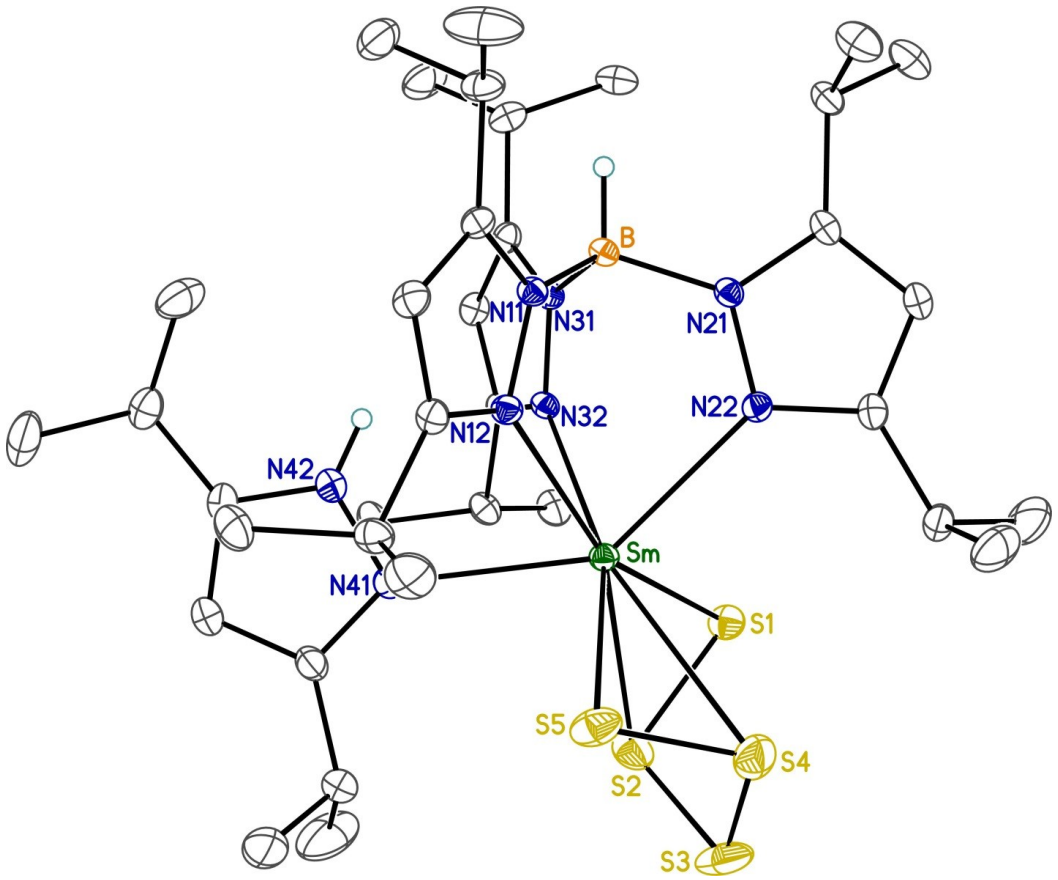
B
N11
N31
N21
N12
N32
N22
N42
Sm
N41
S1
S5
S2
S4
S3

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Table S1. Crystallographic Experimental Details

A. Crystal Data	
formula	$C_{40}H_{70}BN_8OS_5Sm$
formula weight	1000.50
crystal dimensions (mm)	0.31 × 0.19 × 0.12
crystal system	triclinic
space group	$P\bar{1}$ (No. 2)
unit cell parameters[a]	
a (Å)	11.8065 (4)
b (Å)	12.8567 (4)
c (Å)	18.9856 (6)
α (deg)	91.7130 (4)
β (deg)	101.7977 (4)
γ (deg)	116.9095 (3)
V (Å^3)	2490.68 (14)
Z	2
ρ_{calcd} (g cm^{-3})	1.334
μ (mm^{-1})	1.426
B. Data Collection and Refinement Conditions	
diffractometer	Bruker D8/APEX II CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–100
scan type	ω scans (0.3°) (20 s exposures)
data collection 2θ limit (deg)	54.21
total data collected	21641 (-15 ≤ h ≤ 15, -16 ≤ k ≤ 16, -24 ≤ l ≤ 24)
independent reflections	10973 (R_{int} = 0.0171)
number of observed reflections (*NO*)	10149 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method	intrinsic phasing (*SHELXT-2014*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–2014*[d])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	0.8740–0.7483
data/restraints/parameters	10973 / 0 / 505
goodness-of-fit (S)[e] [all data]	1.041
final R indices[f]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0260
wR_2 [all data]	0.0661
largest difference peak and hole	1.219 and –0.857 e Å^{-3}

[a]Obtained from least-squares refinement of 9584 reflections with 4.42° < 2θ < 54.20°.

(continued)

Table S1. Crystallographic Experimental Details (continued)

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

[c]Sheldrick, G. M. *Acta Crystallogr.* **2015**, *A71*, 3–8. (*SHELXT-2014*)

[d]Sheldrick, G. M. *Acta Crystallogr.* **2015**, *C71*, 3–8. (*SHELXL-2014*)

[e]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0346P)^2 + 1.4156P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[f]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

The large differences in the $U_{i,j}$ values between Sm-S and S-S can be explained by a comparatively high flexibility of the S_5^{2-} ligand. However splitting the S sites is not reasonable and does not lead to a satisfying result.

Table S2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters

(a) [{HB(3,5-^{i}Pr$_2$-pyrazolyl)$_3$}Sm(3,5-^{i}Pr$_2$-pyrazole)(S$_5$)] atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Sm	0.25284(2)	0.14496(2)	0.22699(2)	0.02028(4)*
S1	0.30869(6)	0.14263(6)	0.09315(3)	0.03191(13)*
S2	0.41317(7)	0.07620(7)	0.15529(4)	0.04321(16)*
S3	0.59675(7)	0.21768(9)	0.20208(4)	0.0599(2)*
S4	0.54772(7)	0.32224(7)	0.26026(4)	0.04920(18)*
S5	0.47591(6)	0.23772(7)	0.34233(3)	0.04217(16)*
N11	0.01368(16)	0.16973(15)	0.29290(9)	0.0192(3)*
N12	0.12093(16)	0.15037(15)	0.31548(9)	0.0210(3)*
N21	0.05431(16)	0.27552(15)	0.18228(9)	0.0199(3)*
N22	0.17970(16)	0.29417(15)	0.18372(9)	0.0215(3)*
N31	-0.07706(16)	0.05155(14)	0.16611(9)	0.0192(3)*
N32	0.01876(16)	0.02149(14)	0.15811(9)	0.0197(3)*
N41	0.17336(18)	-0.05652(16)	0.27678(10)	0.0260(4)*
N42	0.04501(18)	-0.10969(16)	0.27937(10)	0.0275(4)*
C13	0.1380(2)	0.14950(18)	0.38782(11)	0.0232(4)*
C14	0.0449(2)	0.1696(2)	0.41149(12)	0.0267(4)*
C15	-0.0321(2)	0.18220(18)	0.35068(11)	0.0225(4)*
C16	-0.1517(2)	0.1992(2)	0.34518(12)	0.0313(5)*
C16A	-0.2723(3)	0.0793(3)	0.33686(16)	0.0478(7)*
C16B	-0.1358(3)	0.2799(4)	0.41088(17)	0.0656(10)*
C17	0.2404(2)	0.1234(2)	0.43303(12)	0.0292(5)*
C17A	0.1760(3)	0.0131(2)	0.46883(14)	0.0389(6)*
C17B	0.3390(3)	0.2272(2)	0.49101(14)	0.0415(6)*
C23	0.2363(2)	0.39342(18)	0.15387(12)	0.0251(4)*
C24	0.1481(2)	0.4379(2)	0.13355(13)	0.0294(5)*
C25	0.0345(2)	0.36225(18)	0.15220(11)	0.0244(4)*
C26	-0.0886(2)	0.3739(2)	0.14514(13)	0.0295(5)*
C26A	-0.0684(3)	0.4668(2)	0.20478(15)	0.0419(6)*
C26B	-0.1313(3)	0.4033(2)	0.06960(15)	0.0415(6)*
C27	0.3748(2)	0.4451(2)	0.14646(13)	0.0312(5)*
C27A	0.4646(3)	0.5510(3)	0.20512(18)	0.0513(7)*
C27B	0.3844(3)	0.4801(3)	0.07094(18)	0.0595(9)*
C33	-0.0435(2)	-0.08358(17)	0.11488(11)	0.0219(4)*
C34	-0.1779(2)	-0.12132(18)	0.09612(11)	0.0247(4)*
C35	-0.1966(2)	-0.03413(18)	0.12819(11)	0.0228(4)*
C36	-0.3215(2)	-0.0253(2)	0.11939(13)	0.0295(5)*
C36A	-0.3299(2)	0.0523(2)	0.06111(13)	0.0343(5)*
C36B	-0.4414(2)	-0.1472(3)	0.09925(18)	0.0500(7)*
C37	0.0285(2)	-0.14360(19)	0.09103(12)	0.0272(5)*

Table S2. Atomic Coordinates and Displacement Parameters (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C37A	0.0174(3)	-0.1453(2)	0.00903(13)	0.0345(5)*
C37B	-0.0228(3)	-0.2692(2)	0.10977(15)	0.0416(6)*
C43	0.0079(2)	-0.21358(19)	0.30543(12)	0.0285(5)*
C44	0.1181(2)	-0.2289(2)	0.32156(13)	0.0328(5)*
C45	0.2181(2)	-0.1302(2)	0.30316(13)	0.0297(5)*
C46	0.3576(3)	-0.1039(3)	0.31105(17)	0.0438(7)*
C46A	0.3656(4)	-0.1919(3)	0.2601(3)	0.0974(17)*
C46B	0.4203(3)	-0.1008(4)	0.3902(2)	0.0970(17)*
C47	-0.1310(2)	-0.2889(2)	0.31092(13)	0.0353(5)*
C47A	-0.1346(3)	-0.3658(3)	0.37058(18)	0.0581(8)*
C47B	-0.1999(3)	-0.2160(3)	0.31986(19)	0.0534(8)*
B	-0.0427(2)	0.16881(19)	0.21146(12)	0.0192(4)*

(b) solvent tetrahydrofuran atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
O1S	0.1752(3)	0.5506(2)	0.38338(13)	0.0731(7)*
C1S	0.2285(3)	0.4925(3)	0.34739(15)	0.0478(7)*
C2S	0.3493(3)	0.5073(4)	0.39975(17)	0.0623(9)*
C3S	0.3106(3)	0.5047(3)	0.47129(17)	0.0621(9)*
C4S	0.2305(4)	0.5686(3)	0.46023(18)	0.0706(11)*

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$.

Table S3. Selected Interatomic Distances (Å)

(a) involving [{HB(3,5-^{i}Pr$_2$-pyrazolyl)$_3$}Sm(3,5-^{i}Pr$_2$-pyrazole)(S$_5$)] atoms

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Sm	S1	2.7551(6)	C15	C16	1.507(3)
Sm	S2	2.9519(6)	C16	C16A	1.528(4)
Sm	S4	3.0897(7)	C16	C16B	1.523(4)
Sm	S5	2.7921(6)	C17	C17A	1.531(3)
Sm	N12	2.5326(17)	C17	C17B	1.527(3)
Sm	N22	2.5308(17)	C23	C24	1.395(3)
Sm	N32	2.5090(17)	C23	C27	1.501(3)
Sm	N41	2.6063(18)	C24	C25	1.380(3)
S1	S2	2.0154(9)	C25	C26	1.507(3)
S2	S3	2.0839(12)	C26	C26A	1.522(3)
S3	S4	2.0591(13)	C26	C26B	1.537(3)
S4	S5	2.0334(10)	C27	C27A	1.529(4)
N11	N12	1.385(2)	C27	C27B	1.526(4)
N11	C15	1.354(3)	C33	C34	1.394(3)
N11	B	1.551(3)	C33	C37	1.501(3)
N12	C13	1.348(3)	C34	C35	1.383(3)
N21	N22	1.383(2)	C35	C36	1.506(3)
N21	C25	1.358(3)	C36	C36A	1.530(3)
N21	B	1.544(3)	C36	C36B	1.530(3)
N22	C23	1.350(3)	C37	C37A	1.534(3)
N31	N32	1.384(2)	C37	C37B	1.529(3)
N31	C35	1.361(3)	C43	C44	1.378(3)
N31	B	1.551(3)	C43	C47	1.509(3)
N32	C33	1.352(3)	C44	C45	1.402(3)
N41	N42	1.364(3)	C45	C46	1.497(3)
N41	C45	1.342(3)	C46	C46A	1.514(5)
N42	C43	1.349(3)	C46	C46B	1.524(5)
C13	C14	1.389(3)	C47	C47A	1.520(4)
C13	C17	1.507(3)	C47	C47B	1.518(4)
C14	C15	1.379(3)			

(b) within the solvent tetrahydrofuran molecules

Atom1	Atom2	Distance	Atom1	Atom2	Distance
O1S	C1S	1.412(4)	C2S	C3S	1.516(5)
O1S	C4S	1.436(4)	C3S	C4S	1.498(5)
C1S	C2S	1.490(4)			

Table S4. Selected Interatomic Angles (deg)

(a) involving [{HB(3,5-^{i}Pr$_2$-pyrazolyl)$_3$}Sm(3,5-^{i}Pr$_2$-pyrazole)(S$_5$)] atoms

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
S1	Sm	S2	41.178(19)	C15	N11	B	128.50(17)
S1	Sm	S4	77.20(2)	Sm	N12	N11	120.33(12)
S1	Sm	S5	113.101(19)	Sm	N12	C13	133.35(14)
S1	Sm	N12	155.88(4)	N11	N12	C13	105.97(16)
S1	Sm	N22	84.37(4)	N22	N21	C25	109.89(16)
S1	Sm	N32	84.99(4)	N22	N21	B	121.96(16)
S1	Sm	N41	114.64(4)	C25	N21	B	128.15(17)
S2	Sm	S4	64.06(2)	Sm	N22	N21	120.47(12)
S2	Sm	S5	83.21(2)	Sm	N22	C23	133.03(14)
S2	Sm	N12	159.79(4)	N21	N22	C23	106.28(16)
S2	Sm	N22	122.99(4)	N32	N31	C35	109.70(16)
S2	Sm	N32	106.92(4)	N32	N31	B	121.62(15)
S2	Sm	N41	87.29(4)	C35	N31	B	128.67(17)
S4	Sm	S5	40.05(2)	Sm	N32	N31	121.05(11)
S4	Sm	N12	119.19(4)	Sm	N32	C33	132.21(13)
S4	Sm	N22	94.17(4)	N31	N32	C33	106.47(16)
S4	Sm	N32	160.48(4)	Sm	N41	N42	114.91(13)
S4	Sm	N41	120.54(4)	Sm	N41	C45	140.74(15)
S5	Sm	N12	88.81(4)	N42	N41	C45	104.35(18)
S5	Sm	N22	113.99(4)	N41	N42	C43	113.00(18)
S5	Sm	N32	159.45(4)	N12	C13	C14	110.08(18)
S5	Sm	N41	88.82(4)	N12	C13	C17	122.90(19)
N12	Sm	N22	77.22(5)	C14	C13	C17	126.95(19)
N12	Sm	N32	75.60(5)	C13	C14	C15	106.39(19)
N12	Sm	N41	73.95(6)	N11	C15	C14	107.67(18)
N22	Sm	N32	76.00(5)	N11	C15	C16	123.91(19)
N22	Sm	N41	142.63(6)	C14	C15	C16	128.32(19)
N32	Sm	N41	74.19(5)	C15	C16	C16A	109.4(2)
Sm	S1	S2	74.66(3)	C15	C16	C16B	111.3(2)
Sm	S2	S1	64.17(2)	C16A	C16	C16B	110.9(2)
Sm	S2	S3	98.90(3)	C13	C17	C17A	110.56(19)
S1	S2	S3	106.63(5)	C13	C17	C17B	111.7(2)
S2	S3	S4	101.42(4)	C17A	C17	C17B	109.9(2)
Sm	S4	S3	95.29(3)	N22	C23	C24	109.78(19)
Sm	S4	S5	62.07(2)	N22	C23	C27	122.9(2)
S3	S4	S5	108.54(5)	C24	C23	C27	127.3(2)
Sm	S5	S4	77.88(3)	C23	C24	C25	106.47(19)
N12	N11	C15	109.88(16)	N21	C25	C24	107.59(19)
N12	N11	B	121.53(16)	N21	C25	C26	124.65(19)

Table S4. Selected Interatomic Angles (continued)

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C24	C25	C26	127.69(19)	C33	C37	C37B	111.7(2)
C25	C26	C26A	110.22(19)	C37A	C37	C37B	109.91(19)
C25	C26	C26B	111.0(2)	N42	C43	C44	105.7(2)
C26A	C26	C26B	110.9(2)	N42	C43	C47	121.8(2)
C23	C27	C27A	110.3(2)	C44	C43	C47	132.5(2)
C23	C27	C27B	111.3(2)	C43	C44	C45	106.3(2)
C27A	C27	C27B	110.6(2)	N41	C45	C44	110.6(2)
N32	C33	C34	109.72(18)	N41	C45	C46	122.0(2)
N32	C33	C37	122.51(19)	C44	C45	C46	127.4(2)
C34	C33	C37	127.74(19)	C45	C46	C46A	110.5(3)
C33	C34	C35	106.51(18)	C45	C46	C46B	109.7(2)
N31	C35	C34	107.58(18)	C46A	C46	C46B	112.4(3)
N31	C35	C36	123.98(19)	C43	C47	C47A	110.6(2)
C34	C35	C36	128.23(19)	C43	C47	C47B	112.0(2)
C35	C36	C36A	109.95(18)	C47A	C47	C47B	112.5(3)
C35	C36	C36B	111.1(2)	N11	B	N21	110.73(16)
C36A	C36	C36B	110.0(2)	N11	B	N31	110.64(16)
C33	C37	C37A	110.23(18)	N21	B	N31	110.97(16)

(b) within the solvent tetrahydrofuran molecules

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C1S	O1S	C4S	109.1(2)	C2S	C3S	C4S	102.3(3)
O1S	C1S	C2S	106.6(2)	O1S	C4S	C3S	106.3(3)
C1S	C2S	C3S	101.3(3)				

Table S5. Torsional Angles (deg)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
S4	Sm	S1	S2	65.07(3)	S2	Sm	N12	N11	-145.37(11)
S5	Sm	S1	S2	46.94(4)	S2	Sm	N12	C13	42.5(3)
N12	Sm	S1	S2	-159.18(10)	S4	Sm	N12	N11	120.79(13)
N22	Sm	S1	S2	160.66(5)	S4	Sm	N12	C13	-51.3(2)
N32	Sm	S1	S2	-122.96(5)	S5	Sm	N12	N11	148.09(13)
N41	Sm	S1	S2	-52.90(5)	S5	Sm	N12	C13	-24.03(18)
S1	Sm	S2	S3	104.24(4)	N22	Sm	N12	N11	33.15(13)
S4	Sm	S2	S1	-100.47(3)	N22	Sm	N12	C13	-138.97(19)
S4	Sm	S2	S3	3.77(3)	N32	Sm	N12	N11	-45.44(13)
S5	Sm	S2	S1	-137.40(3)	N32	Sm	N12	C13	142.44(19)
S5	Sm	S2	S3	-33.16(3)	N41	Sm	N12	N11	-122.79(14)
N12	Sm	S2	S1	155.14(11)	N41	Sm	N12	C13	65.08(19)
N12	Sm	S2	S3	-100.61(12)	S1	Sm	N22	N21	123.88(13)
N22	Sm	S2	S1	-23.14(6)	S1	Sm	N22	C23	-49.93(18)
N22	Sm	S2	S3	81.10(6)	S2	Sm	N22	N21	138.95(12)
N32	Sm	S2	S1	60.89(5)	S2	Sm	N22	C23	-34.9(2)
N32	Sm	S2	S3	165.14(5)	S4	Sm	N22	N21	-159.45(13)
N41	Sm	S2	S1	133.47(5)	S4	Sm	N22	C23	26.75(19)
N41	Sm	S2	S3	-122.29(5)	S5	Sm	N22	N21	-123.31(13)
S1	Sm	S4	S3	-45.39(3)	S5	Sm	N22	C23	62.88(19)
S1	Sm	S4	S5	-153.59(4)	N12	Sm	N22	N21	-40.45(13)
S2	Sm	S4	S3	-3.79(3)	N12	Sm	N22	C23	145.75(19)
S2	Sm	S4	S5	-111.99(4)	N32	Sm	N22	N21	37.65(13)
S5	Sm	S4	S3	108.20(5)	N32	Sm	N22	C23	-136.15(19)
N12	Sm	S4	S3	153.67(5)	N41	Sm	N22	N21	-0.26(19)
N12	Sm	S4	S5	45.47(6)	N41	Sm	N22	C23	-174.06(16)
N22	Sm	S4	S3	-128.65(5)	S1	Sm	N32	N31	-128.48(13)
N22	Sm	S4	S5	123.15(5)	S1	Sm	N32	C33	58.35(17)
N32	Sm	S4	S3	-70.00(13)	S2	Sm	N32	N31	-163.76(12)
N32	Sm	S4	S5	-178.20(12)	S2	Sm	N32	C33	23.08(18)
N41	Sm	S4	S3	65.85(6)	S4	Sm	N32	N31	-104.42(16)
N41	Sm	S4	S5	-42.35(6)	S4	Sm	N32	C33	82.4(2)
S1	Sm	S5	S4	28.13(4)	S5	Sm	N32	N31	78.87(18)
S2	Sm	S5	S4	57.11(3)	S5	Sm	N32	C33	-94.3(2)
N12	Sm	S5	S4	-141.50(5)	N12	Sm	N32	N31	37.08(13)
N22	Sm	S5	S4	-66.06(5)	N12	Sm	N32	C33	-136.08(18)
N32	Sm	S5	S4	178.29(11)	N22	Sm	N32	N31	-43.05(13)
N41	Sm	S5	S4	144.53(5)	N22	Sm	N32	C33	143.79(18)
S1	Sm	N12	N11	-8.0(2)	N41	Sm	N32	N31	114.15(14)
S1	Sm	N12	C13	179.87(14)	N41	Sm	N32	C33	-59.02(18)

Table S5. Torsional Angles (continued)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
S1	Sm	N41	N42	-110.91(13)	N22	N21	C25	C24	0.3(2)
S1	Sm	N41	C45	70.1(2)	N22	N21	C25	C26	-176.83(19)
S2	Sm	N41	N42	-142.63(14)	B	N21	C25	C24	-179.39(19)
S2	Sm	N41	C45	38.4(2)	B	N21	C25	C26	3.5(3)
S4	Sm	N41	N42	159.80(12)	N22	N21	B	N11	59.3(2)
S4	Sm	N41	C45	-19.2(3)	N22	N21	B	N31	-64.0(2)
S5	Sm	N41	N42	134.11(14)	C25	N21	B	N11	-121.1(2)
S5	Sm	N41	C45	-44.9(2)	C25	N21	B	N31	115.6(2)
N12	Sm	N41	N42	45.00(14)	Sm	N22	C23	C24	174.45(15)
N12	Sm	N41	C45	-134.0(2)	Sm	N22	C23	C27	-6.6(3)
N22	Sm	N41	N42	4.10(19)	N21	N22	C23	C24	0.0(2)
N22	Sm	N41	C45	-174.9(2)	N21	N22	C23	C27	178.97(19)
N32	Sm	N41	N42	-34.19(14)	C35	N31	N32	Sm	-174.76(13)
N32	Sm	N41	C45	146.8(2)	C35	N31	N32	C33	0.0(2)
Sm	S1	S2	S3	-91.99(3)	B	N31	N32	Sm	6.4(2)
Sm	S2	S3	S4	-5.20(4)	B	N31	N32	C33	-178.89(17)
S1	S2	S3	S4	60.37(5)	N32	N31	C35	C34	0.8(2)
S2	S3	S4	Sm	4.93(4)	N32	N31	C35	C36	-174.36(19)
S2	S3	S4	S5	67.21(5)	B	N31	C35	C34	179.57(19)
S3	S4	S5	Sm	-86.12(4)	B	N31	C35	C36	4.4(3)
C15	N11	N12	Sm	-173.12(13)	N32	N31	B	N11	-65.8(2)
C15	N11	N12	C13	0.9(2)	N32	N31	B	N21	57.5(2)
B	N11	N12	Sm	9.9(2)	C35	N31	B	N11	115.6(2)
B	N11	N12	C13	-176.07(17)	C35	N31	B	N21	-121.1(2)
N12	N11	C15	C14	-0.7(2)	Sm	N32	C33	C34	173.13(14)
N12	N11	C15	C16	-177.27(19)	Sm	N32	C33	C37	-8.6(3)
B	N11	C15	C14	176.08(19)	N31	N32	C33	C34	-0.8(2)
B	N11	C15	C16	-0.5(3)	N31	N32	C33	C37	177.53(18)
N12	N11	B	N21	-68.3(2)	Sm	N41	N42	C43	-179.99(14)
N12	N11	B	N31	55.2(2)	C45	N41	N42	C43	-0.7(2)
C15	N11	B	N21	115.3(2)	Sm	N41	C45	C44	179.43(17)
C15	N11	B	N31	-121.2(2)	Sm	N41	C45	C46	0.1(4)
Sm	N12	C13	C14	172.08(14)	N42	N41	C45	C44	0.4(3)
Sm	N12	C13	C17	-11.0(3)	N42	N41	C45	C46	-178.9(2)
N11	N12	C13	C14	-0.9(2)	N41	N42	C43	C44	0.7(3)
N11	N12	C13	C17	176.10(19)	N41	N42	C43	C47	-178.2(2)
C25	N21	N22	Sm	-175.46(13)	N12	C13	C14	C15	0.5(3)
C25	N21	N22	C23	-0.2(2)	C17	C13	C14	C15	-176.3(2)
B	N21	N22	Sm	4.2(2)	N12	C13	C17	C17A	-118.4(2)
B	N21	N22	C23	179.51(17)	N12	C13	C17	C17B	118.9(2)

Table S5. Torsional Angles (continued)

Atom1	Atom2	Atom3	Atom4	Angle
C14	C13	C17	C17A	58.0(3)
C14	C13	C17	C17B	-64.7(3)
C13	C14	C15	N11	0.1(2)
C13	C14	C15	C16	176.5(2)
N11	C15	C16	C16A	91.6(3)
N11	C15	C16	C16B	-145.4(3)
C14	C15	C16	C16A	-84.3(3)
C14	C15	C16	C16B	38.7(4)
N22	C23	C24	C25	0.2(3)
C27	C23	C24	C25	-178.7(2)
N22	C23	C27	C27A	-102.6(3)
N22	C23	C27	C27B	134.3(3)
C24	C23	C27	C27A	76.2(3)
C24	C23	C27	C27B	-46.9(3)
C23	C24	C25	N21	-0.3(3)
C23	C24	C25	C26	176.7(2)
N21	C25	C26	C26A	100.6(2)
N21	C25	C26	C26B	-136.0(2)
C24	C25	C26	C26A	-75.9(3)
C24	C25	C26	C26B	47.4(3)
N32	C33	C34	C35	1.3(2)
C37	C33	C34	C35	-176.9(2)
N32	C33	C37	C37A	-111.9(2)
N32	C33	C37	C37B	125.6(2)
C34	C33	C37	C37A	66.1(3)
C34	C33	C37	C37B	-56.4(3)
C33	C34	C35	N31	-1.2(2)
C33	C34	C35	C36	173.7(2)
N31	C35	C36	C36A	78.6(3)
N31	C35	C36	C36B	-159.4(2)
C34	C35	C36	C36A	-95.5(3)
C34	C35	C36	C36B	26.5(3)
N42	C43	C44	C45	-0.4(3)
C47	C43	C44	C45	178.3(2)
N42	C43	C47	C47A	-153.8(2)
N42	C43	C47	C47B	-27.4(3)
C44	C43	C47	C47A	27.7(4)
C44	C43	C47	C47B	154.1(3)
C43	C44	C45	N41	0.0(3)
C43	C44	C45	C46	179.3(2)
N41	C45	C46	C46A	-114.0(3)
N41	C45	C46	C46B	121.5(3)
C44	C45	C46	C46A	66.8(4)
C44	C45	C46	C46B	-57.8(4)
C4S	O1S	C1S	C2S	-17.6(4)
C1S	O1S	C4S	C3S	-6.7(4)
O1S	C1S	C2S	C3S	34.1(4)
C1S	C2S	C3S	C4S	-36.8(4)
C2S	C3S	C4S	O1S	27.5(4)

Table S6. Anisotropic Displacement Parameters (U_{ij}, Å^2)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sm	0.01993(6)	0.02282(6)	0.02081(6)	0.00382(4)	0.00622(4)	0.01175(4)
S1	0.0345(3)	0.0404(3)	0.0250(3)	0.0048(2)	0.0107(2)	0.0197(3)
S2	0.0574(4)	0.0579(4)	0.0427(4)	0.0170(3)	0.0267(3)	0.0443(4)
S3	0.0322(3)	0.1133(7)	0.0443(4)	0.0206(4)	0.0158(3)	0.0393(4)
S4	0.0324(3)	0.0477(4)	0.0504(4)	0.0135(3)	0.0011(3)	0.0076(3)
S5	0.0271(3)	0.0613(4)	0.0304(3)	-0.0009(3)	0.0021(2)	0.0166(3)
N11	0.0212(8)	0.0212(8)	0.0177(8)	0.0025(6)	0.0055(6)	0.0119(7)
N12	0.0201(8)	0.0245(9)	0.0199(8)	0.0040(7)	0.0046(7)	0.0116(7)
N21	0.0229(8)	0.0199(8)	0.0196(8)	0.0030(6)	0.0057(7)	0.0121(7)
N22	0.0218(8)	0.0217(8)	0.0222(9)	0.0037(7)	0.0074(7)	0.0105(7)
N31	0.0204(8)	0.0190(8)	0.0196(8)	0.0017(6)	0.0053(6)	0.0102(7)
N32	0.0223(8)	0.0203(8)	0.0200(8)	0.0026(6)	0.0053(7)	0.0129(7)
N41	0.0272(9)	0.0273(9)	0.0275(9)	0.0076(7)	0.0086(7)	0.0152(8)
N42	0.0283(9)	0.0282(10)	0.0278(10)	0.0086(8)	0.0070(8)	0.0144(8)
C13	0.0234(10)	0.0242(10)	0.0195(10)	0.0028(8)	0.0038(8)	0.0096(8)
C14	0.0282(11)	0.0335(12)	0.0191(10)	0.0033(9)	0.0081(8)	0.0143(9)
C15	0.0220(10)	0.0247(10)	0.0218(10)	0.0025(8)	0.0076(8)	0.0109(8)
C16	0.0318(12)	0.0472(14)	0.0249(11)	0.0049(10)	0.0107(9)	0.0254(11)
C16A	0.0303(13)	0.071(2)	0.0453(16)	0.0272(14)	0.0147(11)	0.0229(13)
C16B	0.065(2)	0.107(3)	0.0476(18)	-0.0187(18)	0.0057(15)	0.065(2)
C17	0.0286(11)	0.0398(13)	0.0221(10)	0.0051(9)	0.0047(9)	0.0192(10)
C17A	0.0467(15)	0.0438(14)	0.0298(12)	0.0129(11)	0.0063(11)	0.0250(12)
C17B	0.0354(13)	0.0510(16)	0.0300(13)	0.0014(11)	-0.0032(10)	0.0182(12)
C23	0.0296(11)	0.0212(10)	0.0241(10)	0.0038(8)	0.0080(9)	0.0110(9)
C24	0.0335(12)	0.0234(11)	0.0348(12)	0.0110(9)	0.0108(10)	0.0148(9)
C25	0.0311(11)	0.0210(10)	0.0236(10)	0.0042(8)	0.0050(9)	0.0150(9)
C26	0.0310(11)	0.0255(11)	0.0367(12)	0.0082(9)	0.0073(10)	0.0176(9)
C26A	0.0500(16)	0.0425(15)	0.0444(15)	0.0039(12)	0.0106(12)	0.0315(13)
C26B	0.0474(15)	0.0412(14)	0.0425(15)	0.0088(12)	0.0012(12)	0.0304(13)
C27	0.0305(12)	0.0255(11)	0.0386(13)	0.0096(10)	0.0146(10)	0.0112(9)
C27A	0.0324(14)	0.0390(15)	0.067(2)	-0.0060(14)	0.0120(13)	0.0048(12)
C27B	0.0497(18)	0.078(2)	0.0540(19)	0.0309(17)	0.0297(15)	0.0247(17)
C33	0.0293(10)	0.0195(10)	0.0175(9)	0.0031(7)	0.0042(8)	0.0126(8)
C34	0.0257(10)	0.0210(10)	0.0218(10)	-0.0010(8)	0.0044(8)	0.0071(8)
C35	0.0225(10)	0.0233(10)	0.0201(10)	0.0034(8)	0.0052(8)	0.0084(8)
C36	0.0222(10)	0.0344(12)	0.0282(11)	-0.0023(9)	0.0060(9)	0.0106(9)
C36A	0.0318(12)	0.0461(14)	0.0310(12)	-0.0003(10)	0.0032(10)	0.0256(11)
C36B	0.0245(12)	0.0428(16)	0.070(2)	0.0005(14)	0.0127(13)	0.0055(11)
C37	0.0346(12)	0.0232(11)	0.0262(11)	0.0000(8)	0.0052(9)	0.0167(9)
C37A	0.0480(14)	0.0341(13)	0.0302(12)	0.0024(10)	0.0141(11)	0.0247(11)

Table S6. Anisotropic Displacement Parameters (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C37B	0.0658(18)	0.0295(13)	0.0405(14)	0.0058(11)	0.0155(13)	0.0304(13)
C43	0.0331(12)	0.0236(11)	0.0248(11)	0.0040(8)	0.0076(9)	0.0097(9)
C44	0.0382(13)	0.0281(12)	0.0346(13)	0.0099(10)	0.0091(10)	0.0173(10)
C45	0.0345(12)	0.0300(12)	0.0306(12)	0.0090(9)	0.0086(9)	0.0196(10)
C46	0.0348(13)	0.0450(15)	0.0634(18)	0.0261(14)	0.0186(13)	0.0247(12)
C46A	0.072(3)	0.059(2)	0.192(5)	0.014(3)	0.074(3)	0.039(2)
C46B	0.0369(17)	0.147(4)	0.108(3)	0.090(3)	0.0179(19)	0.040(2)
C47	0.0332(12)	0.0326(12)	0.0307(12)	0.0038(10)	0.0085(10)	0.0072(10)
C47A	0.0543(18)	0.0527(18)	0.0542(19)	0.0240(15)	0.0232(15)	0.0091(15)
C47B	0.0324(14)	0.0529(18)	0.070(2)	0.0054(15)	0.0194(14)	0.0130(13)
B	0.0211(10)	0.0204(11)	0.0184(10)	0.0021(8)	0.0039(8)	0.0120(9)
O1S	0.114(2)	0.0918(19)	0.0539(14)	0.0171(13)	0.0212(14)	0.0814(18)
C1S	0.0636(19)	0.0395(15)	0.0367(14)	0.0032(12)	0.0093(13)	0.0226(14)
C2S	0.0566(19)	0.082(2)	0.0451(18)	0.0076(17)	0.0105(15)	0.0307(18)
C3S	0.060(2)	0.072(2)	0.0410(17)	0.0078(15)	0.0050(15)	0.0237(18)
C4S	0.124(3)	0.0501(19)	0.0443(18)	0.0035(15)	0.033(2)	0.042(2)

The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$

Table S7. Derived Atomic Coordinates and Displacement Parameters for Hydrogen Atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H42N	-0.0081	-0.0794	0.2655	0.033
H14	0.0361	0.1738	0.4600	0.032
H16	-0.1637	0.2365	0.3007	0.038
H16A	-0.3501	0.0903	0.3333	0.057
H16B	-0.2834	0.0306	0.2927	0.057
H16C	-0.2608	0.0401	0.3792	0.057
H16D	-0.2149	0.2892	0.4058	0.079
H16E	-0.1224	0.2453	0.4551	0.079
H16F	-0.0600	0.3571	0.4140	0.079
H17	0.2889	0.1079	0.4001	0.035
H17A	0.2439	-0.0026	0.4980	0.047
H17B	0.1258	0.0257	0.5003	0.047
H17C	0.1172	-0.0543	0.4312	0.047
H17D	0.4039	0.2072	0.5193	0.050
H17E	0.3833	0.2964	0.4676	0.050
H17F	0.2930	0.2447	0.5234	0.050
H24	0.1633	0.5066	0.1113	0.035
H26	-0.1600	0.2966	0.1513	0.035
H26A	-0.1491	0.4736	0.1996	0.050
H26B	-0.0465	0.4438	0.2524	0.050
H26C	0.0032	0.5429	0.2007	0.050
H26D	-0.2113	0.4104	0.0664	0.050
H26E	-0.0616	0.4779	0.0620	0.050
H26F	-0.1481	0.3403	0.0323	0.050
H27	0.4046	0.3838	0.1536	0.037
H27A	0.5547	0.5839	0.1997	0.062
H27B	0.4353	0.6112	0.2001	0.062
H27C	0.4614	0.5259	0.2532	0.062
H27D	0.4757	0.5135	0.0677	0.071
H27E	0.3299	0.4104	0.0342	0.071
H27F	0.3537	0.5389	0.0624	0.071
H34	-0.2438	-0.1929	0.0670	0.030
H36	-0.3206	0.0120	0.1666	0.035
H36A	-0.4114	0.0576	0.0557	0.041
H36B	-0.2549	0.1313	0.0755	0.041
H36C	-0.3287	0.0177	0.0147	0.041
H36D	-0.5212	-0.1390	0.0939	0.060
H36E	-0.4430	-0.1853	0.0533	0.060
H36F	-0.4368	-0.1954	0.1377	0.060
H37	0.1231	-0.0976	0.1169	0.033

Table S7. Derived Parameters for Hydrogen Atoms (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H37A	0.0648	-0.1847	-0.0059	0.041
H37B	-0.0750	-0.1880	-0.0172	0.041
H37C	0.0555	-0.0643	-0.0022	0.041
H37D	0.0262	-0.3056	0.0935	0.050
H37E	-0.0116	-0.2671	0.1625	0.050
H37F	-0.1159	-0.3153	0.0854	0.050
H44	0.1250	-0.2935	0.3412	0.039
H46	0.4059	-0.0239	0.2971	0.053
H46A	0.4575	-0.1734	0.2660	0.117
H46B	0.3162	-0.2715	0.2716	0.117
H46C	0.3284	-0.1877	0.2098	0.117
H46D	0.5116	-0.0836	0.3951	0.116
H46E	0.4176	-0.0395	0.4206	0.116
H46F	0.3721	-0.1775	0.4057	0.116
H47	-0.1797	-0.3429	0.2639	0.042
H47A	-0.2254	-0.4139	0.3733	0.070
H47B	-0.0977	-0.4172	0.3597	0.070
H47C	-0.0829	-0.3157	0.4172	0.070
H47D	-0.2895	-0.2680	0.3232	0.064
H47E	-0.1522	-0.1590	0.3643	0.064
H47F	-0.2024	-0.1739	0.2779	0.064
H1B	-0.1252	0.1751	0.2070	0.023
H1SA	0.2501	0.5277	0.3032	0.057
H1SB	0.1651	0.4078	0.3330	0.057
H2SA	0.4259	0.5832	0.3987	0.075
H2SB	0.3689	0.4419	0.3899	0.075
H3SA	0.2582	0.4229	0.4800	0.075
H3SB	0.3886	0.5461	0.5125	0.075
H4SA	0.1603	0.5366	0.4866	0.085
H4SB	0.2863	0.6536	0.4782	0.085

STRUCTURE REPORT for Compound 4

XCL Code: TAK1422 **Date:** 7 March 2016

Compound: [{HB(3,5-iPr$_2$-pyrazolyl)$_3$}$_2$Sm(3,5-iPr$_2$-pyrazolyl)]•C$_5$H$_{12}$

Formula: C$_{68}$H$_{119}$B$_2$N$_{14}$Sm (C$_{63}$H$_{107}$B$_2$N$_{14}$Sm•C$_5$H$_{12}$)

Supervisor: J. Takats **Crystallographer:** R. McDonald

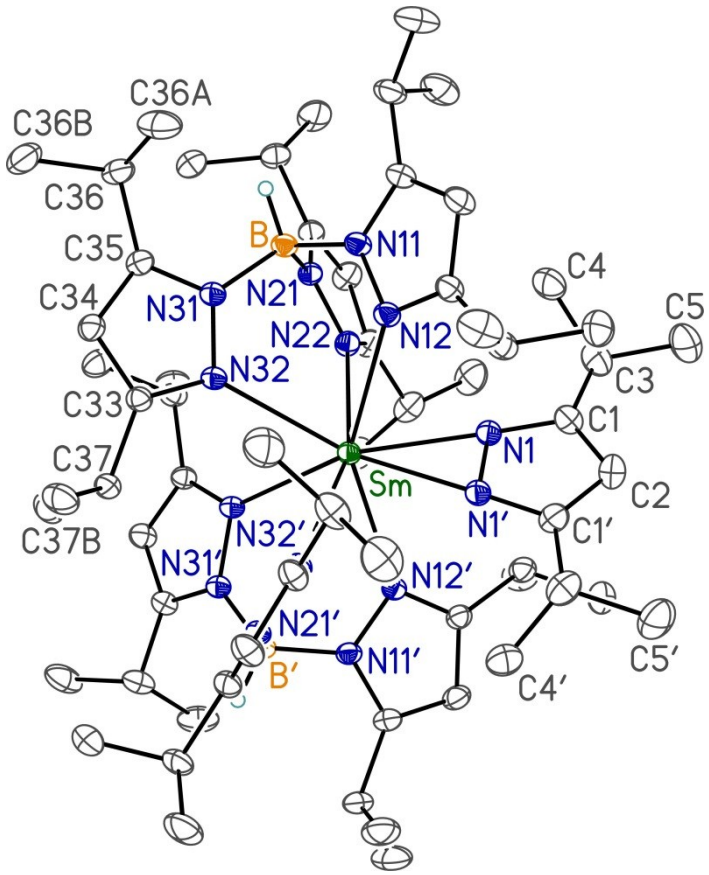
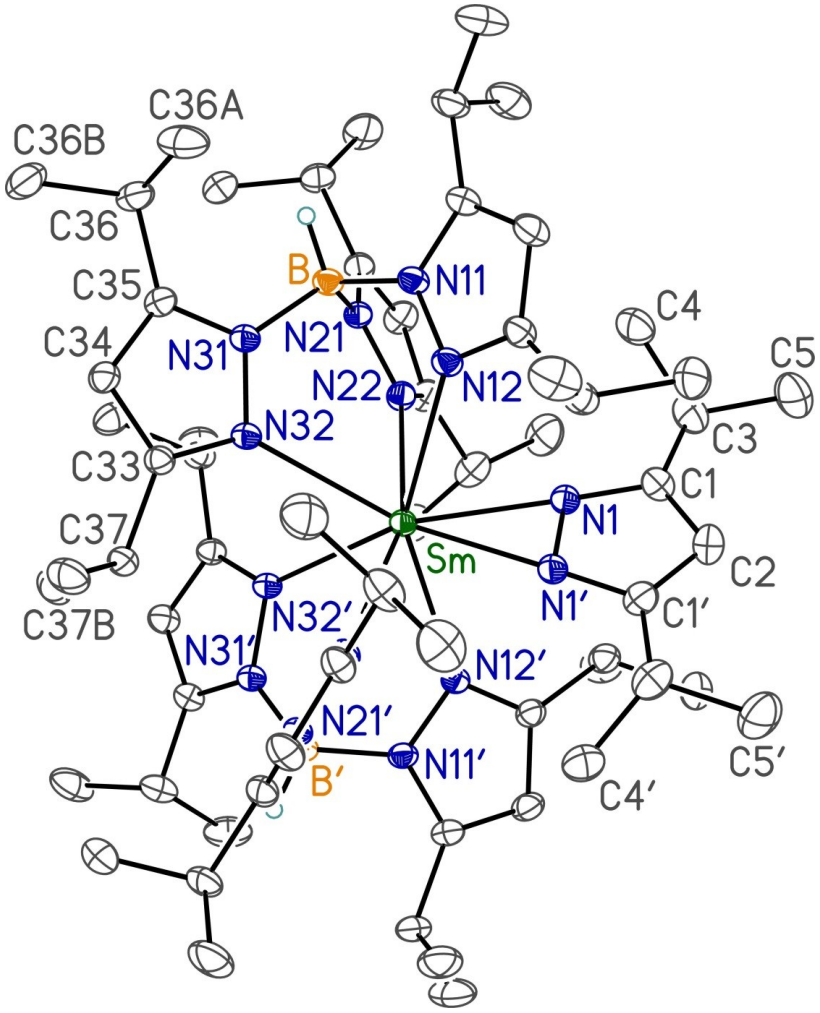


Figure Legends

Figure S4. Perspective view of the [{HB(3,5-iPr$_2$-pyrazolyl)$_3$}$_2$Sm(3,5-iPr$_2$-pyrazolyl)] molecule showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 30% probability level. Hydrogen atoms attached to boron atoms are shown with arbitrarily small thermal parameters; all other hydrogens are not shown. Primed atoms are related to unprimed ones via the crystallographic twofold axis (0, *y*, $^1/_4$) passing through Sm, C2, and the center of the N1–N1' bond.

Figure S5. Alternate view of the molecule approximately along the crystallographic twofold axis.


C36A
C36B
C36
C35
C34
C33
C37
C37B
B
N11
N21
N31
N22
N12
N32
C4
C5
C3
C1
N1
Sm
C2
N1′
C1′
N32′
N31′
N12′
N21′
N11′
B′
C5′
C4′

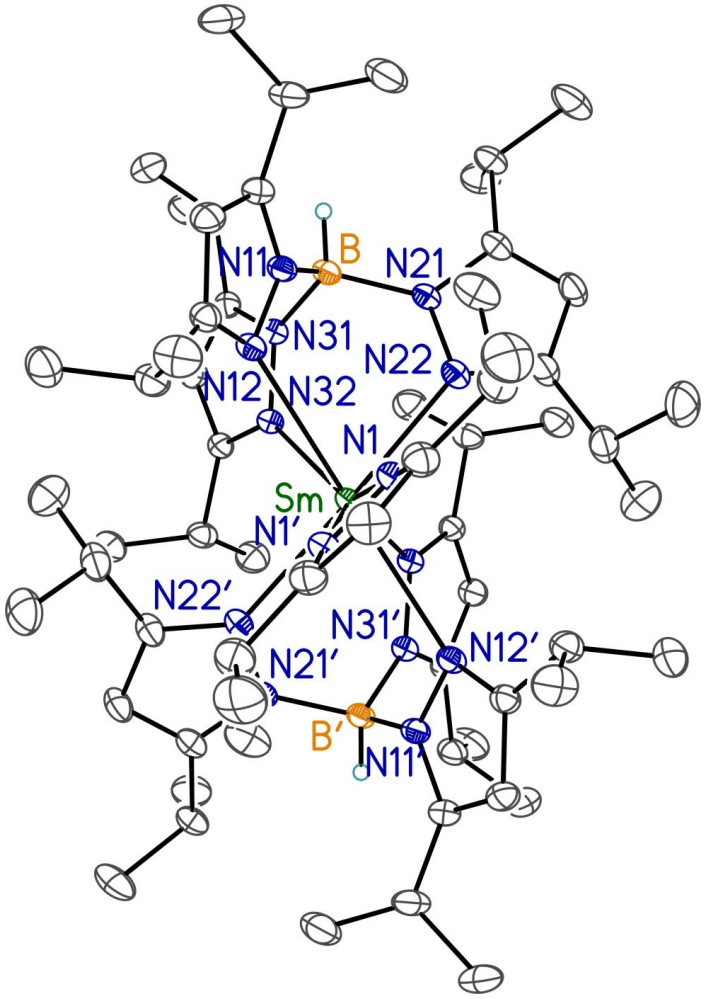

B
N11
N21
N31
N22
N12
N32
N1
Sm
N1′
N22′
N31′
N12′
N21′
B′
N11′

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Table S8. Crystallographic Experimental Details

A. Crystal Data	
formula	$C_{68}H_{119}B_2N_{14}Sm$
formula weight	1304.73
crystal dimensions (mm)	0.25 × 0.17 × 0.15
crystal system	monoclinic
space group	*C*2/*c* (No. 15)
unit cell parameters[a]	
a (Å)	21.5176 (10)
b (Å)	17.2726 (8)
c (Å)	19.2117 (9)
β (deg)	93.2336 (6)
V (Å^3)	7128.9 (6)
Z	4
ρ_{calcd} (g cm^{-3})	1.216
μ (mm^{-1})	0.872
B. Data Collection and Refinement Conditions	
diffractometer	Bruker PLATFORM/APEX II CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–100
scan type	ω scans (0.3°) (15 s exposures)
data collection 2θ limit (deg)	56.55
total data collected	32295 (-28 ≤ *h* ≤ 28, -22 ≤ *k* ≤ 22, -24 ≤ *l* ≤ 25)
independent reflections	8673 (R_{int} = 0.0438)
number of observed reflections (*NO*)	7570 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method	intrinsic phasing (*SHELXT-2014*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–2014*[d])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	0.9263–0.8463
data/restraints/parameters	8673 / 7[e] / 378
goodness-of-fit (*S*)[f] [all data]	1.067
final *R* indices[g]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0364
wR_2 [all data]	0.0968
largest difference peak and hole	0.976 and –1.028 e Å^{-3}

[a]Obtained from least-squares refinement of 9915 reflections with 4.24° < 2θ < 43.60°.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

(continued)

Table S8. Crystallographic Experimental Details (continued)

[c]Sheldrick, G. M. *Acta Crystallogr.* **2015**, *A71*, 3–8.

[d]Sheldrick, G. M. *Acta Crystallogr.* **2015**, *C71*, 3–8.

[e]Distances within the inversion-disordered solvent n-pentane molecule were constrained to idealized values during refinement: d(C1S–C2S) = d(C2S–C3S) = d(C3S–C4S) = d(C4S–C5S) = 1.52(1)Å; d(C1S···C3S) = d(C2S···C4S) = d(C3S···C5S) = 2.48(1) Å.

[f]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0561P)^2 + 1.2805P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[g]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table S9. Atomic Coordinates and Equivalent Isotropic Displacement Parameters

(a) atoms of [{HB(3,5-iPr$_2$-pyrazolyl)$_3$}$_2$Sm(3,5-iPr$_2$-pyrazolyl)]

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Sm	0.0000	0.26981(2)	0.2500	0.02578(7)*
N1	0.02537(9)	0.13915(11)	0.22940(11)	0.0312(4)*
N11	0.15318(9)	0.26560(11)	0.33100(11)	0.0296(4)*
N12	0.09819(9)	0.22907(11)	0.34536(11)	0.0298(4)*
N21	0.14569(9)	0.33283(11)	0.21296(10)	0.0283(4)*
N22	0.09459(9)	0.29448(12)	0.18308(11)	0.0309(4)*
N31	0.10865(8)	0.40157(11)	0.32383(10)	0.0283(4)*
N32	0.04451(8)	0.39408(11)	0.31541(10)	0.0273(4)*
C1	0.04141(13)	0.06422(16)	0.21754(15)	0.0416(6)*
C2	0.0000	0.0158(2)	0.2500	0.0497(10)*
C3	0.09594(15)	0.04560(18)	0.17461(17)	0.0521(7)*
C4	0.15172(14)	0.0966(2)	0.19544(19)	0.0586(8)*
C5	0.11300(18)	-0.0405(2)	0.1795(2)	0.0718(10)*
C13	0.11527(11)	0.16702(14)	0.38413(13)	0.0326(5)*
C14	0.17998(12)	0.16376(16)	0.39459(14)	0.0387(6)*
C15	0.20280(12)	0.22573(14)	0.35999(14)	0.0348(6)*
C16	0.26988(12)	0.24566(18)	0.34852(17)	0.0436(7)*
C16A	0.28842(15)	0.2097(2)	0.28023(19)	0.0585(9)*
C16B	0.31294(15)	0.2163(2)	0.4086(2)	0.0646(10)*
C17	0.07138(12)	0.11076(16)	0.41548(14)	0.0393(6)*
C17A	0.08999(15)	0.02738(18)	0.40078(19)	0.0562(8)*
C17B	0.07192(15)	0.1212(2)	0.49400(17)	0.0604(9)*
C23	0.10472(13)	0.28527(15)	0.11559(14)	0.0360(6)*
C24	0.16226(12)	0.31700(17)	0.10146(14)	0.0408(6)*
C25	0.18713(11)	0.34600(15)	0.16366(13)	0.0346(5)*
C26	0.24781(12)	0.38832(16)	0.17636(15)	0.0397(6)*
C26A	0.29427(14)	0.3638(2)	0.12272(19)	0.0595(9)*
C26B	0.23745(14)	0.47502(17)	0.17454(18)	0.0516(7)*
C27	0.05902(15)	0.24532(19)	0.06550(16)	0.0460(7)*
C27A	0.09321(17)	0.1899(2)	0.01943(17)	0.0630(9)*
C27B	0.02082(17)	0.3034(2)	0.02118(19)	0.0637(9)*
C33	0.02088(11)	0.45474(14)	0.34983(12)	0.0292(5)*
C34	0.06932(11)	0.49887(15)	0.38068(13)	0.0347(5)*
C35	0.12376(11)	0.46440(14)	0.36333(12)	0.0310(5)*
C36	0.18929(12)	0.48851(17)	0.38572(14)	0.0400(6)*
C36A	0.21549(14)	0.4370(2)	0.44541(16)	0.0602(9)*
C36B	0.19154(14)	0.5733(2)	0.40722(19)	0.0609(9)*
C37	-0.04711(11)	0.47526(15)	0.35204(13)	0.0349(5)*
C37A	-0.06431(13)	0.4963(2)	0.42554(15)	0.0498(7)*

Table S9. Atomic Coordinates and Displacement Parameters (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C37B	-0.06386(13)	0.54379(17)	0.30505(16)	0.0474(7)*
B	0.15481(12)	0.34405(16)	0.29324(14)	0.0294(5)*

(b) solvent n-pentane atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C1S[a]	0.4367(10)	0.2213(13)	0.1782(14)	0.187(4)
C2S[a]	0.4723(8)	0.2968(9)	0.1816(8)	0.187(4)
C3S[a]	0.5324(6)	0.2823(10)	0.2283(8)	0.187(4)
C4S[a]	0.5099(8)	0.2584(12)	0.3000(8)	0.187(4)
C5S[a]	0.5657(11)	0.2238(14)	0.3419(10)	0.187(4)

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$. [a]Refined with an occupancy factor of 0.5 and a common isotropic displacement parameter.

Table S10. Selected Interatomic Distances (Å)

(a) within [{HB(3,5-iPr$_2$-pyrazolyl)$_3$}$_2$Sm(3,5-iPr$_2$-pyrazolyl)]

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Sm	N1	2.3606(19)	C3	C5	1.533(5)
Sm	N1’	2.361(2)	C13	C14	1.397(3)
Sm	N12	2.807(2)	C13	C17	1.504(3)
Sm	N12’	2.807(2)	C14	C15	1.366(4)
Sm	N22	2.5045(19)	C15	C16	1.512(4)
Sm	N22’	2.5044(19)	C16	C16A	1.525(5)
Sm	N32	2.6397(19)	C16	C16B	1.526(4)
Sm	N32’	2.6397(19)	C17	C17A	1.525(4)
N1	N1’	1.384(4)	C17	C17B	1.519(4)
N1	C1	1.362(3)	C23	C24	1.395(3)
N11	N12	1.382(3)	C23	C27	1.504(4)
N11	C15	1.363(3)	C24	C25	1.376(4)
N11	B	1.538(3)	C25	C26	1.504(3)
N12	C13	1.345(3)	C26	C26A	1.535(4)
N21	N22	1.380(3)	C26	C26B	1.514(4)
N21	C25	1.356(3)	C27	C27A	1.522(4)
N21	B	1.556(3)	C27	C27B	1.526(5)
N22	C23	1.336(3)	C33	C34	1.396(3)
N31	N32	1.387(2)	C33	C37	1.508(3)
N31	C35	1.353(3)	C34	C35	1.372(3)
N31	B	1.544(3)	C35	C36	1.509(3)
N32	C33	1.353(3)	C36	C36A	1.533(4)
C1	C2	1.395(4)	C36	C36B	1.522(4)
C1	C2’	1.395(4)	C37	C37A	1.524(4)
C1	C3	1.506(4)	C37	C37B	1.520(4)
C3	C4	1.524(4)			

Primed atoms are related to unprimed ones via the crystallographic twofold axis (0, y, $^1/_4$).

(b) within the (disordered) solvent n-pentane molecule

Atom1	Atom2	Distance	Atom1	Atom2	Distance
C1S	C2S	1.512(9)[a]	C3S	C4S	1.541(9)[a]
C2S	C3S	1.553(9)[a]	C4S	C5S	1.528(9)[a]

[a]Distance constrained to a target value of 1.52(1) Å during refinement.

Table S11. Selected Interatomic Angles (deg)

(a) within [{HB(3,5-iPr$_2$-pyrazolyl)$_3$}$_2$Sm(3,5-iPr$_2$-pyrazolyl)]

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
N1	Sm	N1’	34.10(9)	C25	N21	B	128.3(2)
N1	Sm	N12	72.37(6)	Sm	N22	N21	121.30(14)
N1	Sm	N12’	79.84(6)	Sm	N22	C23	131.26(17)
N1	Sm	N22	82.78(7)	N21	N22	C23	106.91(19)
N1	Sm	N22’	116.82(7)	N32	N31	C35	110.26(18)
N1	Sm	N32	140.91(6)	N32	N31	B	123.57(18)
N1	Sm	N32’	141.14(6)	C35	N31	B	126.15(19)
N1’	Sm	N12	79.84(6)	Sm	N32	N31	117.61(13)
N1’	Sm	N12’	72.37(6)	Sm	N32	C33	136.55(15)
N1’	Sm	N22	116.81(7)	N31	N32	C33	105.65(18)
N1’	Sm	N22’	82.78(7)	N1	C1	C2	108.7(2)
N1’	Sm	N32	141.15(6)	N1	C1	C3	120.5(3)
N1’	Sm	N32’	140.90(6)	C2	C1	C3	130.8(3)
N12	Sm	N12’	150.96(8)	C1	C2	C1’	106.3(3)
N12	Sm	N22	76.94(6)	C1	C3	C4	111.0(3)
N12	Sm	N22’	108.13(6)	C1	C3	C5	111.4(3)
N12	Sm	N32	69.73(6)	C4	C3	C5	111.2(3)
N12	Sm	N32’	138.95(6)	N12	C13	C14	110.5(2)
N12’	Sm	N22	108.13(6)	N12	C13	C17	125.4(2)
N12’	Sm	N22’	76.95(6)	C14	C13	C17	124.0(2)
N12’	Sm	N32	138.94(6)	C13	C14	C15	106.3(2)
N12’	Sm	N32’	69.73(6)	N11	C15	C14	107.5(2)
N22	Sm	N22’	160.40(9)	N11	C15	C16	123.9(2)
N22	Sm	N32	79.77(6)	C14	C15	C16	128.4(2)
N22	Sm	N32’	84.31(6)	C15	C16	C16A	109.3(3)
N22’	Sm	N32	84.31(6)	C15	C16	C16B	111.0(3)
N22’	Sm	N32’	79.77(6)	C16A	C16	C16B	109.8(3)
N32	Sm	N32’	71.19(8)	C13	C17	C17A	111.0(2)
Sm	N1	N1’	72.95(5)	C13	C17	C17B	110.6(2)
Sm	N1	C1	178.69(18)	C17A	C17	C17B	108.0(3)
N1’	N1	C1	108.12(15)	N22	C23	C24	109.7(2)
N12	N11	C15	110.34(19)	N22	C23	C27	122.6(2)
N12	N11	B	122.60(19)	C24	C23	C27	127.7(2)
C15	N11	B	126.8(2)	C23	C24	C25	106.3(2)
Sm	N12	N11	112.12(14)	N21	C25	C24	107.9(2)
Sm	N12	C13	137.19(16)	N21	C25	C26	124.5(2)
N11	N12	C13	105.31(19)	C24	C25	C26	127.5(2)
N22	N21	C25	109.25(19)	C25	C26	C26A	110.4(2)
N22	N21	B	121.66(18)	C25	C26	C26B	110.6(2)

Table S11. Selected Interatomic Angles (continued)

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C26A	C26	C26B	111.0(2)	C34	C35	C36	127.4(2)
C23	C27	C27A	109.9(3)	C35	C36	C36A	110.6(2)
C23	C27	C27B	111.6(3)	C35	C36	C36B	111.0(2)
C27A	C27	C27B	110.6(3)	C36A	C36	C36B	110.5(3)
N32	C33	C34	109.8(2)	C33	C37	C37A	111.6(2)
N32	C33	C37	126.0(2)	C33	C37	C37B	111.4(2)
C34	C33	C37	124.2(2)	C37A	C37	C37B	107.6(2)
C33	C34	C35	106.7(2)	N11	B	N21	110.7(2)
N31	C35	C34	107.6(2)	N11	B	N31	110.78(19)
N31	C35	C36	124.9(2)	N21	B	N31	114.17(19)

Primed atoms are related to unprimed ones via the crystallographic twofold axis (0, *y*, $^1/_4$).

(b) within the (disordered) solvent n-pentane molecule

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C1S	C2S	C3S	106.9(8)[a]	C3S	C4S	C5S	107.3(9)[a]
C2S	C3S	C4S	105.4(8)[a]				

[a]Angle includes distances constrained during refinement: d(C1S–C2S) = d(C2S–C3S) = d(C3S–C4S) = d(C4S–C5S) = 1.52(1)Å; d(C1S···C3S) = d(C2S···C4S) = d(C3S···C5S) = 2.48(1) Å.

Table S12. Torsional Angles (deg)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
N12	Sm	N1	N1’	98.01(17)	N12’	Sm	N32	N31	-141.86(13)
N12’	Sm	N1	N1’	-73.49(17)	N12’	Sm	N32	C33	44.2(3)
N22	Sm	N1	N1’	176.55(18)	N22	Sm	N32	N31	-35.93(14)
N22’	Sm	N1	N1’	-3.8(2)	N22	Sm	N32	C33	150.1(2)
N32	Sm	N1	N1’	112.64(16)	N22’	Sm	N32	N31	155.54(15)
N32’	Sm	N1	N1’	-111.91(17)	N22’	Sm	N32	C33	-18.4(2)
N1	Sm	N12	N11	110.44(15)	N32’	Sm	N32	N31	-123.36(17)
N1	Sm	N12	C13	-38.7(2)	N32’	Sm	N32	C33	62.7(2)
N1’	Sm	N12	N11	144.78(15)	N1’	N1	C1	C2	1.3(3)
N1’	Sm	N12	C13	-4.4(2)	N1’	N1	C1	C3	-179.3(3)
N12’	Sm	N12	N11	127.89(14)	C15	N11	N12	Sm	-158.11(16)
N12’	Sm	N12	C13	-21.2(2)	C15	N11	N12	C13	0.7(3)
N22	Sm	N12	N11	23.98(14)	B	N11	N12	Sm	27.0(3)
N22	Sm	N12	C13	-125.1(2)	B	N11	N12	C13	-174.2(2)
N22’	Sm	N12	N11	-136.35(14)	N12	N11	C15	C14	-1.2(3)
N22’	Sm	N12	C13	74.5(2)	N12	N11	C15	C16	174.0(2)
N32	Sm	N12	N11	-59.78(14)	B	N11	C15	C14	173.4(2)
N32	Sm	N12	C13	151.1(2)	B	N11	C15	C16	-11.4(4)
N32’	Sm	N12	N11	-41.10(18)	N12	N11	B	N21	-81.9(3)
N32’	Sm	N12	C13	169.8(2)	N12	N11	B	N31	45.8(3)
N1	Sm	N22	N21	-118.72(17)	C15	N11	B	N21	104.1(3)
N1	Sm	N22	C23	70.8(2)	C15	N11	B	N31	-128.2(2)
N1’	Sm	N22	N21	-116.56(16)	Sm	N12	C13	C14	150.55(19)
N1’	Sm	N22	C23	72.9(2)	Sm	N12	C13	C17	-32.5(4)
N12	Sm	N22	N21	-45.23(16)	N11	N12	C13	C14	0.1(3)
N12	Sm	N22	C23	144.3(2)	N11	N12	C13	C17	177.1(2)
N12’	Sm	N22	N21	164.49(15)	C25	N21	N22	Sm	-173.28(15)
N12’	Sm	N22	C23	-6.0(2)	C25	N21	N22	C23	-0.7(3)
N22’	Sm	N22	N21	62.30(16)	B	N21	N22	Sm	15.9(3)
N22’	Sm	N22	C23	-108.2(2)	B	N21	N22	C23	-171.6(2)
N32	Sm	N22	N21	26.14(16)	N22	N21	C25	C24	0.8(3)
N32	Sm	N22	C23	-144.4(2)	N22	N21	C25	C26	178.4(2)
N32’	Sm	N22	N21	98.00(17)	B	N21	C25	C24	170.9(2)
N32’	Sm	N22	C23	-72.5(2)	B	N21	C25	C26	-11.6(4)
N1	Sm	N32	N31	28.94(19)	N22	N21	B	N11	55.5(3)
N1	Sm	N32	C33	-145.0(2)	N22	N21	B	N31	-70.3(3)
N1’	Sm	N32	N31	84.51(17)	C25	N21	B	N11	-113.4(3)
N1’	Sm	N32	C33	-89.5(2)	C25	N21	B	N31	120.8(3)
N12	Sm	N32	N31	43.81(14)	Sm	N22	C23	C24	171.86(18)
N12	Sm	N32	C33	-130.2(2)	Sm	N22	C23	C27	-8.7(4)

Table S12. Torsional Angles (continued)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
N21	N22	C23	C24	0.3(3)	C13	C14	C15	C16	-173.7(3)
N21	N22	C23	C27	179.8(3)	N11	C15	C16	C16A	-83.2(3)
C35	N31	N32	Sm	-174.71(15)	N11	C15	C16	C16B	155.6(3)
C35	N31	N32	C33	1.0(2)	C14	C15	C16	C16A	91.0(4)
B	N31	N32	Sm	3.9(3)	C14	C15	C16	C16B	-30.3(4)
B	N31	N32	C33	179.6(2)	N22	C23	C24	C25	0.2(3)
N32	N31	C35	C34	-0.4(3)	C27	C23	C24	C25	-179.2(3)
N32	N31	C35	C36	177.3(2)	N22	C23	C27	C27A	-135.7(3)
B	N31	C35	C34	-178.9(2)	N22	C23	C27	C27B	101.3(3)
B	N31	C35	C36	-1.2(4)	C24	C23	C27	C27A	43.7(4)
N32	N31	B	N11	-69.5(3)	C24	C23	C27	C27B	-79.4(4)
N32	N31	B	N21	56.2(3)	C23	C24	C25	N21	-0.6(3)
C35	N31	B	N11	108.8(3)	C23	C24	C25	C26	-178.0(3)
C35	N31	B	N21	-125.4(2)	N21	C25	C26	C26A	155.7(3)
Sm	N32	C33	C34	173.26(17)	N21	C25	C26	C26B	-81.1(3)
Sm	N32	C33	C37	-9.8(4)	C24	C25	C26	C26A	-27.3(4)
N31	N32	C33	C34	-1.2(3)	C24	C25	C26	C26B	95.9(3)
N31	N32	C33	C37	175.7(2)	N32	C33	C34	C35	1.0(3)
N1	C1	C2	C1’	-0.48(12)	C37	C33	C34	C35	-176.0(2)
C3	C1	C2	C1’	-179.9(4)	N32	C33	C37	C37A	135.7(3)
N1	C1	C3	C4	44.7(4)	N32	C33	C37	C37B	-104.0(3)
N1	C1	C3	C5	169.2(3)	C34	C33	C37	C37A	-47.8(3)
C2	C1	C3	C4	-136.0(3)	C34	C33	C37	C37B	72.5(3)
C2	C1	C3	C5	-11.5(4)	C33	C34	C35	N31	-0.3(3)
N12	C13	C14	C15	-0.8(3)	C33	C34	C35	C36	-178.0(2)
C17	C13	C14	C15	-177.8(2)	N31	C35	C36	C36A	-76.4(3)
N12	C13	C17	C17A	131.9(3)	N31	C35	C36	C36B	160.6(3)
N12	C13	C17	C17B	-108.2(3)	C34	C35	C36	C36A	100.8(3)
C14	C13	C17	C17A	-51.5(4)	C34	C35	C36	C36B	-22.2(4)
C14	C13	C17	C17B	68.3(3)	C1S	C2S	C3S	C4S	-61(2)[a]
C13	C14	C15	N11	1.2(3)	C2S	C3S	C4S	C5S	165.8(14)[a]

Primed atoms are related to unprimed ones via the crystallographic twofold axis (0, *y*, $^1/_4$).

[a]Angle includes distances constrained during refinement: d(C1S–C2S) = d(C2S–C3S) = d(C3S–C4S) = d(C4S–C5S) = 1.52(1)Å; d(C1S···C3S) = d(C2S···C4S) = d(C3S···C5S) = 2.48(1) Å.

Table S13. Anisotropic Displacement Parameters (U_{ij}, Å^2)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sm	0.02254(9)	0.02540(9)	0.03012(10)	0.000	0.00795(6)	0.000
N1	0.0280(10)	0.0294(10)	0.0367(11)	-0.0008(8)	0.0061(8)	-0.0002(8)
N11	0.0227(10)	0.0332(11)	0.0331(11)	0.0012(8)	0.0038(8)	0.0021(8)
N12	0.0247(10)	0.0310(10)	0.0342(11)	0.0030(8)	0.0055(8)	0.0005(8)
N21	0.0236(9)	0.0286(9)	0.0332(10)	-0.0001(8)	0.0069(8)	-0.0018(8)
N22	0.0295(10)	0.0306(10)	0.0335(11)	-0.0005(8)	0.0092(8)	-0.0025(8)
N31	0.0241(9)	0.0311(10)	0.0299(10)	-0.0001(8)	0.0035(8)	0.0002(8)
N32	0.0224(9)	0.0312(10)	0.0285(10)	-0.0002(8)	0.0028(8)	0.0003(8)
C1	0.0386(14)	0.0398(14)	0.0463(16)	-0.0005(12)	0.0019(12)	0.0056(11)
C2	0.056(3)	0.0325(19)	0.061(3)	0.000	0.002(2)	0.000
C3	0.0531(18)	0.0500(17)	0.0536(18)	-0.0034(14)	0.0057(14)	0.0125(14)
C4	0.0439(17)	0.0573(19)	0.076(2)	-0.0006(17)	0.0159(16)	0.0086(15)
C5	0.072(2)	0.057(2)	0.087(3)	-0.0162(19)	0.008(2)	0.0183(18)
C13	0.0295(12)	0.0339(12)	0.0347(13)	0.0030(10)	0.0047(10)	0.0040(10)
C14	0.0320(13)	0.0415(14)	0.0422(15)	0.0082(11)	0.0001(11)	0.0084(11)
C15	0.0254(12)	0.0404(14)	0.0386(14)	0.0005(11)	0.0023(10)	0.0047(10)
C16	0.0241(12)	0.0478(15)	0.0589(19)	0.0076(13)	0.0022(12)	0.0048(11)
C16A	0.0377(16)	0.072(2)	0.067(2)	0.0098(18)	0.0188(15)	0.0096(15)
C16B	0.0306(15)	0.090(3)	0.072(2)	0.0099(19)	-0.0081(15)	0.0070(16)
C17	0.0332(13)	0.0409(14)	0.0442(15)	0.0110(12)	0.0051(11)	0.0034(11)
C17A	0.0539(19)	0.0407(16)	0.074(2)	0.0122(15)	0.0049(16)	0.0000(14)
C17B	0.0526(19)	0.079(2)	0.0502(18)	0.0190(17)	0.0132(15)	0.0051(17)
C23	0.0380(14)	0.0370(13)	0.0341(13)	-0.0042(10)	0.0116(11)	-0.0063(11)
C24	0.0404(14)	0.0470(15)	0.0366(14)	-0.0016(12)	0.0165(11)	-0.0086(12)
C25	0.0303(12)	0.0344(12)	0.0402(14)	0.0020(11)	0.0118(10)	-0.0021(10)
C26	0.0281(12)	0.0461(15)	0.0460(15)	0.0029(12)	0.0122(11)	-0.0072(11)
C26A	0.0408(16)	0.064(2)	0.076(2)	-0.0069(17)	0.0287(16)	-0.0127(15)
C26B	0.0405(15)	0.0452(16)	0.069(2)	-0.0002(15)	0.0025(14)	-0.0103(13)
C27	0.0509(18)	0.0521(16)	0.0361(15)	-0.0078(12)	0.0128(13)	-0.0143(14)
C27A	0.075(2)	0.065(2)	0.0496(19)	-0.0195(17)	0.0093(17)	-0.0082(19)
C27B	0.064(2)	0.066(2)	0.060(2)	-0.0053(18)	-0.0089(17)	-0.0068(18)
C33	0.0265(11)	0.0328(12)	0.0285(12)	-0.0031(9)	0.0030(9)	0.0006(9)
C34	0.0319(12)	0.0365(13)	0.0359(13)	-0.0095(10)	0.0022(10)	-0.0019(10)
C35	0.0285(12)	0.0357(12)	0.0289(12)	-0.0028(10)	0.0026(9)	-0.0038(10)
C36	0.0277(12)	0.0537(16)	0.0389(14)	-0.0121(12)	0.0039(11)	-0.0071(11)
C36A	0.0384(16)	0.093(3)	0.0477(18)	-0.0094(17)	-0.0088(13)	0.0041(17)
C36B	0.0414(16)	0.066(2)	0.076(2)	-0.0297(18)	0.0073(15)	-0.0172(15)
C37	0.0272(12)	0.0360(13)	0.0416(14)	-0.0096(11)	0.0041(10)	0.0012(10)
C37A	0.0376(15)	0.0645(19)	0.0482(17)	-0.0081(14)	0.0099(13)	0.0078(14)

Table S13. Anisotropic Displacement Parameters (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C37B	0.0424(15)	0.0467(16)	0.0532(17)	-0.0045(13)	0.0030(13)	0.0123(13)
B	0.0225(12)	0.0329(13)	0.0333(14)	0.0013(11)	0.0048(10)	0.0000(10)

The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$

Table S14. Derived Atomic Coordinates and Displacement Parameters for Hydrogen Atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H2	0.0000	-0.0392	0.2500	0.060
H3	0.0833	0.0571	0.1248	0.063
H4A	0.1865	0.0834	0.1668	0.070
H4B	0.1405	0.1511	0.1881	0.070
H4C	0.1640	0.0881	0.2447	0.070
H5A	0.1485	-0.0508	0.1512	0.086
H5B	0.1240	-0.0539	0.2282	0.086
H5C	0.0773	-0.0717	0.1624	0.086
H14	0.2034	0.1260	0.4206	0.046
H16	0.2740	0.3032	0.3454	0.052
H16A	0.3319	0.2225	0.2727	0.070
H16B	0.2837	0.1533	0.2825	0.070
H16C	0.2616	0.2301	0.2416	0.070
H16D	0.3561	0.2299	0.4000	0.078
H16E	0.3013	0.2403	0.4523	0.078
H16F	0.3091	0.1599	0.4122	0.078
H17	0.0283	0.1201	0.3950	0.047
H17A	0.0608	-0.0081	0.4217	0.067
H17B	0.0890	0.0189	0.3503	0.067
H17C	0.1321	0.0178	0.4209	0.067
H17D	0.0431	0.0841	0.5135	0.072
H17E	0.1141	0.1121	0.5144	0.072
H17F	0.0589	0.1740	0.5047	0.072
H24	0.1806	0.3183	0.0576	0.049
H26	0.2656	0.3741	0.2238	0.048
H26A	0.3335	0.3918	0.1317	0.071
H26B	0.3019	0.3080	0.1266	0.071
H26C	0.2770	0.3760	0.0757	0.071
H26D	0.2774	0.5016	0.1829	0.062
H26E	0.2189	0.4900	0.1288	0.062
H26F	0.2094	0.4896	0.2108	0.062
H27	0.0298	0.2144	0.0932	0.055
H27A	0.0632	0.1641	-0.0130	0.076
H27B	0.1232	0.2189	-0.0069	0.076
H27C	0.1153	0.1510	0.0486	0.076
H27D	-0.0084	0.2756	-0.0108	0.076
H27E	-0.0024	0.3370	0.0516	0.076
H27F	0.0487	0.3350	-0.0057	0.076
H34	0.0654	0.5440	0.4083	0.042
H36	0.2159	0.4818	0.3451	0.048

Table S14. Derived Parameters for Hydrogen Atoms (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H36A	0.2580	0.4534	0.4593	0.072
H36B	0.1893	0.4417	0.4853	0.072
H36C	0.2160	0.3830	0.4298	0.072
H36D	0.2345	0.5876	0.4215	0.073
H36E	0.1768	0.6056	0.3677	0.073
H36F	0.1648	0.5814	0.4463	0.073
H37	-0.0726	0.4296	0.3357	0.042
H37A	-0.1087	0.5092	0.4251	0.060
H37B	-0.0557	0.4521	0.4567	0.060
H37C	-0.0396	0.5409	0.4421	0.060
H37D	-0.1082	0.5557	0.3076	0.057
H37E	-0.0391	0.5889	0.3204	0.057
H37F	-0.0551	0.5310	0.2569	0.057
H1B	0.1975	0.3659	0.3027	0.035
H1SA[a]	0.3982	0.2280	0.1490	0.224
H1SB[a]	0.4623	0.1811	0.1580	0.224
H1SC[a]	0.4264	0.2058	0.2253	0.224
H2SA[a]	0.4469	0.3379	0.2020	0.224
H2SB[a]	0.4829	0.3131	0.1344	0.224
H3SA[a]	0.5577	0.2406	0.2086	0.224
H3SB[a]	0.5580	0.3300	0.2324	0.224
H4SA[a]	0.4938	0.3040	0.3244	0.224
H4SB[a]	0.4761	0.2196	0.2941	0.224
H5SA[a]	0.5530	0.2079	0.3879	0.224
H5SB[a]	0.5812	0.1787	0.3172	0.224
H5SC[a]	0.5988	0.2627	0.3474	0.224

[a]Included with an occupancy factor of 0.5.

STRUCTURE REPORT for Compound 5

Ref. Code: li0003 **Date:** 6 April 2016

Compound: [{{HB(3,5-^{i}Pr$_2$-pyrazolyl)$_3$}$_2$Yb(3,5-^{i}Pr$_2$-pyrazolyl)(3,5-^{i}Pr$_2$-pyrazole)}$_2$(μ-S$_4$)] • 2 *n*-C$_5$H$_{12}$

Formula sum: $C_{100}H_{178}B_2N_{10}S_4Yb_2$

Formula moieties: $C_{90}H_{154}B_2N_{10}S_4Yb_2$, 2 C_5H_{12}

Supervisor: F. T. Edelmann **Crystallographer:** P. Liebing

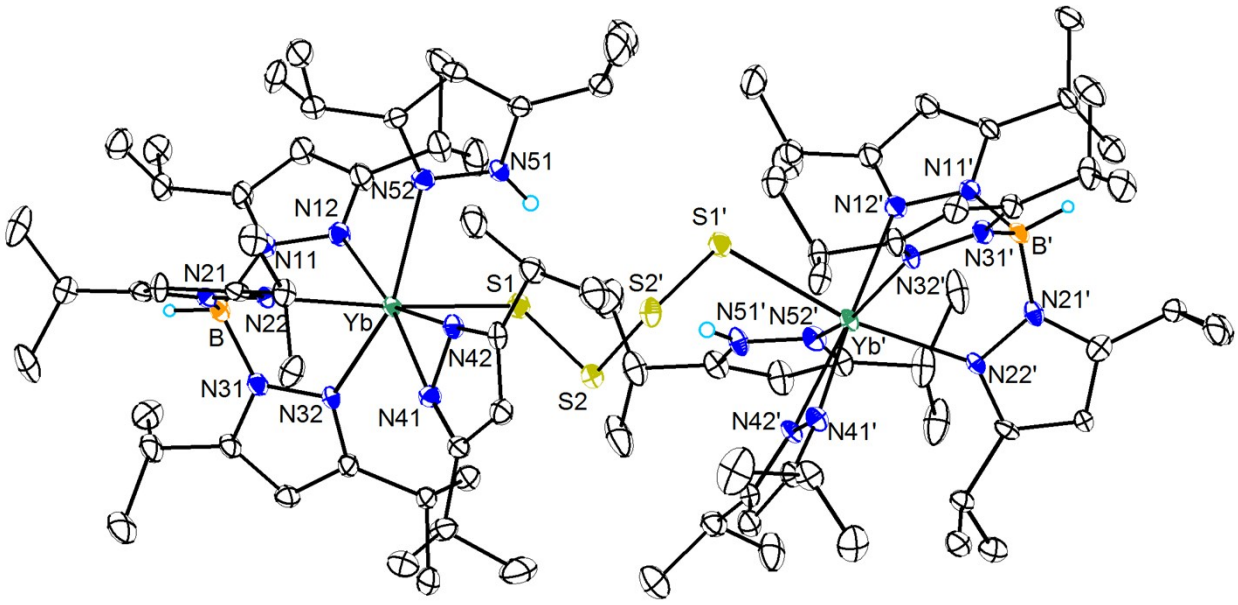

Figure caption

Figure S6. Molecular structure of compound **5** in the crystalline state. Thermal ellipsoids with 30% probability, H atoms attached to C atoms omitted for clarity. Symmetry operator to generate equivalent atoms: ‘ 2–x, y, 1–z.

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Table S15. Crystallographic Experimental Details

A. Crystal Data	
formula	$C_{100}H_{178}B_2N_{10}S_4Yb_2$
formula weight	2156.55
crystal dimensions (mm)	0.49 × 0.22 × 0.14
crystal system	monoclinic
space group	*C*2 (No. 5)
unit cell parameters[a]	
a (Å)	21.7535(5)
b (Å)	17.0849(5)
c (Å)	16.4796(4)
β (deg)	112.597(2)
V (Å^3)	5654.6(3)
Z	2
ρ_{calcd} (g cm^{-3})	1.267
μ (mm^{-1})	1.768
B. Data Collection and Refinement Conditions	
diffractometer	STOE IPDS 2T
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–140
scan type	ω scans (1.5°, 10 min exposure)
completeness of dataset	99.8%
data collection θ limit (deg)	26.138
total data collected	19624 (-26 ≤ *h* ≤ 26, -21 ≤ *k* ≤ 21, -20 ≤ *l* ≤ 20)
independent reflections	11252 (R_{int} = 0.0522)
independent reflections with $I>2\sigma(I)$	10767
structure solution	patterson methods (SHELXS 2013)
refinement method	full-matrix least-squares on F^2 (SHELXL 2014)
absorption correction method	numerical
range of transmission factors	0.6344–0.8078
data/restraints/parameters	11252/ 90[a] / 614
goodness-of-fit (*S*) [all data]	1.067
final *R* indices	
R_1 [all data, $I \geq 2\sigma(I)$]	0.0404, 0.0352
wR_2 [all data, $I \geq 2\sigma(I)$]]	0.1398, 0.1153
largest difference peak and hole	0.839 and –1.991 e Å^{-3}
Flack parameter	–0.01(1)

Refinement special details: Two *n*-pentane molecules are disordered around the special sites (1, *y*, 0) (C46–C50) and (0.5, y, 0.5) (C51–C55) and were refined with a fixed site occupancy factor of 0.5.

[a] restraints for the C-C distances (DFIX) and the anisotropic displacement parameters (SIMU and DELU) of the solvent molecules.

Large U_3/U_1 ratios were obtained for the C atoms of one *n*-pentane molecule (C51–C55) which is considerably disordered. Splitting the C sites does not lead to a satisfying result.

Table S16. Atomic Coordinates and Equivalent Isotropic Displacement Parameters

Atom	x	y	z	Ueq, Å^2
Yb	0.83707(2)	0.31555(3)	0.26640(2)	0.02267(13)
S1	0.95920(11)	0.36827(13)	0.37025(13)	0.0318(4)
S2	1.00921(11)	0.27289(14)	0.44368(15)	0.0344(5)
B	0.7618(5)	0.3734(5)	0.0518(5)	0.0261(17)
N11	0.7842(3)	0.4471(4)	0.1099(5)	0.0268(13)
N12	0.8221(4)	0.4436(4)	0.1984(5)	0.0283(14)
N21	0.7098(3)	0.3265(5)	0.0741(4)	0.0260(16)
N22	0.7270(3)	0.2921(4)	0.1558(4)	0.0229(13)
N31	0.8217(3)	0.3229(6)	0.0605(4)	0.0272(14)
N32	0.8662(3)	0.2968(4)	0.1409(4)	0.0248(15)
N41	0.8572(4)	0.1860(4)	0.3066(5)	0.0285(14)
N42	0.8362(4)	0.2252(4)	0.3648(4)	0.0273(14)
N51	0.8397(4)	0.3943(5)	0.4427(5)	0.0299(15)
N52	0.7932(4)	0.3904(4)	0.3586(5)	0.0293(14)
C1	0.8353(5)	0.5178(6)	0.2258(6)	0.037(2)
C2	0.8066(5)	0.5700(6)	0.1555(6)	0.039(2)
C3	0.7747(5)	0.5239(5)	0.0834(6)	0.0323(18)
C4	0.7296(5)	0.5489(5)	-0.0079(6)	0.0360(19)
C5	0.6579(5)	0.5449(7)	-0.0164(7)	0.047(2)
C6	0.7481(6)	0.6303(6)	-0.0285(7)	0.045(2)
C7	0.8767(6)	0.5413(7)	0.3185(7)	0.043(3)
C8	0.9388(7)	0.5823(8)	0.3246(9)	0.063(4)
C9	0.8366(8)	0.5918(7)	0.3582(8)	0.060(3)
C10	0.6735(4)	0.2510(4)	0.1530(5)	0.0262(16)
C11	0.6227(4)	0.2595(5)	0.0701(5)	0.0299(17)
C12	0.6464(4)	0.3070(7)	0.0222(5)	0.0312(19)
C13	0.6729(5)	0.2011(6)	0.2283(6)	0.0330(19)
C14	0.6053(5)	0.2042(7)	0.2364(7)	0.045(2)
C15	0.6932(5)	0.1177(7)	0.2200(8)	0.043(2)
C16	0.6117(4)	0.3335(5)	-0.0711(6)	0.034(2)
C17	0.6085(7)	0.2694(8)	-0.1337(7)	0.057(3)
C18	0.5420(5)	0.3648(9)	-0.0868(8)	0.059(3)
C19	0.9149(4)	0.2604(6)	0.1255(5)	0.0310(17)
C20	0.9024(4)	0.2617(6)	0.0365(6)	0.0340(18)
C21	0.8422(4)	0.2981(5)	-0.0036(5)	0.030(2)
C22	0.9768(4)	0.2293(6)	0.1985(5)	0.0340(19)
C23	1.0303(5)	0.2932(6)	0.2217(7)	0.041(2)
C24	1.0042(5)	0.1562(7)	0.1751(7)	0.042(2)
C25	0.8049(4)	0.3193(11)	-0.0992(5)	0.043(2)
C26	0.8144(6)	0.2561(9)	-0.1582(8)	0.053(3)
C27	0.8257(7)	0.3986(8)	-0.1208(8)	0.051(3)
C28	0.8408(4)	0.1750(5)	0.4312(5)	0.0301(17)
C29	0.8643(5)	0.1039(6)	0.4144(6)	0.0362(19)
C30	0.8736(5)	0.1131(6)	0.3367(6)	0.0306(19)

Table S16 (continued). Atomic Coordinates and Equivalent Isotropic Displacement Parameters

Atom	x	y	z	Ueq, Å^2
C31	0.8218(6)	0.2008(7)	0.5056(8)	0.037(2)
C32	0.7471(6)	0.2150(11)	0.4753(8)	0.058(4)
C33	0.8473(8)	0.1449(9)	0.5828(8)	0.057(3)
C34	0.8995(6)	0.0560(6)	0.2876(7)	0.041(2)
C35	0.9709(7)	0.0309(11)	0.3467(13)	0.080(5)
C36	0.8554(7)	-0.0144(7)	0.2568(9)	0.056(3)
C37	0.8146(6)	0.4226(6)	0.4996(7)	0.032(2)
C38	0.7485(5)	0.4373(7)	0.4509(7)	0.041(2)
C39	0.7362(5)	0.4163(5)	0.3640(6)	0.0341(18)
C40	0.8585(5)	0.4345(7)	0.5944(6)	0.042(2)
C41	0.8217(8)	0.4142(12)	0.6537(8)	0.072(4)
C42	0.8856(9)	0.5150(10)	0.6110(10)	0.072(4)
C43	0.6728(5)	0.4209(8)	0.2842(7)	0.051(3)
C44	0.6135(6)	0.4197(10)	0.3135(9)	0.065(4)
C45	0.6684(7)	0.4936(12)	0.2291(8)	0.065(5)
C46	0.9514(17)	0.512(2)	0.113(2)	0.072(8)
C47	0.9974(12)	0.4951(13)	0.0639(16)	0.055(5)
C48	1.0000	0.5576(10)	0.0000	0.056(4)
C49	1.0478(12)	0.5458(14)	-0.0446(16)	0.055(5)
C50	1.0369(17)	0.4725(16)	-0.1006(19)	0.063(7)
C51	0.617(4)	0.314(3)	0.556(4)	0.158(14)
C52	0.562(3)	0.270(4)	0.482(6)	0.26(3)
C53	0.5000	0.293(4)	0.5000	0.27(2)
C54	0.431(3)	0.312(6)	0.431(5)	0.27(3)
C55	0.399(6)	0.351(4)	0.489(8)	0.27(3)

Table S17. Selected Interatomic Distances (Å)

atom1	atom2	distance (Å)	atom1	atom2	distance (Å)
Yb	S1	2.703(2)	N32	N31	1.380(9)
Yb	N12	2.423(7)	N42	N41	1.383(10)
Yb	N22	2.421(7)	N51	N52	1.367(11)
Yb	N32	2.406(6)	N11	C3	1.374(11)
Yb	N41	2.304(7)	N12	C1	1.339(12)
Yb	N42	2.244(7)	N21	C12	1.355(11)
Yb	N52	2.443(7)	N22	C10	1.346(11)
S1	S2	2.072(3)	N31	C21	1.362(10)
S2	S2'	2.044(5)	N32	C19	1.334(11)
B	N11	1.543(11)	N41	C30	1.336(12)
B	N21	1.541(11)	N42	C28	1.364(11)
B	N31	1.524(12)	N51	C37	1.345(12)
N12	N11	1.373(10)	N52	C39	1.352(12)
N22	N21	1.382(9)			

Table S18. Selected Interatomic Angles

atom1	atom2	atom3	angle (deg.)	atom1	atom2	atom3	angle (deg.)
S1	Yb	N12	85.22(18)	N52	Yb	N32	154.0(2)
S1	Yb	N22	168.23(16)	N52	Yb	N41	113.6(2)
S1	Yb	N32	93.97(16)	N52	Yb	N42	78.3(3)
S1	Yb	N41	96.08(19)	Yb	S1	S2	105.99(11)
S1	Yb	N42	92.9(2)	S1	S2	S2	106.75(12)
S1	Yb	N52	87.45(19)	N11	B	N21	111.3(7)
N12	Yb	N52	78.5(2)	N21	B	N31	111.3(7)
N12	Yb	N22	83.3(2)	N11	B	N31	110.4(7)
N12	Yb	N32	75.8(2)	Yb	N12	N11	116.7(5)
N12	Yb	N41	167.9(3)	Yb	N22	N21	118.9(5)
N12	Yb	N42	156.7(3)	Yb	N32	N31	117.6(5)
N22	Yb	N41	94.7(2)	Yb	N41	N42	69.9(4)
N22	Yb	N32	80.9(2)	Yb	N42	N41	74.7(4)
N22	Yb	N42	98.6(2)	Yb	N52	N51	110.0(5)
N32	Yb	N41	92.0(2)	B	N11	N12	122.8(6)
N32	Yb	N42	127.4(2)	B	N21	N22	120.2(6)
N41	Yb	N42	35.4(3)	B	N31	N32	122.1(6)
N52	Yb	N22	92.6(2)				

Table S19. Selected Torsional Angles

atom1	atom2	atom3	atom4	angle (deg.)	atom1	atom2	atom3	atom4	angle (deg.)
N31	B	N11	N12	-54.8(9)	B	N11	N12	Yb	-10.2(9)
N21	B	N11	N12	69.3(10)	C12	N21	N22	C10	0.3(9)
N31	B	N11	C3	120.5(9)	B	N21	N22	C10	-175.4(7)
N21	B	N11	C3	-115.4(9)	C12	N21	N22	Yb	-179.4(6)
N31	B	N21	C12	-116.0(11)	B	N21	N22	Yb	4.9(9)
N11	B	N21	C12	120.4(10)	C21	N31	N32	C19	3.3(10)
N31	B	N21	N22	58.8(9)	B	N31	N32	C19	-174.9(8)
N11	B	N21	N22	-64.8(10)	C21	N31	N32	Yb	-172.0(5)
N21	B	N31	C21	113.1(10)	B	N31	N32	Yb	9.8(10)
N11	B	N31	C21	-122.8(9)	C30	N41	N42	C28	0.6(10)
N21	B	N31	N32	-69.1(10)	Yb	N41	N42	C28	-174.2(7)
N11	B	N31	N32	55.0(10)	C30	N41	N42	Yb	174.9(7)
C3	N11	N12	C1	0.3(10)	C39	N52	N51	C37	-1.0(11)
B	N11	N12	C1	176.3(8)	Yb	N52	N51	C37	-169.0(7)
C3	N11	N12	Yb	173.7(6)					

Table S20. Anisotropic Displacement Parameters (U_{ij}, Å^2)

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Yb	0.02712(18)	0.02485(18)	0.01574(17)	0.00070(14)	0.00789(12)	0.00292(14)
S1	0.0329(10)	0.0371(11)	0.0245(9)	0.0013(8)	0.0099(8)	0.0002(8)
S2	0.0335(10)	0.0396(12)	0.0264(10)	-0.0044(9)	0.0074(8)	0.0051(9)
B	0.035(4)	0.027(4)	0.017(4)	0.003(3)	0.010(3)	-0.002(4)
N11	0.032(3)	0.023(3)	0.023(3)	0.002(3)	0.009(3)	-0.001(3)
N12	0.034(3)	0.027(3)	0.024(3)	0.002(3)	0.010(3)	0.000(3)
N21	0.029(3)	0.034(5)	0.017(3)	0.000(3)	0.010(2)	0.006(3)
N22	0.027(3)	0.027(3)	0.016(3)	0.003(2)	0.010(2)	0.002(2)
N31	0.030(3)	0.034(4)	0.019(3)	-0.002(3)	0.011(2)	-0.001(3)
N32	0.028(3)	0.029(4)	0.015(3)	0.000(2)	0.006(2)	0.002(2)
N41	0.033(3)	0.029(3)	0.025(3)	0.001(3)	0.012(3)	0.005(3)
N42	0.035(4)	0.030(3)	0.018(3)	0.005(3)	0.011(3)	0.003(3)
N52	0.034(4)	0.030(4)	0.027(3)	0.000(3)	0.014(3)	0.005(3)
N51	0.035(4)	0.038(4)	0.017(3)	-0.001(3)	0.010(3)	0.009(3)
C1	0.049(5)	0.031(4)	0.027(4)	0.000(4)	0.009(4)	-0.003(4)
C2	0.054(6)	0.024(4)	0.031(5)	0.007(4)	0.008(4)	0.001(4)
C3	0.042(5)	0.032(4)	0.021(4)	0.009(3)	0.009(4)	0.002(3)
C4	0.053(5)	0.028(4)	0.020(4)	0.010(3)	0.006(4)	0.006(3)
C5	0.049(6)	0.041(5)	0.044(6)	0.012(4)	0.009(5)	0.007(4)
C6	0.061(6)	0.033(5)	0.039(6)	0.013(4)	0.019(5)	0.001(5)
C7	0.058(6)	0.031(5)	0.030(5)	0.002(4)	0.003(5)	-0.008(4)
C8	0.063(8)	0.051(7)	0.051(7)	-0.005(6)	-0.006(6)	-0.012(6)
C9	0.093(10)	0.038(6)	0.041(6)	-0.014(5)	0.016(6)	-0.001(6)
C10	0.044(4)	0.016(3)	0.023(4)	0.003(3)	0.018(3)	0.003(3)
C11	0.028(4)	0.035(4)	0.021(4)	0.007(3)	0.003(3)	-0.005(3)
C12	0.029(3)	0.034(5)	0.034(4)	-0.011(4)	0.017(3)	0.000(4)
C13	0.033(4)	0.041(6)	0.027(5)	0.007(4)	0.014(4)	-0.003(4)
C14	0.044(6)	0.053(6)	0.041(5)	0.008(5)	0.020(4)	-0.005(4)
C15	0.038(5)	0.041(5)	0.045(6)	0.015(4)	0.010(4)	0.002(4)
C16	0.031(4)	0.035(6)	0.034(4)	0.005(3)	0.011(3)	-0.002(3)
C17	0.084(8)	0.055(7)	0.021(5)	-0.002(4)	0.009(5)	-0.019(6)
C18	0.036(5)	0.083(9)	0.049(6)	0.035(6)	0.007(4)	0.009(5)
C19	0.027(4)	0.046(5)	0.020(4)	0.000(3)	0.009(3)	0.007(3)
C20	0.029(4)	0.045(5)	0.032(4)	-0.008(4)	0.016(3)	0.002(4)
C21	0.030(4)	0.043(6)	0.020(3)	-0.003(3)	0.014(3)	-0.001(3)
C22	0.029(4)	0.050(5)	0.022(4)	-0.003(4)	0.008(3)	0.011(4)
C23	0.032(4)	0.053(6)	0.038(5)	-0.005(4)	0.012(4)	0.005(4)
C24	0.028(4)	0.054(6)	0.037(5)	-0.008(4)	0.005(4)	0.001(4)
C25	0.036(4)	0.074(6)	0.022(3)	-0.007(6)	0.015(3)	0.002(7)
C26	0.056(7)	0.079(9)	0.032(6)	-0.007(5)	0.026(5)	-0.003(6)
C27	0.057(7)	0.066(8)	0.042(6)	0.016(6)	0.031(6)	0.017(6)
C28	0.029(4)	0.035(5)	0.021(4)	0.003(3)	0.004(3)	-0.004(3)
C29	0.041(5)	0.032(5)	0.030(4)	0.003(4)	0.008(4)	0.004(4)
C30	0.036(4)	0.029(5)	0.026(4)	-0.001(3)	0.011(3)	0.003(4)
C31	0.044(6)	0.039(6)	0.032(5)	0.001(4)	0.017(5)	-0.001(4)
C32	0.046(6)	0.099(11)	0.031(6)	-0.006(6)	0.016(5)	0.005(6)
C33	0.072(8)	0.066(8)	0.036(6)	0.006(6)	0.023(6)	0.006(6)
C34	0.047(5)	0.032(5)	0.044(5)	0.001(4)	0.018(5)	0.012(4)
C35	0.050(7)	0.083(11)	0.101(13)	-0.028(9)	0.024(8)	0.021(7)

Table S20 (continued). Anisotropic Displacement Parameters (U_{ij}, Å2)

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C36	0.064(7)	0.043(6)	0.054(7)	-0.013(5)	0.015(6)	0.006(5)
C37	0.040(5)	0.031(5)	0.027(5)	0.000(4)	0.015(4)	0.010(4)
C38	0.042(5)	0.055(6)	0.029(5)	-0.007(4)	0.017(4)	0.016(5)
C39	0.037(5)	0.034(4)	0.032(4)	0.000(4)	0.013(4)	0.013(4)
C40	0.045(5)	0.054(6)	0.028(5)	0.000(4)	0.014(4)	0.018(5)
C41	0.073(9)	0.116(13)	0.030(6)	0.013(7)	0.021(6)	0.019(8)
C42	0.080(10)	0.076(10)	0.050(8)	-0.021(7)	0.012(7)	-0.012(8)
C43	0.035(5)	0.071(7)	0.038(5)	-0.018(5)	0.005(4)	0.018(5)
C44	0.034(5)	0.102(11)	0.051(7)	-0.025(7)	0.007(5)	0.016(6)
C45	0.047(8)	0.095(14)	0.037(7)	0.006(6)	-0.003(6)	0.030(7)
C46	0.09(2)	0.061(18)	0.08(2)	-0.009(16)	0.047(17)	-0.001(16)
C47	0.043(11)	0.050(12)	0.069(14)	0.000(10)	0.018(10)	-0.001(9)
C48	0.051(9)	0.049(9)	0.073(11)	0.000	0.028(8)	0.000
C49	0.059(13)	0.056(13)	0.048(12)	-0.001(10)	0.021(10)	-0.009(11)
C50	0.09(2)	0.050(14)	0.061(16)	0.011(11)	0.039(15)	0.021(14)
C51	0.30(4)	0.05(2)	0.21(4)	0.05(2)	0.18(3)	0.09(3)
C52	0.34(5)	0.07(3)	0.35(5)	0.05(3)	0.12(4)	0.02(3)
C53	0.33(4)	0.08(3)	0.37(4)	0.000	0.11(4)	0.000
C54	0.34(5)	0.07(3)	0.38(5)	-0.01(4)	0.10(4)	0.01(3)
C55	0.37(6)	0.07(4)	0.40(9)	0.07(5)	0.17(7)	0.02(5)

Table S21. Derived Atomic Coordinates and Displacement Parameters for Hydrogen Atoms

Atom	x	y	z	Ueq, Å2
H1	0.7404	0.3909	-0.0107	0.031
H2	0.8087	0.6256	0.1575	0.046
H3	0.7354	0.5112	-0.0509	0.043
H4	0.6472	0.4912	-0.0059	0.057
H5	0.6516	0.5800	0.0268	0.057
H6	0.6286	0.5611	-0.0758	0.057
H7	0.7942	0.6300	-0.0247	0.053
H8	0.7183	0.6454	-0.0880	0.053
H9	0.7438	0.6678	0.0140	0.053
H10	0.8900	0.4923	0.3543	0.052
H11	0.9646	0.5968	0.3859	0.076
H12	0.9654	0.5475	0.3038	0.076
H13	0.9273	0.6296	0.2882	0.076
H14	0.8246	0.6415	0.3261	0.072
H15	0.7960	0.5639	0.3535	0.072
H16	0.8637	0.6023	0.4202	0.072
H17	0.5796	0.2365	0.0507	0.036
H18	0.7067	0.2233	0.2837	0.040
H19	0.5953	0.2583	0.2466	0.054
H20	0.5708	0.1848	0.1819	0.054
H21	0.6065	0.1713	0.2857	0.054
H22	0.6621	0.0951	0.1649	0.052
H23	0.6924	0.0867	0.2697	0.052
H24	0.7383	0.1173	0.2201	0.052
H25	0.6382	0.3773	-0.0816	0.041

Table S21 (continued). Derived Atomic Coordinates and Displacement Parameters for Hydrogen Atoms

Atom	x	y	z	Ueq, Å^2
H26	0.5856	0.2882	-0.1941	0.068
H27	0.5840	0.2249	-0.1233	0.068
H28	0.6538	0.2529	-0.1250	0.068
H29	0.5214	0.3852	-0.1468	0.070
H30	0.5145	0.3224	-0.0788	0.070
H31	0.5455	0.4069	-0.0448	0.070
H32	0.9302	0.2415	0.0088	0.041
H33	0.9661	0.2186	0.2513	0.041
H34	10.423	0.3029	0.1710	0.050
H35	10.698	0.2760	0.2718	0.050
H36	10.130	0.3414	0.2372	0.050
H37	0.9706	0.1147	0.1604	0.050
H38	10.160	0.1663	0.1243	0.050
H39	10.440	0.1397	0.2251	0.050
H40	0.7564	0.3219	-0.1103	0.052
H41	0.8006	0.2055	-0.1430	0.064
H42	0.8614	0.2537	-0.1501	0.064
H43	0.7872	0.2685	-0.2197	0.064
H44	0.8734	0.3980	-0.1088	0.062
H45	0.8006	0.4104	-0.1830	0.062
H46	0.8165	0.4387	-0.0844	0.062
H47	0.8723	0.0579	0.4493	0.043
H48	0.8442	0.2522	0.5267	0.045
H49	0.7336	0.2560	0.4302	0.070
H50	0.7230	0.1666	0.4507	0.070
H51	0.7366	0.2317	0.5254	0.070
H52	0.8285	0.0927	0.5639	0.069
H53	0.8339	0.1636	0.6298	0.069
H54	0.8960	0.1422	0.6045	0.069
H55	0.9013	0.0833	0.2349	0.049
H56	0.9700	0.0026	0.3980	0.096
H57	0.9888	-0.0033	0.3134	0.096
H58	0.9991	0.0774	0.3663	0.096
H59	0.8108	0.0022	0.2174	0.067
H60	0.8526	-0.0416	0.3077	0.067
H61	0.8740	-0.0499	0.2254	0.067
H62	0.8815	0.3798	0.4578	0.036
H63	0.7170	0.4578	0.4723	0.049
H64	0.8970	0.3977	0.6088	0.051
H65	0.8044	0.3607	0.6413	0.087
H66	0.7847	0.4508	0.6427	0.087
H67	0.8524	0.4181	0.7153	0.087
H68	0.8488	0.5526	0.5953	0.087
H69	0.9141	0.5207	0.6734	0.087
H70	0.9119	0.5250	0.5753	0.087
H71	0.6698	0.3737	0.2470	0.061
H72	0.5718	0.4227	0.2617	0.078
H73	0.6144	0.3711	0.3455	0.078

Table S21 (continued). Derived Atomic Coordinates and Displacement Parameters for Hydrogen Atoms

Atom	x	y	z	Ueq, Å^2
H74	0.6166	0.4646	0.3519	0.078
H75	0.6260	0.4934	0.1781	0.079
H76	0.6708	0.5404	0.2647	0.079
H77	0.7054	0.4939	0.2091	0.079
H78	0.9533	0.4688	0.1523	0.087
H79	0.9056	0.5189	0.0702	0.087
H80	0.9660	0.5606	0.1472	0.087
H81	0.9829	0.4454	0.0312	0.066
H82	10.431	0.4870	0.1080	0.066
H83	0.9595	0.5905	-0.0229	0.067
H84	10.405	0.5905	0.0229	0.067
H85	10.450	0.5918	-0.0824	0.065
H86	10.935	0.5442	0.0009	0.065
H87	10.409	0.4262	-0.0637	0.075
H88	0.9923	0.4740	-0.1473	0.075
H89	10.703	0.4701	-0.1268	0.075
H90	0.6188	0.2955	0.6129	0.189
H91	0.6078	0.3701	0.5501	0.189
H92	0.6600	0.3039	0.5512	0.189
H93	0.5582	0.2880	0.4231	0.312
H94	0.5693	0.2127	0.4864	0.312
H95A	0.4930	0.2493	0.5354	0.324
H95B	0.5070	0.2493	0.4646	0.324
H96A	0.5133	0.3386	0.5395	0.324
H96B	0.4867	0.3386	0.4605	0.324
H97	0.4337	0.3488	0.3860	0.329
H98	0.4066	0.2645	0.4019	0.329
H99	0.3985	0.3134	0.5341	0.328
H100	0.3537	0.3669	0.4533	0.328
H101	0.4255	0.3969	0.5183	0.328