

Supporting Information for the manuscript

**Reversible C-C coupling in phenanthroline
complexes of divalent samarium and thulium**

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1. General considerations.

All reactions were performed using standard Schlenk-line techniques or in an argon filled glovebox (MBraun). All glassware was dried at 120 °C for at least 12 h prior to use. $[1,2,4-(\text{Me}_3\text{C})_3\text{C}_5\text{H}_2]_2\text{Sm}^1$ and $[1,2,4-(\text{Me}_3\text{C})_3\text{C}_5\text{H}_2]_2\text{Tm}(\text{thf})^2$ and $\text{Cp}^*_2\text{Sm}(\text{OEt}_2)^3$ were prepared according published procedure. Toluene, thf, toluene- d_8 , C_6D_6 , pyridine- d_5 , thf- d_8 and pentane were dried over sodium and transferred under reduced pressure in a cold flask. All solvents were degassed prior to use. Pyridine, was degassed and let stirred on molecular sieves for 24h, transferred under reduce pressure in a cold flask and stored on molecular sieves in the glovebox. NMR spectra were recorded in 5 mm tube adapted with a J.Young valve on a Bruker 300 MHz Avance III spectrometer. Chemical shifts are expressed relative to TMS in ppm. Elemental analyses were obtained from the London Metropolitan University Science Centre. Cyclic Voltammetry studies were conducted in a N_2 filled glovebox using a Princeton Applied Research VersaSTAT4 potentiostat. Measurements were performed in a 5 mL THF solution of 5 mM of the complex and ~ 0.1 M of $[\text{NBu}_4][\text{PF}_6]$ with a 5 mm platinum disk working electrode and a silver wire as quasi reference electrode.

2. Syntheses.

$[\text{Cp}^*_2\text{Sm}(\text{phen})]_2$ (1). A toluene solution of phenanthroline (52 mg, 0.30 mmol) was added to a green toluene solution of $\text{Cp}^*_2\text{Sm}(\text{OEt}_2)$ (144 mg, 0.30 mmol) at room temperature. The solution turned dark green immediately and a dark precipitate formed gradually with time. The solution was let stand at room temperature overnight and the dark precipitate was filtered, washed several time with toluene and dried under reduced pressure to yield 102 mg (0.17 mmol, 56 %). The black powder is very scarcely solution in toluene of thf but yields to a deep green solution in pyridine. A recrystallization in pyridine yields dark green crystals that were not suitable for X-ray but that were used for further analyses. Dark green X-ray suitable crystals were obtained from a slow diffusion of a phenanthroline solution into a diluted toluene solution of $\text{Cp}^*_2\text{Sm}(\text{OEt}_2)$ at room temperature.

Despite our efforts, the combustion analysis of the crystals (those recrystallized from pyridine and those obtained from slow diffusion of the ligand) always came back off whereas the ^1H NMR shows little impurities. We were not able to find a recrystallization solvent to overcome this problem.

^1H (δ , ppm, py- d_5 , 298 K) 9.48, 1H, d, $J = 8$ Hz, **I**; 8.95, 1H, d, $J = 7$ Hz, **II**; 8.33, 1H, d, $J = 7$ Hz, **I**; 8.30, 1H, d, $J = 7$ Hz, **II**; 7.72, 1H, d, $J = 7$ Hz, **II**; 7.55, 1H, d, $J = 7$ Hz, **I**; 5.75, 1H, s,

II; 5.53, 1H, s, **I**; 4.59, 1H, s, **II**; 4.28, 1H, s, **I**; 3.32, 1H, s, **I**; 3.20, 1H, s, **II**; 1.16, 30H, s, **I** and **II**; 1.08, 15H, s, **I**; 0.75, 15H, s, **II**; -11.06, 1H, s, **I**; -11.12, 1H, s, **II**; -14.90, 1H, s, **I**; -15.11, 1H, s, **II**. **I** stands for the major isomer, **II** for the minor one.

[Cp^{III}₂Sm(phen)]₂ (3). Phenanthroline (36.6 mg, 0.202 mmol) was added to a purple pentane solution of Cp^{III}₂Sm(thf) (140.0 mg, 0.202 mmol) at room temperature. The solution turned dark purple immediately and a dark precipitate formed. The solution was let stand at -35 °C overnight and the dark precipitate was filtered, washed several time with cold pentane and dried under reduced pressure to yield 107 mg (0.134 mmol, 67 %). A recrystallization in toluene yields dark purple X-ray suitable crystals. Anal. Calcd for C₄₆H₆₆N₂Sm: C, 69.29; H, 8.34 ; N, 3.51. Found: C, 69.13; H, 8.29 ; N, 3.60.

¹H (δ, ppm, py-d₅, 298 K) 17.92, 1H, s, **II**; 16.36, 1H, s, **I**; 14.13, 1H, s, **II**; 14.03, 0.3H, s, **M**; 12.92, 1H, s, **I**; 12.66, 1H, s, **I**; 12.26, 1H, s, **II**; 11.94, 1H, s, **II**; 10.10, 1H, s, **I**; 9.33, 1H, d, J = 9 Hz, **I**; 8.45, 1H, d, J = 9 Hz, **I**; 7.95, 1H, m, **II**; 7.32, 2H, m, **I** and **II**; 7.16, 1H, s, **II**; 4.89, 1H, s, **I**; 4.79, 1H, s, **II**; 4.45, 1H, s, **I**; 3.37, 1H, s, **II**; 3.08, 9H, s, **II**; 2.43, 9H, s, **II**; 2.31, 9H, s, **I**; 2.03, 9H, s, **I**; 1.89, 9H, s, **I**; 1.47, 6H, s, **M**; 1.30, 1H, s, **I**; 0.37, 9H, s, **II**; 0.29, 18H, s, **I** and **II**; -0.73, 9H, s, **I**; -1.78, 18H, s, **I** and **II**; -2.42, 9H, s, **II**; -7.94, 1H, s, **II**; -9.35, 1H, s, **I**; -12.27, 1H, s, **I**; -12.41, 1H, s, **II**; -85.56, 0.15H, s, **M**; -178.9, 0.15H, s, **M**.

I stands for the major isomer, **II** for the minor one, and **M** for the monomer, several resonances are missing for the monomer, **M**, at room temperature and one resonance of the phenanthroline ligand is missing for **II**.

[Cp^{II}₂Sm(phen)]₂ (5). KCp^{II} (406 mg, 1.86 mmol) was added to SmI₂ (376 mg, 0.93 mmol) in a J.Young flask and thf was condensed over the solid mixture at 77 K. The reaction mixture was warmed to room temperature and the green suspension turned deep purple in 2 h. The reaction was stirred overnight at room temperature and the thf was removed under reduced pressure to yield a dark purple residue, which was extracted to pentane to yield a purple solution and a white solid. After filtration, the filtrate was concentrated to 5 mL and cooled at -35 °C to yield a green powder that was filtered and dried under reduced pressure (582 mg of Cp^{II}₂Sm(thf), 1.30 mmol, 70%). Phenanthroline (11.5 mg, 0.064 mmol) was added to a purple pentane solution of Cp^{II}₂Sm(thf) (37.0 mg, 0.064 mmol) at room temperature. The solution

turned dark purple immediately and a dark precipitate formed. The solution was let stand at -35 °C overnight and the dark precipitate was filtered, washed several time with cold pentane and dried under reduced pressure to yield 25 mg (0.036 mmol, 58 %). A recrystallization in thf yields dark purple X-ray suitable crystals. Anal. Calcd for C₃₈H₅₀N₂Sm: C, 66.61; H, 7.35 ; N, 4.09. Found: C, 66.68; H, 7.30; N, 4.07.

The ratio between the two isomers was found to be 38:62 but we were not able to attribute all resonances to their corresponding isomers, especially for the Cp-H protons because of overlaps. One proton of the phenanthroline ligand could not be found.

¹H (δ, ppm, py-d₅, 298 K): 16.91, s, Cp-H; 16.04, s, Cp-H; 15.12, s, Cp-H; 15.02, s, Cp-H; 14.55, s, Cp-H; 14.12, s, Cp-H; 13.93, s, Cp-H; 13.57, s, Cp-H; 13.05, s, Cp-H; 12.46, s, Cp-H; 12.14, s, Cp-H; 11.39, s, Cp-H; 9.50, s, phen; 9.02, s, phen; 8.47, s, phen; 8.24, s, phen; 7.96, s, phen; 7.79, s, phen; 7.56, s, phen; 5.72, s, phen; 5.52, s, phen; 4.44, s, phen; 3.75, s, phen; 1.47, s, ^tBu; 1.16, s, ^tBu; 1.05, s, ^tBu; 0.82, s, ^tBu; 0.04, s, ^tBu; -0.17, s, ^tBu; -1.18, s, ^tBu; -1.52, s, ^tBu; -8.52, s, phen; -9.69, s, phen; -11.65, s, phen; -11.92, s, phen.

[Cp^{ttt}₂Tm(phen)]₂ (7). Phenanthroline (18.4 mg, 0.102 mmol) was added to a deep purple toluene solution of Cp^{ttt}₂Tm(thf) (72 mg, 0.102 mmol) at room temperature. The solution turned dark bleu/purple, almost black, immediately and a dark precipitate formed. The solution was let stand at -35 °C overnight and the dark microcrystalline powder was filtered, washed several time with cold pentane and dried under reduce pressure to yield 25 mg (0.031 mmol, 30 %). X-ray suitable crystals were obtained from recrystallization in toluene at -35 °C. Despite our efforts, the combustion analysis never came back satisfactory. The NMR analyses showed very broad peaks that were not attributed but their number is in agreement with the dimeric form present at room temperature. A toluene solution of the crystal at room temperature and at lower temperature (273 K) is blue while upon heating to the boiling point of toluene (383 K), the solution turns to purple (See Figure S17 for the visible spectra).

Crossover experiments.

[Cp^{*}₂Sm(phen)]₂, 1 and [Cp^{ttt}₂Sm(phen)]₂, 3. The complex [Cp^{ttt}₂Sm(phen)]₂ (**3**) (32 mg, 0.0201 mmol) was added to a toluene-d₈ suspension of [Cp^{*}₂Sm(phen)]₂ (**1**) (24.1 mg, 0.0201 mmol) at room temperature. The dark blue/purple resulting solution was heated to 100 °C for several minutes and slowly cooled to room temperature. The ¹H NMR spectrum of the

solution shows about 120 resonances (see Figure S14). As a reminder, **1** shows 20 peaks while **3** shows 36 resonances. If nothing happens between both, one expects 56 resonances. If a mixed dimer is formed, 28 other resonances are expected. The presence of additional peaks shows that the mixed dimer $\text{Cp}^*_2\text{Sm}(\text{phen})\text{-(phen)SmCp}^{\text{ttt}}_2$ is formed. However, it also means that other mixed dimers are formed. These could be the results of an exchange of the Cp ligands to form the other mixed dimer $\text{Cp}^*\text{Cp}^{\text{ttt}}\text{Sm}(\text{phen})\text{-(phen)SmCp}^*\text{Cp}^{\text{ttt}}$, for which another set of 28 set is expected. These four dimers represent 114 resonances, which is close to the 120 resonances that we counted. Two additional dimers are possible: $\text{Cp}^*\text{Cp}^{\text{ttt}}\text{Sm}(\text{phen})\text{-(phen)SmCp}^*_2$ and $\text{Cp}^*\text{Cp}^{\text{ttt}}\text{Sm}(\text{phen})\text{-(phen)SmCp}^{\text{ttt}}_2$ but statistically less probable.

When this mixture was heated to 80 °C, the presence of three different sets of monomers are observed (See Figure S15) and attributed to $\text{Cp}^*_2\text{Sm}(\text{phen})$, $\text{Cp}^{\text{ttt}}_2\text{Sm}(\text{phen})$ and the mixed complex $\text{Cp}^*\text{Cp}^{\text{ttt}}\text{Sm}(\text{phen})$, attesting of the formation of the latter complex.

$[\text{Cp}^{\text{ttt}}_2\text{Sm}(\text{phen})]_2$, **3 and $[\text{Cp}^{\text{ttt}}_2\text{Tm}(\text{phen})]_2$, **7**.** The complex $[\text{Cp}^{\text{ttt}}_2\text{Tm}(\text{phen})]_2$ (**7**) (10.6 mg, 0.007 mmol) was added to a toluene- d_8 solution of $[\text{Cp}^{\text{ttt}}_2\text{Sm}(\text{phen})]_2$ (**3**) (10.3 mg, 0.007 mmol) at room temperature. The dark blue/purple resulting solution was heated to 100 °C for several minutes and slowly cooled to room temperature. The color turned purple while heating and came back to blue/purple at room temperature. The ^1H NMR spectrum is different to that of **3** and to that of **7**, and several additional resonances are present (see Figure S16). These resonances are attributed to the heterodimer $[\text{Cp}^{\text{ttt}}_2\text{Sm}(\text{phen})\text{-(phen)SmCp}^{\text{ttt}}_2]$.

3. NMR studies.

Figure S1. ^1H NMR spectrum of **1** at 298 K. Yellow and green marks are to distinguish between the two different isomers for the phenanthroline resonances and blue and red for the methyl resonances.

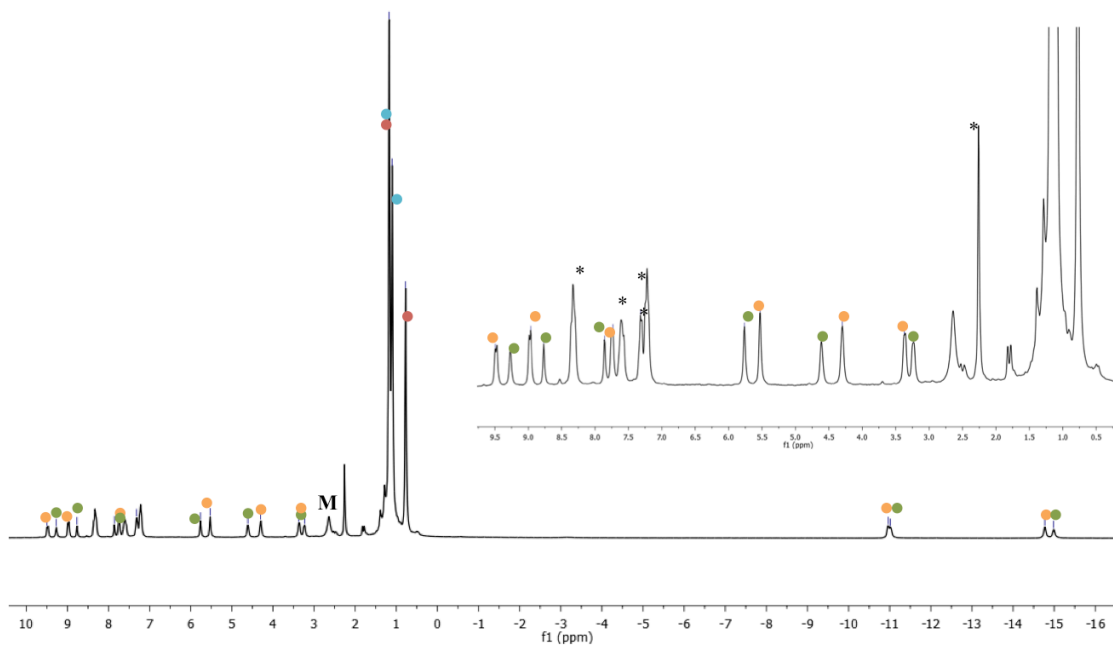


Figure S2. ^1H NMR spectrum of **1** at 60 °C (333 K).

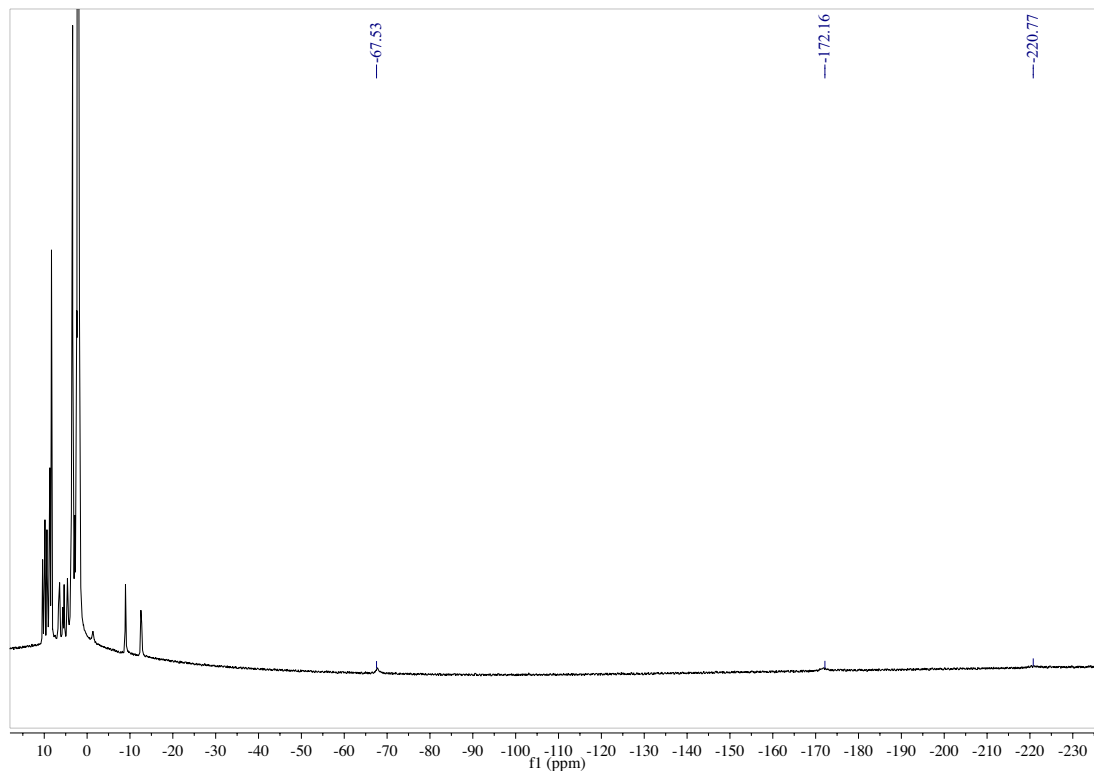


Figure S5. ^1H NMR Spectrum of **3** at different temperatures that shows the signals of the monomers that are increasing in intensity with the temperature (right) while the signals of the dimer are decreasing in intensity (left).

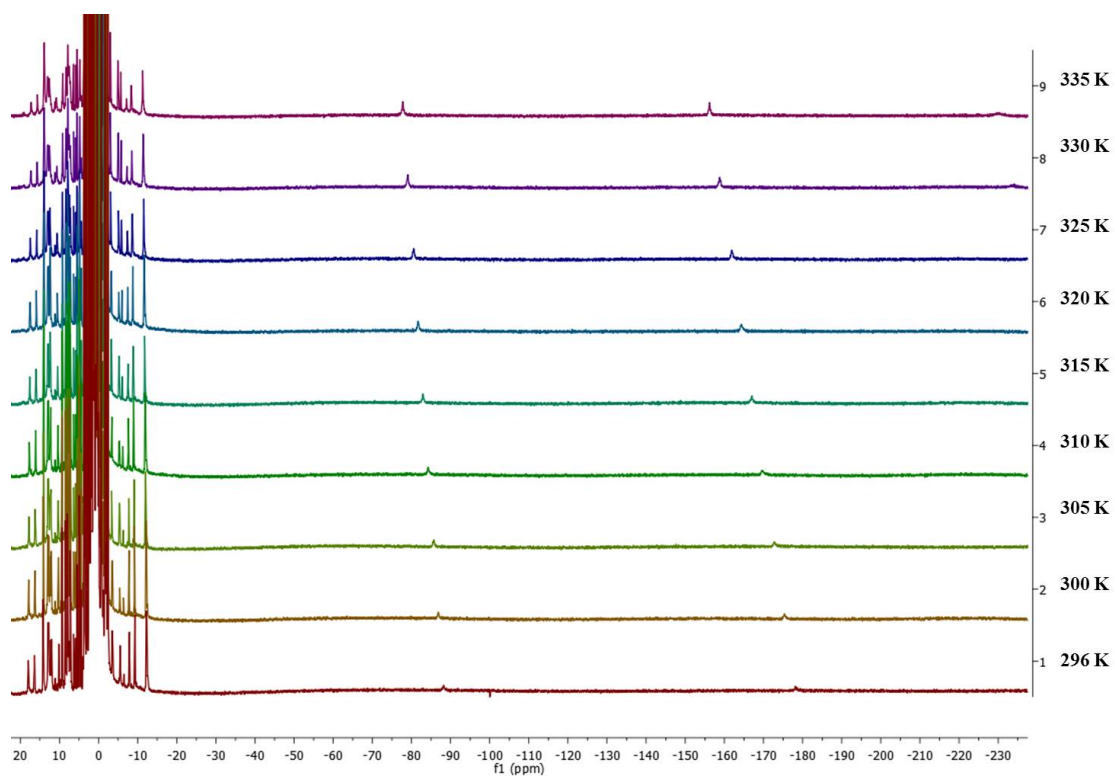


Figure S6. ^1H NMR Spectrum of **5** at 298 K. Light blue and red marks are to distinguish between the two different isomers of the ^tBu groups of Cp resonances, asterisks are for solvents.

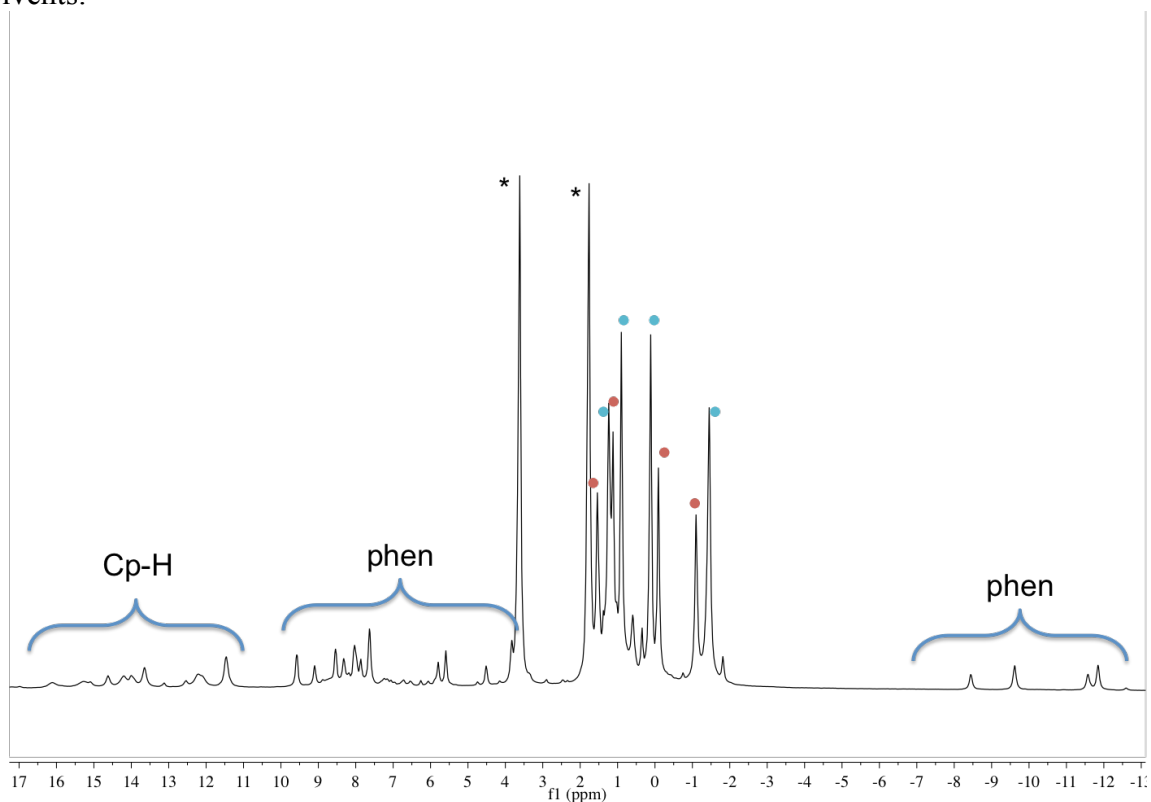


Figure S7. ^1H NMR Spectrum of **5** at 335 K. The letter “M” marks the resonances attributed to the monomer.

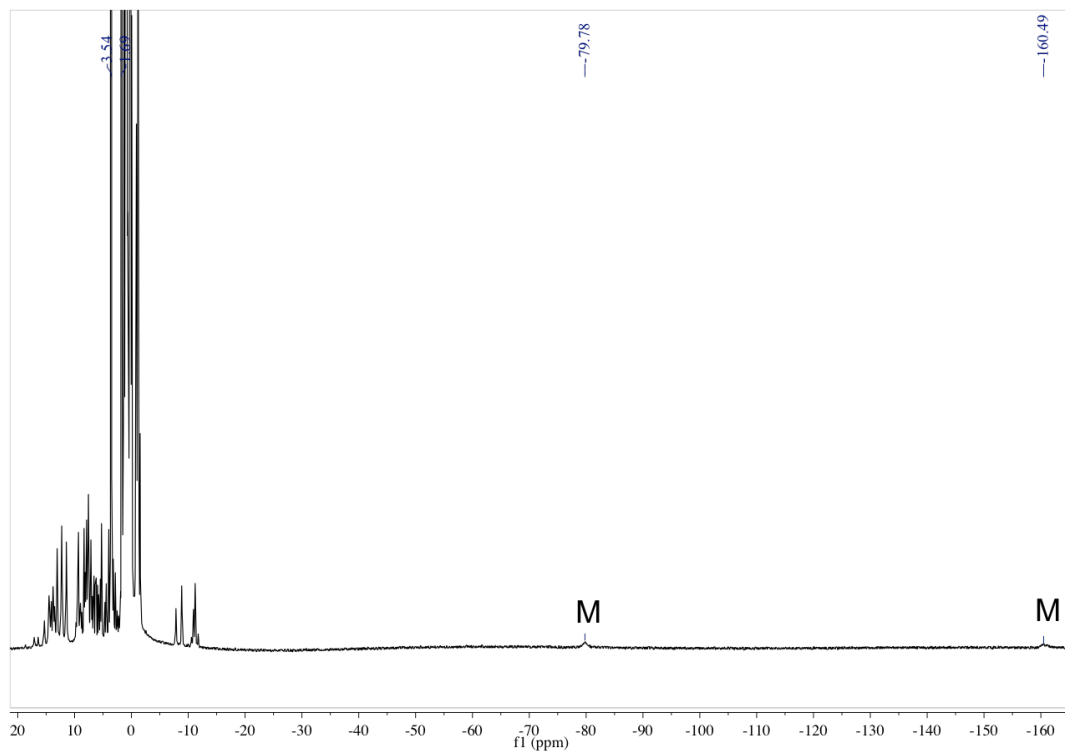


Figure S8. ^1H NMR Spectrum of **7** at 295 K in thf-d_8 . Tm(III) complexes usually show such very broad ^1H NMR. This experiment was performed on crystals of **7**. The observation of multiple signals with similar integration is attributed to the presence of the dimer in solution at this temperature.

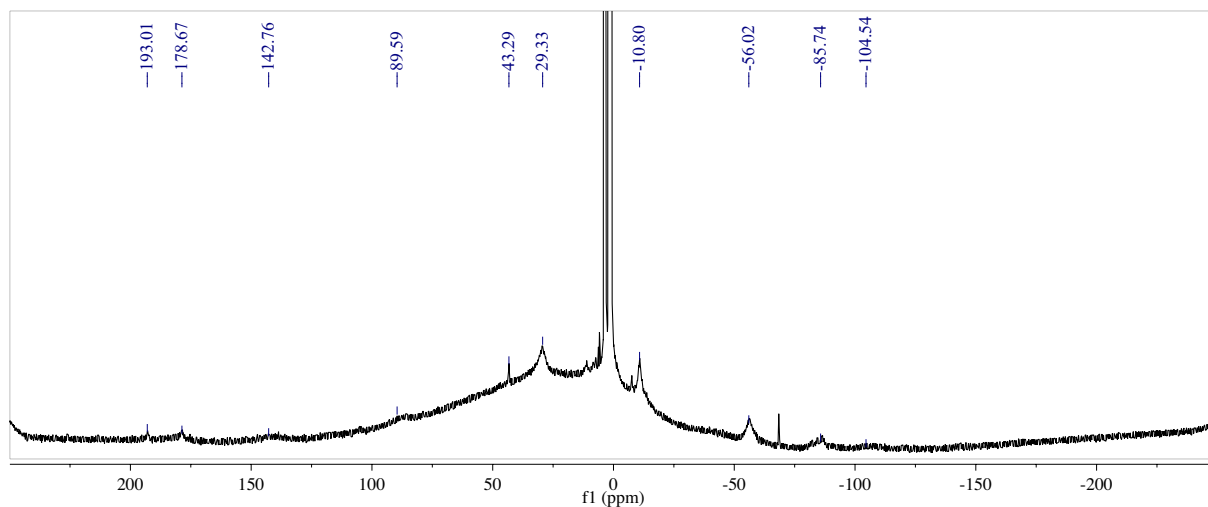


Figure S9. ^1H NMR Spectrum of **7** at 333 K in thf-d_8 . The blue arrows show the signals that increased with temperature and that can be attributed to the monomeric form in solution. Note that these peaks are not present at 295 K (See Figure S8, above). The two experiments were performed in the same tube on the same day at different temperatures.

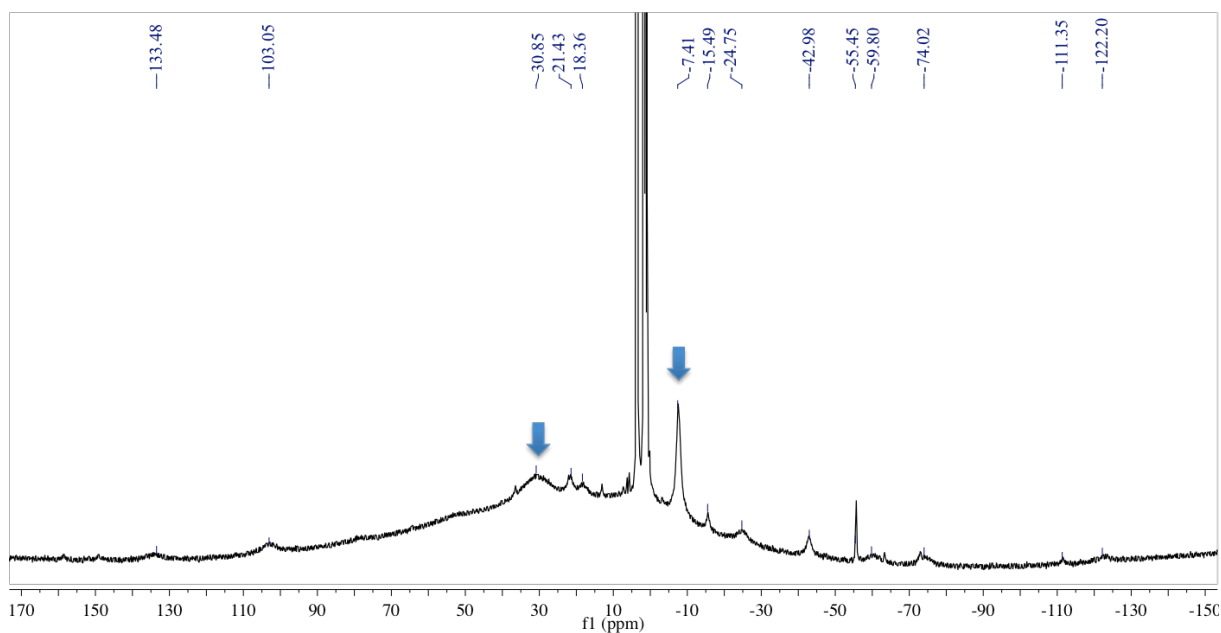


Figure S10. ^1H NMR Spectra of **7** at different temperature in toluene- d_8 . The blue arrows show the signals that increased with temperature and that can be attributed to the monomeric form in solution. The red dots represent 9 on the 12 resonances (attributed based on the integration at 353 K) of the peaks attributed to the ^1Bu resonances of the dimer.

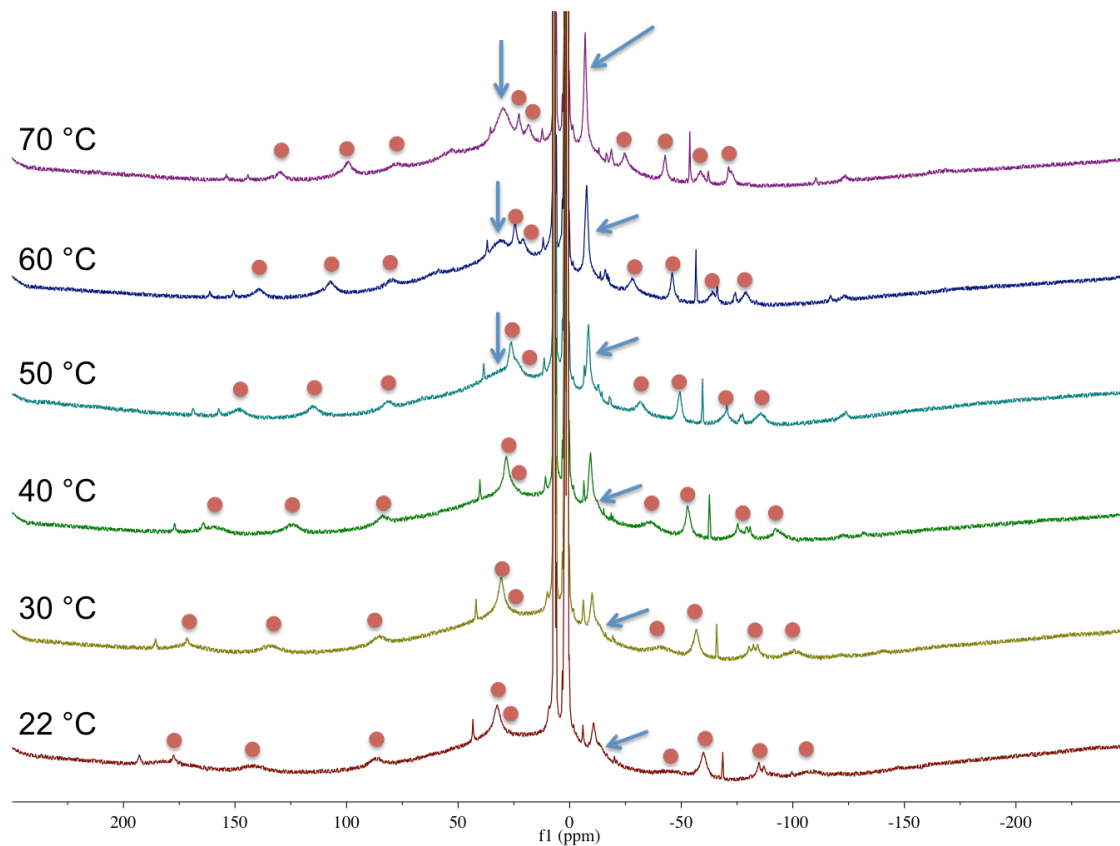


Figure S11. Van't Hoff plot of the dimerization reaction $2 = 2 \ 1$

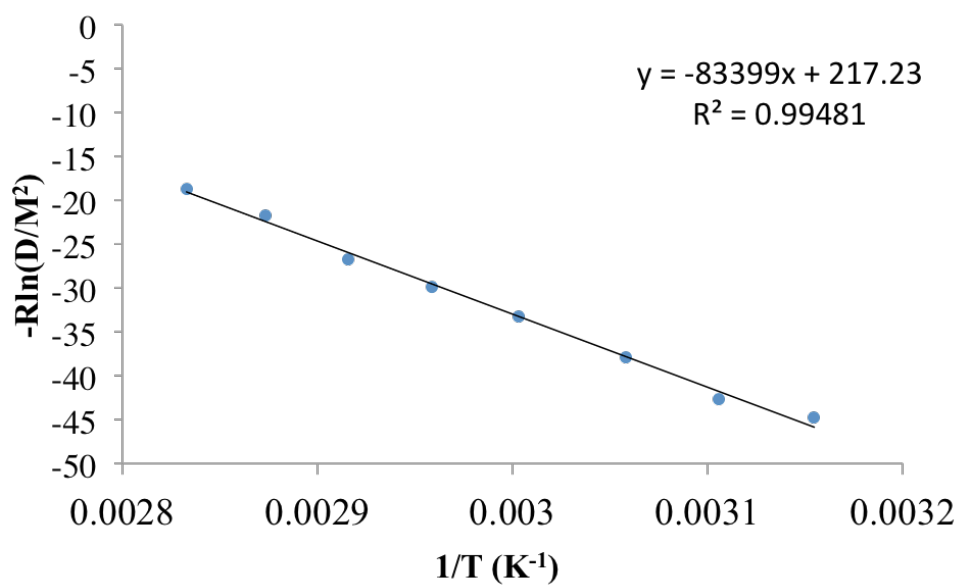


Figure S12. Van't Hoff plot of the dimerization reaction $4 = 2 \ 3$

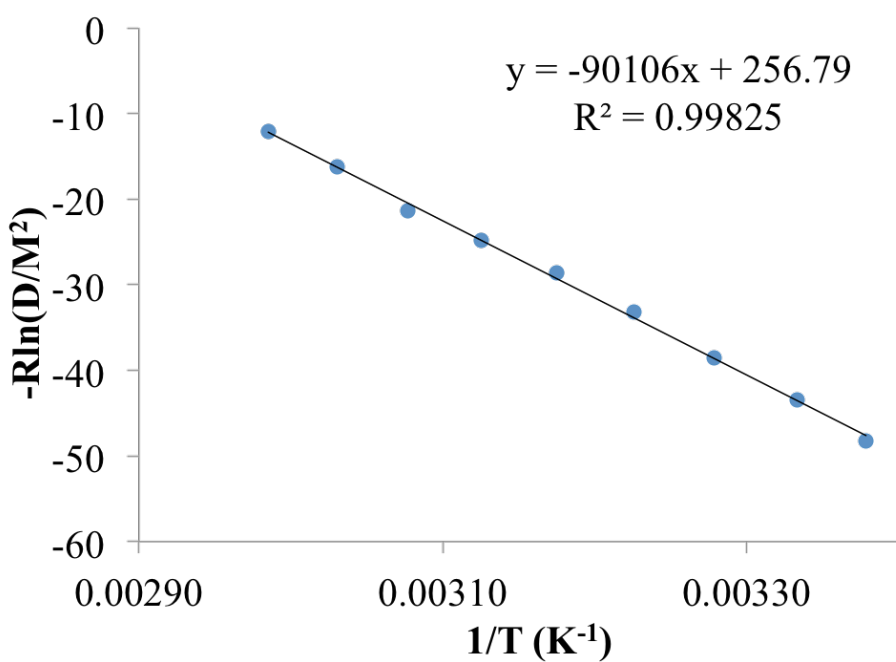


Figure S13. Van't Hoff plot of the dimerization reaction $6 = 2 \mathbf{5}$

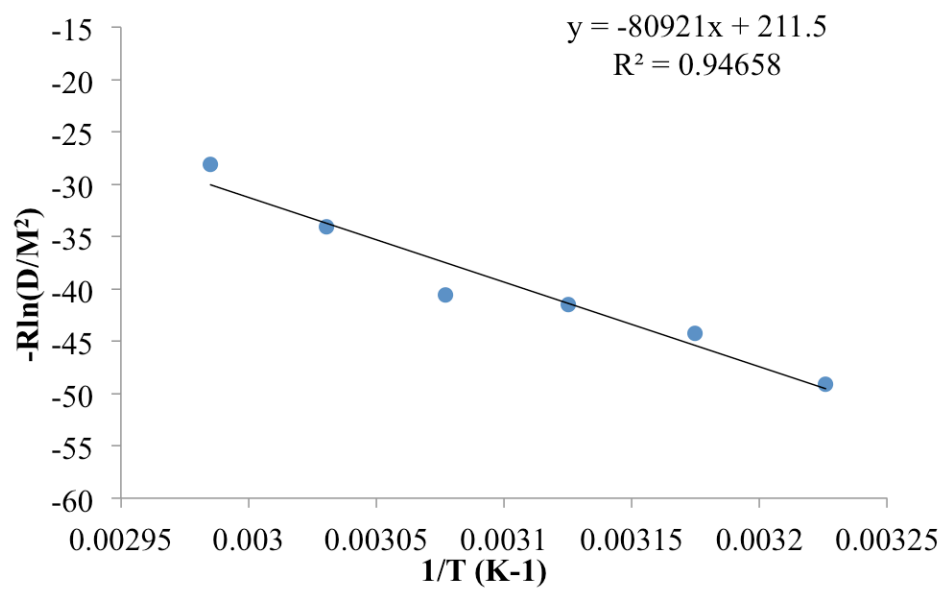


Figure S14. Room temperature (295 K) ^1H NMR spectrum of the crossover experiment between **1** and **3**.

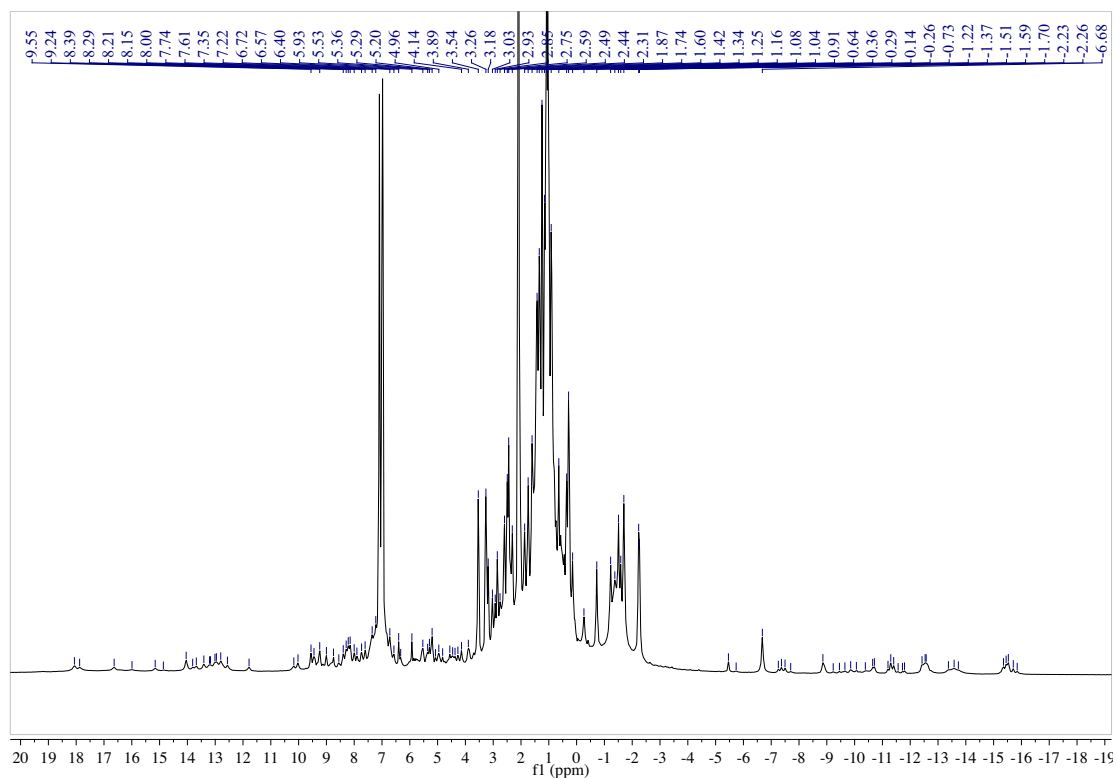


Figure S15. High temperature (353 K) ^1H NMR spectrum of the crossover experiment between **1** and **3**.

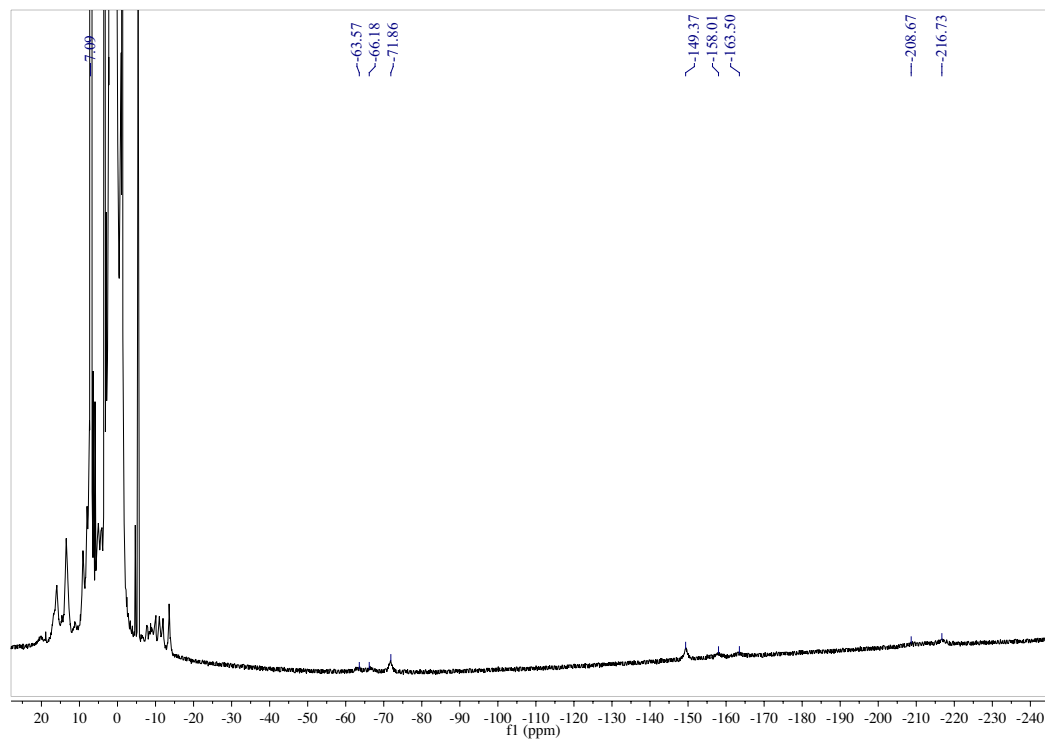


Figure S16. Room temperature (295 K) ^1H NMR spectrum of the crossover experiment between **3** and **7**. Several additional ^tBu resonances are present, in particular between -4 ppm and -21 ppm. The ^1H NMR spectrum of **3** is given below for an easier comparison. At this concentration the resonances of **5** are not observed.

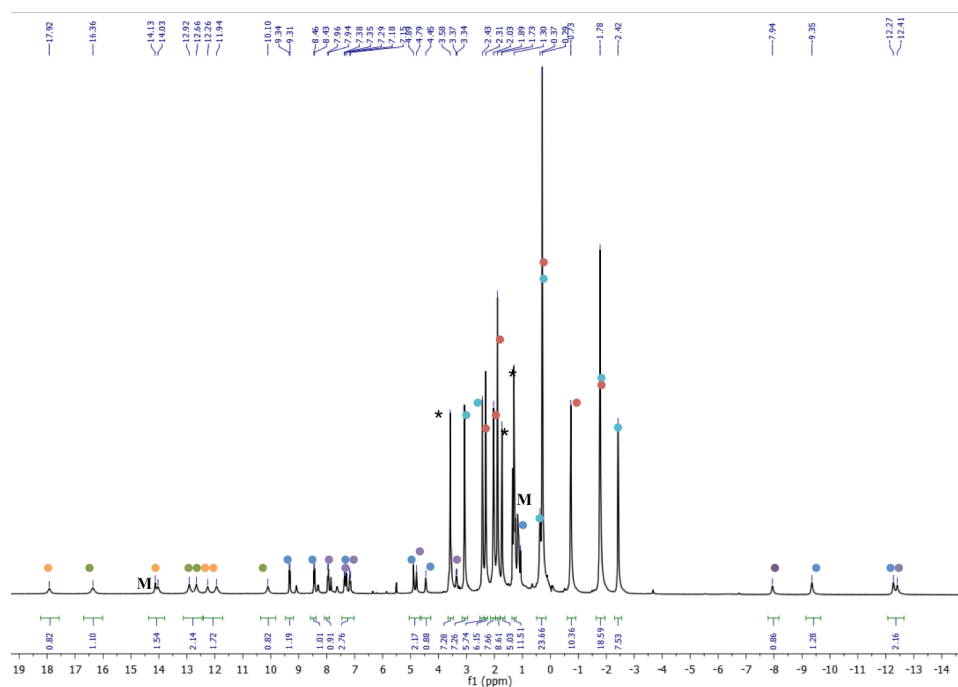
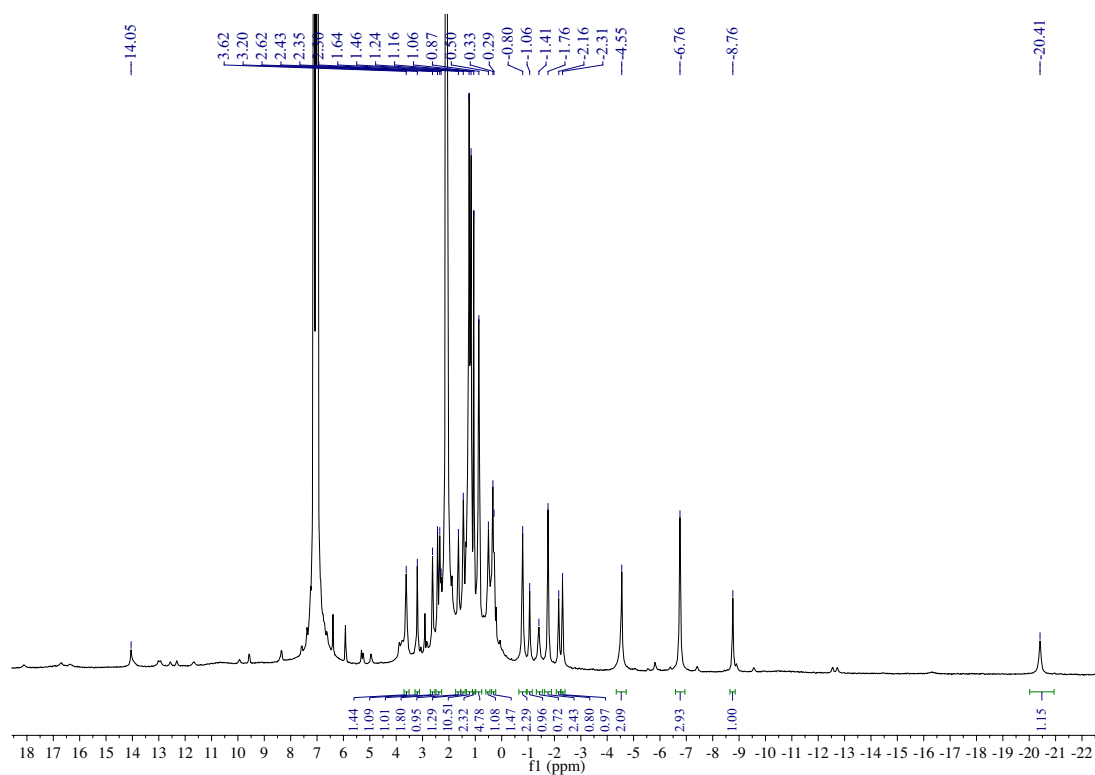
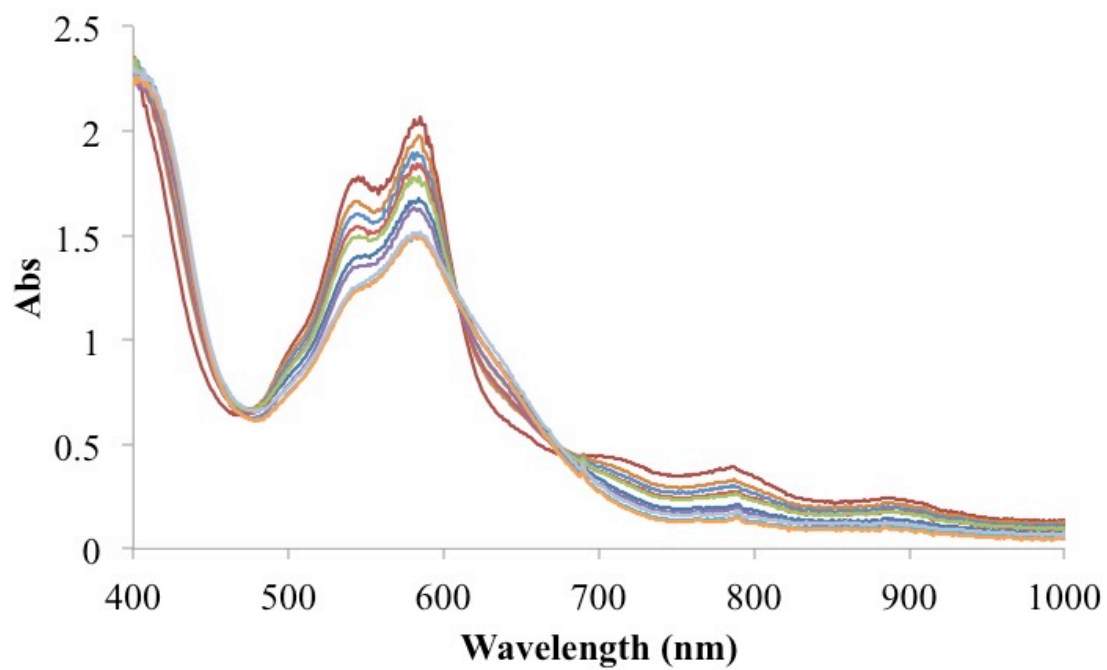


Figure S17. Visible spectra of **7** recorded from around 273 K (ice bath, orange line) to around 373 K (boiling water, red line) in toluene. The temperature was not monitored and the information is only qualitative. The blue line corresponds to the room temperature spectrum. The important point is the evolution of the spectra that agrees with the color evolution of **7** with the temperature (from blue to purple). This shows that equilibrium is present because the evolution is reversible.



4. X-ray structures.

Table S1. Selected Crystal Data Collection Parameters for **1, 3, 5** and **7**.

	[Cp* ₂ Sm(phen)] ₂ (1)	[Cp ^{III} ₂ Sm(phen)] ₂ •2(C ₇ H ₈) (3)	[Cp ^{II} ₂ Sm(phen)] ₂ •4.5(C ₄ H ₈ O) (5)	[Cp ^{III} ₂ Tm(phen)] ₂ •3(C ₇ H ₈) (7)
Formula	C ₆₄ H ₇₆ N ₄ Sm ₂	C ₉₂ H ₁₃₂ N ₄ Sm ₂ •2(C ₇ H ₈)	C ₇₆ H ₁₀₀ N ₄ Sm ₂ •4.5(C ₄ H ₈ O)	C ₉₂ H ₁₃₂ N ₄ Tm ₂ •3(C ₇ H ₈)
Crystal size (mm)	0.15 x 0.12 x 0.10	0.06 x 0.06 x 0.02	0.30 x 0.10 x 0.03	0.18 x 0.11 x 0.04
cryst system	Orthorhombic	Triclinic	Monoclinic	Triclinic
space group	<i>Pbca</i>	<i>P-1</i>	<i>P2₁/c</i>	<i>P-1</i>
volume (Å ³)	5405.33(16)	2575.8(4)	4053.23(12)	2538.9(4)
<i>a</i> (Å)	16.6036(3)	10.225(1)	10.9726(2)	10.148(1)
<i>b</i> (Å)	17.8851(3)	12.304(1)	18.7116(3)	12.286(1)
<i>c</i> (Å)	18.2024(3)	20.627(1)	19.7467(3)	20.481(1)
<i>a</i> (deg)	90.00	87.886(1)	90.00	87.531(1)
<i>b</i> (deg)	90.00	87.688(1)	91.3117(9)	88.273(1)
<i>g</i> (deg)	90.00	83.688(1)	90.00	84.590(1)
Z	4	1	2	1
formula weight (g/mol)	1201.98	1963.24	1694.76	1908.27
density (calcd) (g cm ⁻³)	1.477	1.266	1.389	1.248
absorption coefficient (mm ⁻¹)	2.19	1.179	1.490	1.783
F(000)	2448	1036	1776	1000
absorption correction	Multi-scan	Multi-scan	Multi-scan	Multi-scan
Tmin / Tmax	0.734 / 0.81	0.759 / 1.369	0.936 / 1.077	0.889 / 1.102
Diffractometer	KappaCCD	KappaCCD	KappaCCD	KappaCCD
X-ray source	MoKa	MoKa	MoKa	MoKa
λ(Å)	0.71069	0.71069	0.71069	0.71069
Monochromator	graphite	graphite	graphite	graphite
T (K)	150.0(1)	150.0(1)	150.0(1)	150.0(1)
Scan mode	phi and omega scans	phi and omega scans	phi and omega scans	phi and omega scans
Maximum q	30.00	27.46	30.06	30.10
HKL ranges	-23 23; -25 25 ; -25 25	-13 13; -15 15 ; -23 26	-15 15 ; -26 26 ; -27 27	-14 14; -17 17 ; -28 28
Reflections measured	54313	18460	56778	56322
Reflections used	6081[0.076]	11083 [0.0419]	11870 [0.0678]	14831 [0.0845]
Refinement type	Fsqd	Fsqd	Fsqd	Fsqd
wR2	0.162	0.1456	0.1168	0.1597
R1	0.053	0.0563	0.0482	0.0644
GoF	1.23	1.132	1.068	1.080
difference peak / hole (e Å ⁻³)	1.16/ -1.59	1.163/ -0.819	0.569/ -0.912	3.796/ -1.459

Figure S18. ORTEP of **1**. Carbon atoms are shown in grey, samarium in green and nitrogen in blue. Thermal ellipsoids are represented at 50 % level and hydrogen atoms are omitted for clarity.

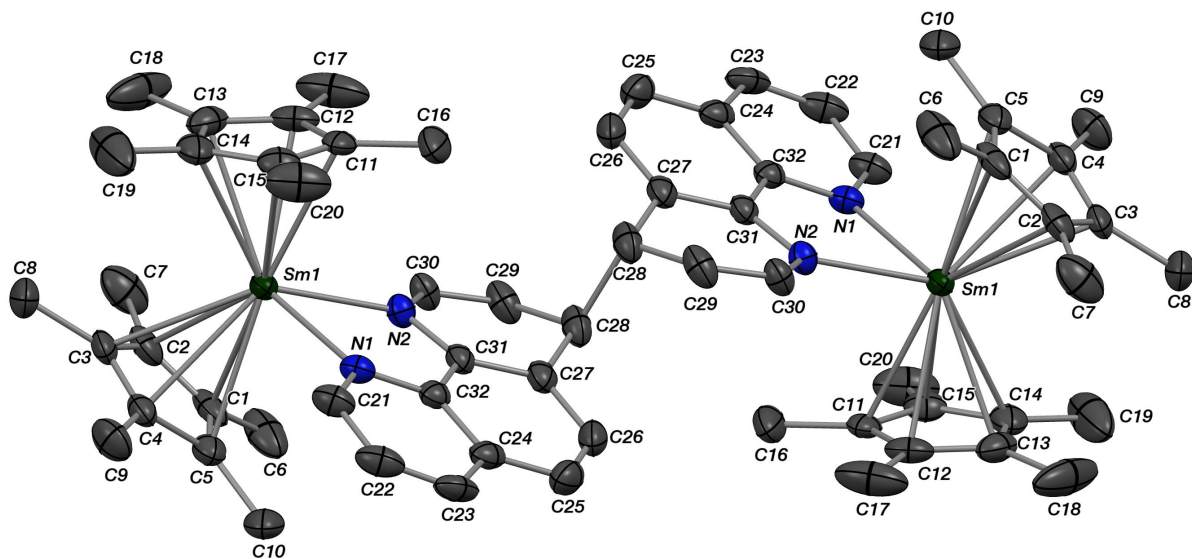


Figure S19. ORTEP of **3**. Carbon atoms are shown in grey, samarium in green and nitrogen in blue. Thermal ellipsoids are represented at 50 % level and hydrogen atoms are omitted for clarity.

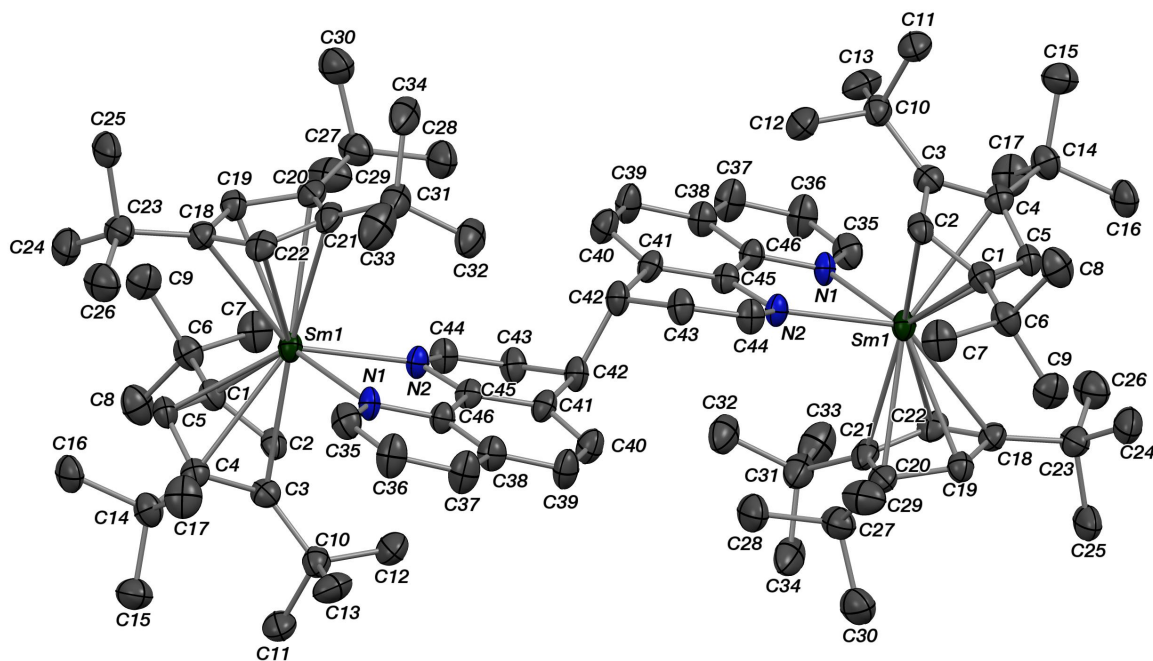


Figure S20. ORTEP of **5**. Carbon atoms are shown in grey, samarium in green and nitrogen in blue. Thermal ellipsoids are represented at 50 % level and hydrogen atoms are omitted for clarity.

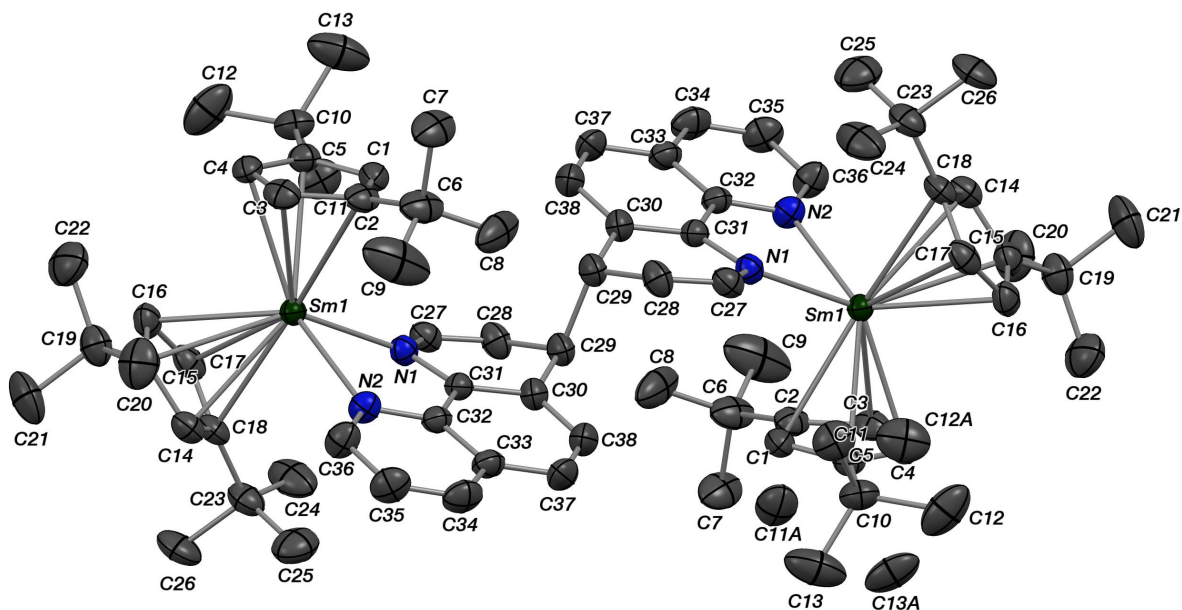


Figure S21. ORTEP of **7**. Carbon atoms are shown in grey, samarium in green and nitrogen in blue. Thermal ellipsoids are represented at 50 % level and hydrogen atoms are omitted for clarity.

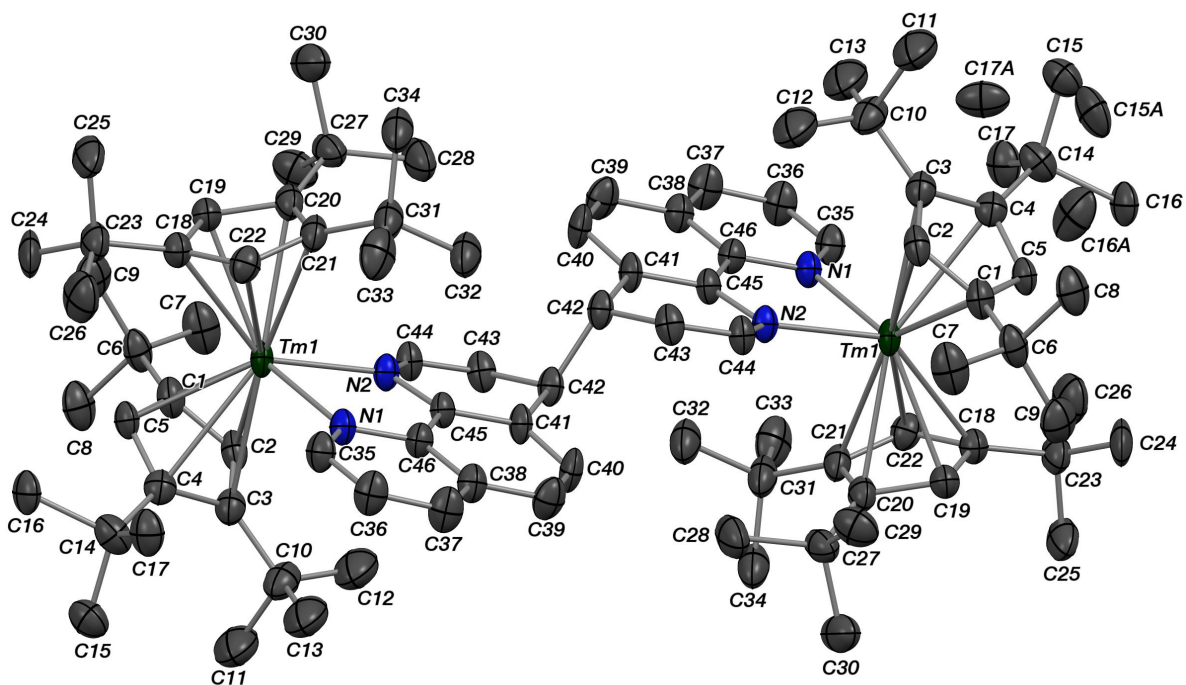


Table S2. Bond lengths (Å) and angles (deg) of **1**.

C3—C4	1.405 (8)	C4—Sm1	2.736 (5)
C3—C2	1.413 (8)	C28—C29	1.493 (8)
C3—C8	1.517 (8)	C28—C27	1.507 (8)
C3—Sm1	2.713 (5)	C28—C28 ⁱ	1.614 (11)
C12—C13	1.395 (9)	C1—C5	1.410 (9)
C12—C11	1.414 (8)	C1—C6	1.515 (8)
C12—C17	1.508 (9)	C1—Sm1	2.686 (5)
C12—Sm1	2.679 (5)	C5—Sm1	2.733 (5)
C10—C5	1.499 (9)	Sm1—N2	2.376 (4)
C14—C13	1.420 (10)	Sm1—N1	2.482 (4)
C14—C15	1.433 (9)	N2—C31	1.378 (7)
C14—C19	1.524 (9)	N2—C30	1.395 (6)
C14—Sm1	2.752 (6)	N1—C21	1.319 (7)
C2—C1	1.397 (9)	N1—C32	1.374 (7)
C2—C7	1.531 (9)	C27—C31	1.388 (7)
C2—Sm1	2.688 (6)	C27—C26	1.421 (8)
C11—C15	1.414 (8)	C32—C24	1.427 (7)
C11—C16	1.497 (8)	C32—C31	1.432 (7)
C11—Sm1	2.697 (5)	C30—C29	1.346 (7)
C13—C18	1.505 (9)	C22—C23	1.366 (10)
C13—Sm1	2.727 (6)	C22—C21	1.395 (8)
C15—C20	1.500 (9)	C26—C25	1.364 (10)
C15—Sm1	2.731 (5)	C24—C23	1.406 (9)
C4—C5	1.447 (8)	C24—C25	1.406 (9)
C4—C9	1.502 (8)		
C4—C3—C2	108.8 (5)	C2—Sm1—C11	143.71 (18)
C4—C3—C8	124.2 (6)	N2—Sm1—C3	134.90 (16)
C2—C3—C8	126.6 (6)	N1—Sm1—C3	117.94 (16)
C4—C3—Sm1	76.0 (3)	C12—Sm1—C3	119.55 (19)
C2—C3—Sm1	73.8 (3)	C1—Sm1—C3	49.78 (17)
C8—C3—Sm1	122.4 (4)	C2—Sm1—C3	30.32 (18)
C13—C12—C11	108.9 (5)	C11—Sm1—C3	139.11 (17)
C13—C12—C17	124.1 (7)	N2—Sm1—C13	116.54 (18)
C11—C12—C17	127.0 (7)	N1—Sm1—C13	132.98 (16)
C13—C12—Sm1	77.0 (3)	C12—Sm1—C13	29.89 (19)
C11—C12—Sm1	75.5 (3)	C1—Sm1—C13	124.81 (19)
C17—C12—Sm1	116.1 (4)	C2—Sm1—C13	96.16 (18)

C13—C14—C15	107.2 (5)	C11—Sm1—C13	49.82 (17)
C13—C14—C19	127.9 (7)	C3—Sm1—C13	91.96 (18)
C15—C14—C19	124.3 (7)	N2—Sm1—C15	108.31 (17)
C13—C14—Sm1	74.0 (3)	N1—Sm1—C15	83.55 (16)
C15—C14—Sm1	74.0 (3)	C12—Sm1—C15	49.95 (17)
C19—C14—Sm1	124.8 (4)	C1—Sm1—C15	166.48 (18)
C1—C2—C3	107.9 (5)	C2—Sm1—C15	138.82 (19)
C1—C2—C7	124.7 (6)	C11—Sm1—C15	30.20 (18)
C3—C2—C7	127.3 (6)	C3—Sm1—C15	116.73 (18)
C1—C2—Sm1	74.9 (3)	C13—Sm1—C15	49.76 (17)
C3—C2—Sm1	75.8 (3)	N2—Sm1—C5	93.82 (16)
C7—C2—Sm1	117.7 (4)	N1—Sm1—C5	78.49 (17)
C15—C11—C12	107.7 (5)	C12—Sm1—C5	162.98 (19)
C15—C11—C16	124.5 (6)	C1—Sm1—C5	30.15 (19)
C12—C11—C16	127.7 (6)	C2—Sm1—C5	49.91 (19)
C15—C11—Sm1	76.2 (3)	C11—Sm1—C5	166.34 (18)
C12—C11—Sm1	74.0 (3)	C3—Sm1—C5	49.84 (17)
C16—C11—Sm1	117.9 (4)	C13—Sm1—C5	141.60 (18)
C12—C13—C14	108.4 (5)	C15—Sm1—C5	143.74 (18)
C12—C13—C18	124.6 (8)	N2—Sm1—C4	124.22 (16)
C14—C13—C18	126.7 (8)	N1—Sm1—C4	88.13 (16)
C12—C13—Sm1	73.1 (3)	C12—Sm1—C4	146.17 (19)
C14—C13—Sm1	75.9 (3)	C1—Sm1—C4	50.10 (17)
C18—C13—Sm1	121.5 (4)	C2—Sm1—C4	49.97 (18)
C11—C15—C14	107.8 (5)	C11—Sm1—C4	148.70 (17)
C11—C15—C20	125.9 (6)	C3—Sm1—C4	29.88 (17)
C14—C15—C20	125.8 (6)	C13—Sm1—C4	116.37 (18)
C11—C15—Sm1	73.6 (3)	C15—Sm1—C4	118.52 (17)
C14—C15—Sm1	75.7 (3)	C5—Sm1—C4	30.68 (17)
C20—C15—Sm1	122.8 (4)	N2—Sm1—C14	132.14 (16)
C3—C4—C5	107.1 (5)	N1—Sm1—C14	109.46 (18)
C3—C4—C9	126.6 (5)	C12—Sm1—C14	49.70 (19)
C5—C4—C9	125.8 (6)	C1—Sm1—C14	137.92 (18)
C3—C4—Sm1	74.1 (3)	C2—Sm1—C14	108.58 (19)
C5—C4—Sm1	74.5 (3)	C11—Sm1—C14	49.93 (17)
C9—C4—Sm1	122.9 (4)	C3—Sm1—C14	90.12 (17)
C29—C28—C27	108.7 (4)	C13—Sm1—C14	30.0 (2)
C29—C28—C28 ⁱ	111.3 (6)	C15—Sm1—C14	30.29 (18)
C27—C28—C28 ⁱ	110.9 (6)	C5—Sm1—C14	133.59 (18)
C2—C1—C5	109.1 (5)	C4—Sm1—C14	102.90 (17)

C2—C1—C6	125.4 (6)	C31—N2—C30	114.1 (4)
C5—C1—C6	125.1 (6)	C31—N2—Sm1	119.8 (3)
C2—C1—Sm1	75.0 (3)	C30—N2—Sm1	125.4 (3)
C5—C1—Sm1	76.8 (3)	C21—N1—C32	118.5 (5)
C6—C1—Sm1	120.2 (4)	C21—N1—Sm1	124.9 (4)
C1—C5—C4	107.0 (5)	C32—N1—Sm1	115.8 (3)
C1—C5—C10	126.4 (6)	C31—C27—C26	119.4 (5)
C4—C5—C10	126.6 (6)	C31—C27—C28	118.6 (5)
C1—C5—Sm1	73.1 (3)	C26—C27—C28	121.8 (5)
C4—C5—Sm1	74.8 (3)	N1—C32—C24	121.1 (5)
C10—C5—Sm1	119.8 (4)	N1—C32—C31	117.9 (4)
N2—Sm1—N1	68.06 (14)	C24—C32—C31	121.0 (5)
N2—Sm1—C12	87.51 (18)	C29—C30—N2	125.2 (5)
N1—Sm1—C12	117.48 (17)	C23—C22—C21	117.8 (6)
N2—Sm1—C1	85.21 (16)	N1—C21—C22	124.4 (6)
N1—Sm1—C1	101.91 (18)	C25—C26—C27	122.9 (5)
C12—Sm1—C1	133.55 (19)	C23—C24—C25	123.9 (5)
N2—Sm1—C2	107.99 (17)	C23—C24—C32	117.1 (5)
N1—Sm1—C2	128.32 (17)	C25—C24—C32	119.0 (5)
C12—Sm1—C2	113.65 (19)	N2—C31—C27	124.3 (5)
C1—Sm1—C2	30.14 (19)	N2—C31—C32	117.6 (4)
N2—Sm1—C11	82.52 (16)	C27—C31—C32	118.0 (5)
N1—Sm1—C11	87.95 (15)	C30—C29—C28	120.1 (5)
C12—Sm1—C11	30.51 (18)	C26—C25—C24	119.2 (5)
C1—Sm1—C11	160.11 (18)	C22—C23—C24	121.0 (5)

Table S3. Bond lengths (Å) and angles (deg) of 3.

Sm(1)–N(2)	2.385(4)	Sm(1)–N(1)	2.517(4)
Sm(1)–C(19)	2.731(5)	Sm(1)–C(2)	2.773(5)
Sm(1)–C(20)	2.784(5)	Sm(1)–C(5)	2.786(5)
Sm(1)–C(1)	2.794(5)	Sm(1)–C(22)	2.812(5)
Sm(1)–C(18)	2.812(5)	Sm(1)–C(3)	2.852(5)
Sm(1)–C(4)	2.863(5)	Sm(1)–C(21)	2.863(5)
N(1)–C(35)	1.334(6)	N(1)–C(46)	1.370(6)
N(2)–C(45)	1.386(6)	N(2)–C(44)	1.397(6)
C(1)–C(2)	1.409(7)	C(1)–C(5)	1.412(7)
C(1)–C(6)	1.509(7)	C(2)–C(3)	1.424(7)
C(2)–H(2)	0.9500	C(3)–C(4)	1.448(7)
C(3)–C(10)	1.536(7)	C(4)–C(5)	1.427(7)
C(4)–C(14)	1.549(7)	C(5)–H(5)	0.9500
C(6)–C(8)	1.525(8)	C(6)–C(7)	1.537(7)
C(6)–C(9)	1.542(8)	C(7)–H(7A)	0.9800
C(7)–H(7B)	0.9800	C(7)–H(7C)	0.9800
C(8)–H(8A)	0.9800	C(8)–H(8B)	0.9800
C(8)–H(8C)	0.9800	C(9)–H(9A)	0.9800
C(9)–H(9B)	0.9800	C(9)–H(9C)	0.9800
C(10)–C(12)	1.525(8)	C(10)–C(13)	1.530(8)
C(10)–C(11)	1.535(7)	C(11)–H(11A)	0.9800
C(11)–H(11B)	0.9800	C(11)–H(11C)	0.9800
C(12)–H(12A)	0.9800	C(12)–H(12B)	0.9800
C(12)–H(12C)	0.9800	C(13)–H(13A)	0.9800
C(13)–H(13B)	0.9800	C(13)–H(13C)	0.9800
C(14)–C(17)	1.528(8)	C(14)–C(15)	1.545(8)
C(14)–C(16)	1.553(8)	C(15)–H(15A)	0.9800
C(15)–H(15B)	0.9800	C(15)–H(15C)	0.9800
C(16)–H(16A)	0.9800	C(16)–H(16B)	0.9800
C(16)–H(16C)	0.9800	C(17)–H(17A)	0.9800
C(17)–H(17B)	0.9800	C(17)–H(17C)	0.9800
C(18)–C(19)	1.407(7)	C(18)–C(22)	1.409(7)
C(18)–C(23)	1.530(7)	C(19)–C(20)	1.424(7)
C(19)–H(19)	0.9500	C(20)–C(21)	1.431(8)
C(20)–C(27)	1.547(8)	C(21)–C(22)	1.413(8)
C(21)–C(31)	1.557(8)	C(22)–H(22)	0.9500
C(23)–C(24)	1.51(1)	C(23)–C(26)	1.544(8)
C(23)–C(25)	1.546(8)	C(24)–H(24A)	0.9800
C(24)–H(24B)	0.9800	C(24)–H(24C)	0.9800
C(25)–H(25A)	0.9800	C(25)–H(25B)	0.9800
C(25)–H(25C)	0.9800	C(26)–H(26A)	0.9800
C(26)–H(26B)	0.9800	C(26)–H(26C)	0.9800
C(27)–C(30)	1.540(8)	C(27)–C(29)	1.54(1)
C(27)–C(28)	1.543(8)	C(28)–H(28A)	0.9800
C(28)–H(28B)	0.9800	C(28)–H(28C)	0.9800
C(29)–H(29A)	0.9800	C(29)–H(29B)	0.9800
C(29)–H(29C)	0.9800	C(30)–H(30A)	0.9800
C(30)–H(30B)	0.9800	C(30)–H(30C)	0.9800
C(31)–C(32)	1.531(8)	C(31)–C(33)	1.54(1)
C(31)–C(34)	1.54(1)	C(32)–H(32A)	0.9800
C(32)–H(32B)	0.9800	C(32)–H(32C)	0.9800
C(33)–H(33A)	0.9800	C(33)–H(33B)	0.9800
C(33)–H(33C)	0.9800	C(34)–H(34A)	0.9800
C(34)–H(34B)	0.9800	C(34)–H(34C)	0.9800
C(35)–C(36)	1.400(8)	C(35)–H(35)	0.9500
C(36)–C(37)	1.367(8)	C(36)–H(36)	0.9500
C(37)–C(38)	1.410(7)	C(37)–H(37)	0.9500
C(38)–C(39)	1.406(7)	C(38)–C(46)	1.432(7)
C(39)–C(40)	1.375(8)	C(39)–H(39)	0.9500
C(40)–C(41)	1.418(7)	C(40)–H(40)	0.9500
C(41)–C(45)	1.402(6)	C(41)–C(42)	1.507(7)
C(42)–C(43)	1.505(7)	C(42)–C(42)#2	1.57(1)
C(42)–H(42)	1.0000	C(43)–C(44)	1.320(7)
C(43)–H(43)	0.9500	C(44)–H(44)	0.9500
C(45)–C(46)	1.427(6)		

N (2) -Sm (1) -N (1)	67.5 (1)	N (2) -Sm (1) -C (19)	117.6 (1)
N (1) -Sm (1) -C (19)	125.2 (1)	N (2) -Sm (1) -C (2)	79.4 (1)
N (1) -Sm (1) -C (2)	111.5 (1)	C (19) -Sm (1) -C (2)	123.2 (2)
N (2) -Sm (1) -C (20)	90.3 (2)	N (1) -Sm (1) -C (20)	105.3 (2)
C (19) -Sm (1) -C (20)	29.9 (2)	C (2) -Sm (1) -C (20)	133.9 (2)
N (2) -Sm (1) -C (5)	126.9 (1)	N (1) -Sm (1) -C (5)	125.9 (1)
C (19) -Sm (1) -C (5)	95.5 (2)	C (2) -Sm (1) -C (5)	47.5 (1)
C (20) -Sm (1) -C (5)	123.9 (2)	N (2) -Sm (1) -C (1)	102.5 (1)
N (1) -Sm (1) -C (1)	137.9 (1)	C (19) -Sm (1) -C (1)	96.2 (2)
C (2) -Sm (1) -C (1)	29.3 (2)	C (20) -Sm (1) -C (1)	115.8 (2)
C (5) -Sm (1) -C (1)	29.3 (1)	N (2) -Sm (1) -C (22)	117.1 (1)
N (1) -Sm (1) -C (22)	80.0 (1)	C (19) -Sm (1) -C (22)	47.7 (2)
C (2) -Sm (1) -C (22)	163.1 (2)	C (20) -Sm (1) -C (22)	48.0 (2)
C (5) -Sm (1) -C (22)	115.8 (2)	C (1) -Sm (1) -C (22)	135.1 (2)
N (2) -Sm (1) -C (18)	137.5 (1)	N (1) -Sm (1) -C (18)	107.3 (1)
C (19) -Sm (1) -C (18)	29.4 (2)	C (2) -Sm (1) -C (18)	135.2 (2)
C (20) -Sm (1) -C (18)	49.0 (2)	C (5) -Sm (1) -C (18)	91.3 (2)
C (1) -Sm (1) -C (18)	106.2 (2)	C (22) -Sm (1) -C (18)	29.0 (2)
N (2) -Sm (1) -C (3)	86.7 (1)	N (1) -Sm (1) -C (3)	88.8 (1)
C (19) -Sm (1) -C (3)	143.0 (2)	C (2) -Sm (1) -C (3)	29.3 (2)
C (20) -Sm (1) -C (3)	163.1 (2)	C (5) -Sm (1) -C (3)	48.4 (2)
C (1) -Sm (1) -C (3)	49.1 (2)	C (22) -Sm (1) -C (3)	146.4 (2)
C (18) -Sm (1) -C (3)	135.8 (2)	N (2) -Sm (1) -C (4)	115.9 (1)
N (1) -Sm (1) -C (4)	97.1 (1)	C (19) -Sm (1) -C (4)	120.9 (2)
C (2) -Sm (1) -C (4)	47.8 (1)	C (20) -Sm (1) -C (4)	150.8 (2)
C (5) -Sm (1) -C (4)	29.2 (2)	C (1) -Sm (1) -C (4)	48.7 (1)
C (22) -Sm (1) -C (4)	120.6 (2)	C (18) -Sm (1) -C (4)	106.7 (1)
C (3) -Sm (1) -C (4)	29.4 (1)	N (2) -Sm (1) -C (21)	90.8 (1)
N (1) -Sm (1) -C (21)	78.5 (2)	C (19) -Sm (1) -C (21)	48.3 (2)
C (2) -Sm (1) -C (21)	161.4 (2)	C (20) -Sm (1) -C (21)	29.3 (2)
C (5) -Sm (1) -C (21)	139.4 (2)	C (1) -Sm (1) -C (21)	143.6 (2)
C (22) -Sm (1) -C (21)	28.8 (2)	C (18) -Sm (1) -C (21)	48.3 (2)
C (3) -Sm (1) -C (21)	167.1 (2)	C (4) -Sm (1) -C (21)	149.3 (2)
C (35) -N (1) -C (46)	118.4 (4)	C (35) -N (1) -Sm (1)	125.9 (3)
C (46) -N (1) -Sm (1)	115.7 (3)	C (45) -N (2) -C (44)	113.4 (4)
C (45) -N (2) -Sm (1)	120.4 (3)	C (44) -N (2) -Sm (1)	125.0 (3)
C (2) -C (1) -C (5)	105.2 (5)	C (2) -C (1) -C (6)	126.8 (4)
C (5) -C (1) -C (6)	124.9 (5)	C (2) -C (1) -Sm (1)	74.5 (3)
C (5) -C (1) -Sm (1)	75.0 (3)	C (6) -C (1) -Sm (1)	130.8 (3)
C (1) -C (2) -C (3)	111.8 (4)	C (1) -C (2) -Sm (1)	76.1 (3)
C (3) -C (2) -Sm (1)	78.4 (3)	C (1) -C (2) -H (2)	124.1
C (3) -C (2) -H (2)	124.1	Sm (1) -C (2) -H (2)	113.1
C (2) -C (3) -C (4)	105.4 (4)	C (2) -C (3) -C (10)	120.0 (4)
C (4) -C (3) -C (10)	132.8 (5)	C (2) -C (3) -Sm (1)	72.3 (3)
C (4) -C (3) -Sm (1)	75.7 (3)	C (10) -C (3) -Sm (1)	127.9 (3)
C (5) -C (4) -C (3)	106.9 (4)	C (5) -C (4) -C (14)	120.4 (4)
C (3) -C (4) -C (14)	132.3 (5)	C (5) -C (4) -Sm (1)	72.4 (3)
C (3) -C (4) -Sm (1)	74.9 (3)	C (14) -C (4) -Sm (1)	123.3 (3)
C (1) -C (5) -C (4)	110.6 (4)	C (1) -C (5) -Sm (1)	75.6 (3)
C (4) -C (5) -Sm (1)	78.4 (3)	C (1) -C (5) -H (5)	124.7
C (4) -C (5) -H (5)	124.7	Sm (1) -C (5) -H (5)	113.2
C (1) -C (6) -C (8)	107.2 (4)	C (1) -C (6) -C (7)	112.1 (5)
C (8) -C (6) -C (7)	108.3 (4)	C (1) -C (6) -C (9)	113.2 (4)
C (8) -C (6) -C (9)	107.6 (5)	C (7) -C (6) -C (9)	108.2 (5)
C (6) -C (7) -H (7A)	109.5	C (6) -C (7) -H (7B)	109.5
H (7A) -C (7) -H (7B)	109.5	C (6) -C (7) -H (7C)	109.5
H (7A) -C (7) -H (7C)	109.5	H (7B) -C (7) -H (7C)	109.5
C (6) -C (8) -H (8A)	109.5	C (6) -C (8) -H (8B)	109.5
H (8A) -C (8) -H (8B)	109.5	C (6) -C (8) -H (8C)	109.5
H (8A) -C (8) -H (8C)	109.5	H (8B) -C (8) -H (8C)	109.5
C (6) -C (9) -H (9A)	109.5	C (6) -C (9) -H (9B)	109.5
H (9A) -C (9) -H (9B)	109.5	C (6) -C (9) -H (9C)	109.5
H (9A) -C (9) -H (9C)	109.5	H (9B) -C (9) -H (9C)	109.5
C (12) -C (10) -C (13)	107.0 (5)	C (12) -C (10) -C (11)	106.1 (5)
C (13) -C (10) -C (11)	108.9 (5)	C (12) -C (10) -C (3)	111.4 (5)
C (13) -C (10) -C (3)	115.5 (4)	C (11) -C (10) -C (3)	107.6 (4)
C (10) -C (11) -H (11A)	109.5	C (10) -C (11) -H (11B)	109.5

H (11A) -C (11) -H (11B)	109.5	C (10) -C (11) -H (11C)	109.5
H (11A) -C (11) -H (11C)	109.5	H (11B) -C (11) -H (11C)	109.5
C (10) -C (12) -H (12A)	109.5	C (10) -C (12) -H (12B)	109.5
H (12A) -C (12) -H (12B)	109.5	C (10) -C (12) -H (12C)	109.5
H (12A) -C (12) -H (12C)	109.5	H (12B) -C (12) -H (12C)	109.5
C (10) -C (13) -H (13A)	109.5	C (10) -C (13) -H (13B)	109.5
H (13A) -C (13) -H (13B)	109.5	C (10) -C (13) -H (13C)	109.5
H (13A) -C (13) -H (13C)	109.5	H (13B) -C (13) -H (13C)	109.5
C (17) -C (14) -C (15)	110.8 (5)	C (17) -C (14) -C (4)	111.7 (5)
C (15) -C (14) -C (4)	112.9 (5)	C (17) -C (14) -C (16)	105.7 (5)
C (15) -C (14) -C (16)	105.2 (5)	C (4) -C (14) -C (16)	110.0 (4)
C (14) -C (15) -H (15A)	109.5	C (14) -C (15) -H (15B)	109.5
H (15A) -C (15) -H (15B)	109.5	C (14) -C (15) -H (15C)	109.5
H (15A) -C (15) -H (15C)	109.5	H (15B) -C (15) -H (15C)	109.5
C (14) -C (16) -H (16A)	109.5	C (14) -C (16) -H (16B)	109.5
H (16A) -C (16) -H (16B)	109.5	C (14) -C (16) -H (16C)	109.5
H (16A) -C (16) -H (16C)	109.5	H (16B) -C (16) -H (16C)	109.5
C (14) -C (17) -H (17A)	109.5	C (14) -C (17) -H (17B)	109.5
H (17A) -C (17) -H (17B)	109.5	C (14) -C (17) -H (17C)	109.5
H (17A) -C (17) -H (17C)	109.5	H (17B) -C (17) -H (17C)	109.5
C (19) -C (18) -C (22)	105.7 (4)	C (19) -C (18) -C (23)	125.9 (5)
C (22) -C (18) -C (23)	124.9 (5)	C (19) -C (18) -Sm (1)	72.1 (3)
C (22) -C (18) -Sm (1)	75.5 (3)	C (23) -C (18) -Sm (1)	133.9 (3)
C (18) -C (19) -C (20)	110.0 (5)	C (18) -C (19) -Sm (1)	78.5 (3)
C (20) -C (19) -Sm (1)	77.1 (3)	C (18) -C (19) -H (19)	125.0
C (20) -C (19) -H (19)	125.0	Sm (1) -C (19) -H (19)	111.6
C (19) -C (20) -C (21)	106.9 (5)	C (19) -C (20) -C (27)	118.8 (5)
C (21) -C (20) -C (27)	133.5 (5)	C (19) -C (20) -Sm (1)	73.0 (3)
C (21) -C (20) -Sm (1)	78.4 (3)	C (27) -C (20) -Sm (1)	121.2 (3)
C (22) -C (21) -C (20)	106.4 (5)	C (22) -C (21) -C (31)	119.1 (5)
C (20) -C (21) -C (31)	132.4 (5)	C (22) -C (21) -Sm (1)	73.6 (3)
C (20) -C (21) -Sm (1)	72.3 (3)	C (31) -C (21) -Sm (1)	132.0 (4)
C (18) -C (22) -C (21)	110.8 (5)	C (18) -C (22) -Sm (1)	75.5 (3)
C (21) -C (22) -Sm (1)	77.6 (3)	C (18) -C (22) -H (22)	124.6
C (21) -C (22) -H (22)	124.6	Sm (1) -C (22) -H (22)	114.2
C (24) -C (23) -C (18)	113.6 (5)	C (24) -C (23) -C (26)	110.3 (5)
C (18) -C (23) -C (26)	111.1 (5)	C (24) -C (23) -C (25)	108.2 (5)
C (18) -C (23) -C (25)	105.8 (4)	C (26) -C (23) -C (25)	107.6 (5)
C (23) -C (24) -H (24A)	109.5	C (23) -C (24) -H (24B)	109.5
H (24A) -C (24) -H (24B)	109.5	C (23) -C (24) -H (24C)	109.5
H (24A) -C (24) -H (24C)	109.5	H (24B) -C (24) -H (24C)	109.5
C (23) -C (25) -H (25A)	109.5	C (23) -C (25) -H (25B)	109.5
H (25A) -C (25) -H (25B)	109.5	C (23) -C (25) -H (25C)	109.5
H (25A) -C (25) -H (25C)	109.5	H (25B) -C (25) -H (25C)	109.5
C (23) -C (26) -H (26A)	109.5	C (23) -C (26) -H (26B)	109.5
H (26A) -C (26) -H (26B)	109.5	C (23) -C (26) -H (26C)	109.5
H (26A) -C (26) -H (26C)	109.5	H (26B) -C (26) -H (26C)	109.5
C (30) -C (27) -C (29)	107.3 (5)	C (30) -C (27) -C (28)	109.5 (5)
C (29) -C (27) -C (28)	106.4 (5)	C (30) -C (27) -C (20)	108.8 (5)
C (29) -C (27) -C (20)	109.0 (5)	C (28) -C (27) -C (20)	115.5 (5)
C (27) -C (28) -H (28A)	109.5	C (27) -C (28) -H (28B)	109.5
H (28A) -C (28) -H (28B)	109.5	C (27) -C (28) -H (28C)	109.5
H (28A) -C (28) -H (28C)	109.5	H (28B) -C (28) -H (28C)	109.5
C (27) -C (29) -H (29A)	109.5	C (27) -C (29) -H (29B)	109.5
H (29A) -C (29) -H (29B)	109.5	C (27) -C (29) -H (29C)	109.5
H (29A) -C (29) -H (29C)	109.5	H (29B) -C (29) -H (29C)	109.5
C (27) -C (30) -H (30A)	109.5	C (27) -C (30) -H (30B)	109.5
H (30A) -C (30) -H (30B)	109.5	C (27) -C (30) -H (30C)	109.5
H (30A) -C (30) -H (30C)	109.5	H (30B) -C (30) -H (30C)	109.5
C (32) -C (31) -C (33)	105.9 (5)	C (32) -C (31) -C (34)	110.1 (5)
C (33) -C (31) -C (34)	106.3 (5)	C (32) -C (31) -C (21)	116.4 (5)
C (33) -C (31) -C (21)	110.6 (5)	C (34) -C (31) -C (21)	107.1 (5)
C (31) -C (32) -H (32A)	109.5	C (31) -C (32) -H (32B)	109.5
H (32A) -C (32) -H (32B)	109.5	C (31) -C (32) -H (32C)	109.5
H (32A) -C (32) -H (32C)	109.5	H (32B) -C (32) -H (32C)	109.5
C (31) -C (33) -H (33A)	109.5	C (31) -C (33) -H (33B)	109.5
H (33A) -C (33) -H (33B)	109.5	C (31) -C (33) -H (33C)	109.5
H (33A) -C (33) -H (33C)	109.5	H (33B) -C (33) -H (33C)	109.5

C (31) -C (34) -H (34A)	109.5	C (31) -C (34) -H (34B)	109.5
H (34A) -C (34) -H (34B)	109.5	C (31) -C (34) -H (34C)	109.5
H (34A) -C (34) -H (34C)	109.5	H (34B) -C (34) -H (34C)	109.5
N (1) -C (35) -C (36)	123.8 (5)	N (1) -C (35) -H (35)	118.1
C (36) -C (35) -H (35)	118.1	C (37) -C (36) -C (35)	118.9 (5)
C (37) -C (36) -H (36)	120.6	C (35) -C (36) -H (36)	120.6
C (36) -C (37) -C (38)	119.7 (5)	C (36) -C (37) -H (37)	120.1
C (38) -C (37) -H (37)	120.1	C (39) -C (38) -C (37)	122.1 (5)
C (39) -C (38) -C (46)	119.7 (5)	C (37) -C (38) -C (46)	118.2 (5)
C (40) -C (39) -C (38)	118.7 (5)	C (40) -C (39) -H (39)	120.6
C (38) -C (39) -H (39)	120.6	C (39) -C (40) -C (41)	123.2 (5)
C (39) -C (40) -H (40)	118.4	C (41) -C (40) -H (40)	118.4
C (45) -C (41) -C (40)	118.8 (5)	C (45) -C (41) -C (42)	120.6 (4)
C (40) -C (41) -C (42)	120.5 (4)	C (43) -C (42) -C (41)	107.5 (4)
C (43) -C (42) -C (42) #2	112.7 (5)	C (41) -C (42) -C (42) #2	110.8 (5)
C (43) -C (42) -H (42)	108.6	C (41) -C (42) -H (42)	108.6
C (42) #2 -C (42) -H (42)	108.6	C (44) -C (43) -C (42)	121.4 (4)
C (44) -C (43) -H (43)	119.3	C (42) -C (43) -H (43)	119.3
C (43) -C (44) -N (2)	126.4 (5)	C (43) -C (44) -H (44)	116.8
N (2) -C (44) -H (44)	116.8	N (2) -C (45) -C (41)	123.5 (4)
N (2) -C (45) -C (46)	117.5 (4)	C (41) -C (45) -C (46)	118.9 (4)
N (1) -C (46) -C (45)	118.6 (4)	N (1) -C (46) -C (38)	121.0 (4)
C (45) -C (46) -C (38)	120.3 (4)		

Table S4. Bond lengths (Å) and angles (deg) of 5.

Sm(1)-N(1)	2.356(3)	Sm(1)-N(2)	2.498(3)
Sm(1)-C(17)	2.699(4)	Sm(1)-C(16)	2.707(4)
Sm(1)-C(4)	2.709(4)	Sm(1)-C(3)	2.726(4)
Sm(1)-C(5)	2.759(4)	Sm(1)-C(18)	2.769(4)
Sm(1)-C(14)	2.775(4)	Sm(1)-C(15)	2.782(4)
Sm(1)-C(1)	2.790(4)	Sm(1)-C(2)	2.821(4)
N(1)-C(31)	1.384(4)	N(1)-C(27)	1.394(5)
N(2)-C(36)	1.329(5)	N(2)-C(32)	1.365(5)
C(1)-C(2)	1.416(6)	C(1)-C(5)	1.419(5)
C(1)-H(1)	0.9500	C(2)-C(3)	1.427(6)
C(2)-C(6)	1.518(6)	C(3)-C(4)	1.409(5)
C(3)-H(3)	0.9500	C(4)-C(5)	1.411(5)
C(4)-H(4)	0.9500	C(5)-C(10)	1.528(5)
C(6)-C(8)	1.524(8)	C(6)-C(9)	1.533(8)
C(6)-C(7)	1.543(6)	C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800	C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800	C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800	C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800	C(9)-H(9C)	0.9800
C(10)-C(13A)	1.49(1)	C(10)-C(11)	1.509(8)
C(10)-C(13)	1.51(1)	C(10)-C(12A)	1.53(1)
C(10)-C(12)	1.57(1)	C(10)-C(11A)	1.61(1)
C(11)-H(11A)	0.9800	C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800	C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800	C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800	C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800	C(11A)-H(11D)	0.9800
C(11A)-H(11E)	0.9800	C(11A)-H(11F)	0.9800
C(12A)-H(12D)	0.9800	C(12A)-H(12E)	0.9800
C(12A)-H(12F)	0.9800	C(13A)-H(13D)	0.9800
C(13A)-H(13E)	0.9800	C(13A)-H(13F)	0.9800
C(14)-C(18)	1.409(5)	C(14)-C(15)	1.411(6)
C(14)-H(14)	0.9500	C(15)-C(16)	1.405(6)
C(15)-C(19)	1.534(6)	C(16)-C(17)	1.410(6)
C(16)-H(16)	0.9500	C(17)-C(18)	1.411(6)
C(17)-H(17)	0.9500	C(18)-C(23)	1.524(6)
C(19)-C(22)	1.526(7)	C(19)-C(20)	1.530(7)
C(19)-C(21)	1.534(6)	C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800	C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800	C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800	C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800	C(22)-H(22C)	0.9800
C(23)-C(25)	1.518(7)	C(23)-C(24)	1.530(6)
C(23)-C(26)	1.535(6)	C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800	C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800	C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800	C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800	C(26)-H(26C)	0.9800
C(27)-C(28)	1.332(5)	C(27)-H(27)	0.9500
C(28)-C(29)	1.497(6)	C(28)-H(28)	0.9500
C(29)-C(30)	1.504(5)	C(29)-C(29)#3	1.581(8)
C(29)-H(29)	1.0000	C(30)-C(31)	1.397(5)
C(30)-C(38)	1.406(6)	C(31)-C(32)	1.433(5)
C(32)-C(33)	1.415(5)	C(33)-C(37)	1.413(6)
C(33)-C(34)	1.415(6)	C(34)-C(35)	1.353(6)
C(34)-H(34)	0.9500	C(35)-C(36)	1.406(6)
C(35)-H(35)	0.9500	C(36)-H(36)	0.9500
C(37)-C(38)	1.365(6)	C(37)-H(37)	0.9500
C(38)-H(38)	0.9500		

N (1) -Sm (1) -N (2)	68.3 (1)	N (1) -Sm (1) -C (17)	99.5 (1)
N (2) -Sm (1) -C (17)	118.0 (1)	N (1) -Sm (1) -C (16)	129.5 (1)
N (2) -Sm (1) -C (16)	127.1 (1)	C (17) -Sm (1) -C (16)	30.3 (1)
N (1) -Sm (1) -C (4)	128.1 (1)	N (2) -Sm (1) -C (4)	132.2 (1)
C (17) -Sm (1) -C (4)	103.9 (1)	C (16) -Sm (1) -C (4)	80.4 (1)
N (1) -Sm (1) -C (3)	125.7 (1)	N (2) -Sm (1) -C (3)	102.2 (1)
C (17) -Sm (1) -C (3)	128.6 (1)	C (16) -Sm (1) -C (3)	99.8 (1)
C (4) -Sm (1) -C (3)	30.1 (1)	N (1) -Sm (1) -C (5)	99.1 (1)
N (2) -Sm (1) -C (5)	135.3 (1)	C (17) -Sm (1) -C (5)	106.2 (1)
C (16) -Sm (1) -C (5)	94.6 (1)	C (4) -Sm (1) -C (5)	29.9 (1)
C (3) -Sm (1) -C (5)	49.3 (1)	N (1) -Sm (1) -C (18)	90.5 (1)
N (2) -Sm (1) -C (18)	88.2 (1)	C (17) -Sm (1) -C (18)	29.9 (1)
C (16) -Sm (1) -C (18)	49.3 (1)	C (4) -Sm (1) -C (18)	129.6 (1)
C (3) -Sm (1) -C (18)	143.7 (1)	C (5) -Sm (1) -C (18)	136.0 (1)
N (1) -Sm (1) -C (14)	112.1 (1)	N (2) -Sm (1) -C (14)	78.8 (1)
C (17) -Sm (1) -C (14)	48.8 (1)	C (16) -Sm (1) -C (14)	48.5 (1)
C (4) -Sm (1) -C (14)	118.3 (1)	C (3) -Sm (1) -C (14)	118.2 (1)
C (5) -Sm (1) -C (14)	141.8 (1)	C (18) -Sm (1) -C (14)	29.4 (1)
N (1) -Sm (1) -C (15)	139.3 (1)	N (2) -Sm (1) -C (15)	100.8 (1)
C (17) -Sm (1) -C (15)	49.5 (1)	C (16) -Sm (1) -C (15)	29.6 (1)
C (4) -Sm (1) -C (15)	89.0 (1)	C (3) -Sm (1) -C (15)	94.6 (1)
C (5) -Sm (1) -C (15)	113.4 (1)	C (18) -Sm (1) -C (15)	49.2 (1)
C (14) -Sm (1) -C (15)	29.4 (1)	N (1) -Sm (1) -C (1)	81.8 (1)
N (2) -Sm (1) -C (1)	106.2 (1)	C (17) -Sm (1) -C (1)	132.9 (1)
C (16) -Sm (1) -C (1)	124.1 (1)	C (4) -Sm (1) -C (1)	48.7 (1)
C (3) -Sm (1) -C (1)	48.4 (1)	C (5) -Sm (1) -C (1)	29.6 (1)
C (18) -Sm (1) -C (1)	159.5 (1)	C (14) -Sm (1) -C (1)	166.1 (1)
C (15) -Sm (1) -C (1)	137.6 (1)	N (1) -Sm (1) -C (2)	96.1 (1)
N (2) -Sm (1) -C (2)	88.3 (1)	C (17) -Sm (1) -C (2)	152.9 (1)
C (16) -Sm (1) -C (2)	128.2 (1)	C (4) -Sm (1) -C (2)	49.4 (1)
C (3) -Sm (1) -C (2)	29.8 (1)	C (5) -Sm (1) -C (2)	49.3 (1)
C (18) -Sm (1) -C (2)	170.7 (1)	C (14) -Sm (1) -C (2)	141.3 (1)
C (15) -Sm (1) -C (2)	123.4 (1)	C (1) -Sm (1) -C (2)	29.2 (1)
C (31) -N (1) -C (27)	113.7 (3)	C (31) -N (1) -Sm (1)	117.6 (2)
C (27) -N (1) -Sm (1)	128.5 (2)	C (36) -N (2) -C (32)	118.5 (3)
C (36) -N (2) -Sm (1)	126.8 (3)	C (32) -N (2) -Sm (1)	114.3 (2)
C (2) -C (1) -C (5)	110.2 (3)	C (2) -C (1) -Sm (1)	76.6 (2)
C (5) -C (1) -Sm (1)	74.0 (2)	C (2) -C (1) -H (1)	124.9
C (5) -C (1) -H (1)	124.9	Sm (1) -C (1) -H (1)	116.4
C (1) -C (2) -C (3)	105.4 (3)	C (1) -C (2) -C (6)	127.0 (4)
C (3) -C (2) -C (6)	126.5 (4)	C (1) -C (2) -Sm (1)	74.2 (2)
C (3) -C (2) -Sm (1)	71.4 (2)	C (6) -C (2) -Sm (1)	128.4 (3)
C (4) -C (3) -C (2)	109.3 (3)	C (4) -C (3) -Sm (1)	74.3 (2)
C (2) -C (3) -Sm (1)	78.8 (2)	C (4) -C (3) -H (3)	125.3
C (2) -C (3) -H (3)	125.3	Sm (1) -C (3) -H (3)	113.7
C (3) -C (4) -C (5)	108.3 (3)	C (3) -C (4) -Sm (1)	75.6 (2)
C (5) -C (4) -Sm (1)	77.0 (2)	C (3) -C (4) -H (4)	125.8
C (5) -C (4) -H (4)	125.8	Sm (1) -C (4) -H (4)	113.8
C (4) -C (5) -C (1)	106.7 (3)	C (4) -C (5) -C (10)	127.0 (4)
C (1) -C (5) -C (10)	126.1 (4)	C (4) -C (5) -Sm (1)	73.1 (2)
C (1) -C (5) -Sm (1)	76.4 (2)	C (10) -C (5) -Sm (1)	120.6 (2)
C (2) -C (6) -C (8)	111.4 (4)	C (2) -C (6) -C (9)	112.0 (4)
C (8) -C (6) -C (9)	110.2 (5)	C (2) -C (6) -C (7)	108.0 (4)
C (8) -C (6) -C (7)	107.8 (4)	C (9) -C (6) -C (7)	107.3 (5)
C (6) -C (7) -H (7A)	109.5	C (6) -C (7) -H (7B)	109.5
H (7A) -C (7) -H (7B)	109.5	C (6) -C (7) -H (7C)	109.5
H (7A) -C (7) -H (7C)	109.5	H (7B) -C (7) -H (7C)	109.5
C (6) -C (8) -H (8A)	109.5	C (6) -C (8) -H (8B)	109.5
H (8A) -C (8) -H (8B)	109.5	C (6) -C (8) -H (8C)	109.5
H (8A) -C (8) -H (8C)	109.5	H (8B) -C (8) -H (8C)	109.5
C (6) -C (9) -H (9A)	109.5	C (6) -C (9) -H (9B)	109.5
H (9A) -C (9) -H (9B)	109.5	C (6) -C (9) -H (9C)	109.5
H (9A) -C (9) -H (9C)	109.5	H (9B) -C (9) -H (9C)	109.5
C (11) -C (10) -C (13)	109.5 (6)	C (13A) -C (10) -C (5)	111.2 (6)
C (11) -C (10) -C (5)	111.6 (4)	C (13) -C (10) -C (5)	110.0 (5)
C (13A) -C (10) -C (12A)	114 (1)	C (5) -C (10) -C (12A)	110.5 (6)

C(11)-C(10)-C(12)	106.1(6)	C(13)-C(10)-C(12)	110.0(7)
C(5)-C(10)-C(12)	109.5(4)	C(13A)-C(10)-C(11A)	106(1)
C(5)-C(10)-C(11A)	107.8(6)	C(12A)-C(10)-C(11A)	107(1)
C(10)-C(11)-H(11A)	109.5	C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5	C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5	H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5	C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5	C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5	H(12B)-C(12)-H(12C)	109.5
C(10)-C(13)-H(13A)	109.5	C(10)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5	C(10)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5	H(13B)-C(13)-H(13C)	109.5
C(10)-C(11A)-H(11D)	109.5	C(10)-C(11A)-H(11E)	109.5
H(11D)-C(11A)-H(11E)	109.5	C(10)-C(11A)-H(11F)	109.5
H(11D)-C(11A)-H(11F)	109.5	H(11E)-C(11A)-H(11F)	109.5
C(10)-C(12A)-H(12D)	109.5	C(10)-C(12A)-H(12E)	109.5
H(12D)-C(12A)-H(12E)	109.5	C(10)-C(12A)-H(12F)	109.5
H(12D)-C(12A)-H(12F)	109.5	H(12E)-C(12A)-H(12F)	109.5
C(10)-C(13A)-H(13D)	109.5	C(10)-C(13A)-H(13E)	109.5
H(13D)-C(13A)-H(13E)	109.5	C(10)-C(13A)-H(13F)	109.5
H(13D)-C(13A)-H(13F)	109.5	H(13E)-C(13A)-H(13F)	109.5
C(18)-C(14)-C(15)	109.9(4)	C(18)-C(14)-Sm(1)	75.1(2)
C(15)-C(14)-Sm(1)	75.5(2)	C(18)-C(14)-H(14)	125.1
C(15)-C(14)-H(14)	125.1	Sm(1)-C(14)-H(14)	116.2
C(16)-C(15)-C(14)	106.2(4)	C(16)-C(15)-C(19)	127.9(4)
C(14)-C(15)-C(19)	125.0(4)	C(16)-C(15)-Sm(1)	72.2(2)
C(14)-C(15)-Sm(1)	75.0(2)	C(19)-C(15)-Sm(1)	126.5(3)
C(15)-C(16)-C(17)	109.2(4)	C(15)-C(16)-Sm(1)	78.1(2)
C(17)-C(16)-Sm(1)	74.5(2)	C(15)-C(16)-H(16)	125.4
C(17)-C(16)-H(16)	125.4	Sm(1)-C(16)-H(16)	114.0
C(16)-C(17)-C(18)	108.0(3)	C(16)-C(17)-Sm(1)	75.2(2)
C(18)-C(17)-Sm(1)	77.8(2)	C(16)-C(17)-H(17)	126.0
C(18)-C(17)-H(17)	126.0	Sm(1)-C(17)-H(17)	113.4
C(14)-C(18)-C(17)	106.7(4)	C(14)-C(18)-C(23)	124.9(4)
C(17)-C(18)-C(23)	127.2(4)	C(14)-C(18)-Sm(1)	75.5(2)
C(17)-C(18)-Sm(1)	72.3(2)	C(23)-C(18)-Sm(1)	127.2(3)
C(22)-C(19)-C(20)	109.2(4)	C(22)-C(19)-C(15)	112.1(4)
C(20)-C(19)-C(15)	111.0(4)	C(22)-C(19)-C(21)	108.5(4)
C(20)-C(19)-C(21)	108.3(4)	C(15)-C(19)-C(21)	107.7(4)
C(19)-C(20)-H(20A)	109.5	C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5	C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5	H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5	C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5	C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5	H(21B)-C(21)-H(21C)	109.5
C(19)-C(22)-H(22A)	109.5	C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5	C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5	H(22B)-C(22)-H(22C)	109.5
C(25)-C(23)-C(18)	112.1(4)	C(25)-C(23)-C(24)	108.7(4)
C(18)-C(23)-C(24)	111.9(4)	C(25)-C(23)-C(26)	108.8(4)
C(18)-C(23)-C(26)	107.1(4)	C(24)-C(23)-C(26)	108.1(4)
C(23)-C(24)-H(24A)	109.5	C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5	C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5	H(24B)-C(24)-H(24C)	109.5
C(23)-C(25)-H(25A)	109.5	C(23)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5	C(23)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5	H(25B)-C(25)-H(25C)	109.5
C(23)-C(26)-H(26A)	109.5	C(23)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5	C(23)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5	H(26B)-C(26)-H(26C)	109.5
C(28)-C(27)-N(1)	125.5(4)	C(28)-C(27)-H(27)	117.2
N(1)-C(27)-H(27)	117.2	C(27)-C(28)-C(29)	119.9(4)
C(27)-C(28)-H(28)	120.1	C(29)-C(28)-H(28)	120.1
C(28)-C(29)-C(30)	108.3(3)	C(28)-C(29)-C(29)#3	111.3(4)
C(30)-C(29)-C(29)#3	110.6(4)	C(28)-C(29)-H(29)	108.8
C(30)-C(29)-H(29)	108.8	C(29)#3-C(29)-H(29)	108.8
C(31)-C(30)-C(38)	119.6(4)	C(31)-C(30)-C(29)	118.5(3)
C(38)-C(30)-C(29)	121.8(3)	N(1)-C(31)-C(30)	123.7(3)

N(1)-C(31)-C(32)	118.0(3)	C(30)-C(31)-C(32)	118.2(3)
N(2)-C(32)-C(33)	121.4(3)	N(2)-C(32)-C(31)	118.0(3)
C(33)-C(32)-C(31)	120.6(3)	C(37)-C(33)-C(34)	122.8(4)
C(37)-C(33)-C(32)	119.3(4)	C(34)-C(33)-C(32)	117.9(4)
C(35)-C(34)-C(33)	120.0(4)	C(35)-C(34)-H(34)	120.0
C(33)-C(34)-H(34)	120.0	C(34)-C(35)-C(36)	118.9(4)
C(34)-C(35)-H(35)	120.6	C(36)-C(35)-H(35)	120.6
N(2)-C(36)-C(35)	123.3(4)	N(2)-C(36)-H(36)	118.4
C(35)-C(36)-H(36)	118.4	C(38)-C(37)-C(33)	119.2(4)
C(38)-C(37)-H(37)	120.4	C(33)-C(37)-H(37)	120.4
C(37)-C(38)-C(30)	122.7(4)	C(37)-C(38)-H(38)	118.6
C(30)-C(38)-H(38)	118.6		

Table S5. Bond lengths (Å) and angles (deg) of 7.

Tm(1)-N(2)	2.288(4)	Tm(1)-N(1)	2.391(4)
Tm(1)-C(19)	2.625(5)	Tm(1)-C(1)	2.668(5)
Tm(1)-C(2)	2.673(5)	Tm(1)-C(5)	2.683(5)
Tm(1)-C(20)	2.709(6)	Tm(1)-C(22)	2.711(5)
Tm(1)-C(18)	2.717(5)	Tm(1)-C(21)	2.780(5)
Tm(1)-C(3)	2.787(6)	Tm(1)-C(4)	2.798(5)
N(1)-C(35)	1.332(7)	N(1)-C(46)	1.377(6)
N(2)-C(45)	1.384(6)	N(2)-C(44)	1.395(6)
C(1)-C(2)	1.402(8)	C(1)-C(5)	1.417(7)
C(1)-C(6)	1.527(8)	C(2)-C(3)	1.404(8)
C(2)-H(2)	0.9500	C(3)-C(4)	1.452(8)
C(3)-C(10)	1.534(8)	C(4)-C(5)	1.406(8)
C(4)-C(14)	1.553(8)	C(5)-H(5)	0.9500
C(6)-C(7)	1.516(8)	C(6)-C(9)	1.53(1)
C(6)-C(8)	1.551(8)	C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800	C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800	C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800	C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800	C(9)-H(9C)	0.9800
C(10)-C(12)	1.50(1)	C(10)-C(11)	1.53(1)
C(10)-C(13)	1.56(1)	C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800	C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800	C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800	C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800	C(13)-H(13C)	0.9800
C(14)-C(16A)	1.43(2)	C(14)-C(17)	1.50(1)
C(14)-C(15A)	1.51(2)	C(14)-C(15)	1.54(1)
C(14)-C(17A)	1.63(2)	C(14)-C(16)	1.64(1)
C(15)-H(15A)	0.9800	C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800	C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800	C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800	C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800	C(15A)-H(15D)	0.9800
C(15A)-H(15E)	0.9800	C(15A)-H(15F)	0.9800
C(16A)-H(16D)	0.9800	C(16A)-H(16E)	0.9800
C(16A)-H(16F)	0.9800	C(17A)-H(17D)	0.9800
C(17A)-H(17E)	0.9800	C(17A)-H(17F)	0.9800
C(18)-C(22)	1.413(7)	C(18)-C(19)	1.420(7)
C(18)-C(23)	1.519(7)	C(19)-C(20)	1.420(7)
C(19)-H(19)	0.9500	C(20)-C(21)	1.436(8)
C(20)-C(27)	1.535(8)	C(21)-C(22)	1.416(8)
C(21)-C(31)	1.551(8)	C(22)-H(22)	0.9500
C(23)-C(25)	1.53(1)	C(23)-C(24)	1.54(1)
C(23)-C(26)	1.54(1)	C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800	C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800	C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800	C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800	C(26)-H(26C)	0.9800
C(27)-C(28)	1.53(1)	C(27)-C(29)	1.54(1)
C(27)-C(30)	1.55(1)	C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800	C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800	C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800	C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800	C(30)-H(30C)	0.9800
C(31)-C(32)	1.53(1)	C(31)-C(34)	1.54(1)
C(31)-C(33)	1.55(1)	C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800	C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800	C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800	C(34)-H(34A)	0.9800

C (34) -H (34B)	0.9800	C (34) -H (34C)	0.9800
C (35) -C (36)	1.400 (8)	C (35) -H (35)	0.9500
C (36) -C (37)	1.360 (8)	C (36) -H (36)	0.9500
C (37) -C (38)	1.408 (8)	C (37) -H (37)	0.9500
C (38) -C (46)	1.410 (7)	C (38) -C (39)	1.413 (8)
C (39) -C (40)	1.361 (8)	C (39) -H (39)	0.9500
C (40) -C (41)	1.415 (7)	C (40) -H (40)	0.9500
C (41) -C (45)	1.410 (7)	C (41) -C (42)	1.504 (7)
C (42) -C (43)	1.503 (7)	C (42) -C (42) #2	1.58 (1)
C (42) -H (42)	1.0000	C (43) -C (44)	1.336 (7)
C (43) -H (43)	0.9500	C (44) -H (44)	0.9500
C (45) -C (46)	1.425 (7)		

N (2) -Tm (1) -N (1)	70.6 (1)	N (2) -Tm (1) -C (19)	116.8 (2)
N (1) -Tm (1) -C (19)	127.2 (2)	N (2) -Tm (1) -C (1)	102.8 (2)
N (1) -Tm (1) -C (1)	136.7 (2)	C (19) -Tm (1) -C (1)	94.6 (2)
N (2) -Tm (1) -C (2)	79.0 (2)	N (1) -Tm (1) -C (2)	110.2 (2)
C (19) -Tm (1) -C (2)	122.6 (2)	C (1) -Tm (1) -C (2)	30.4 (2)
N (2) -Tm (1) -C (5)	128.4 (2)	N (1) -Tm (1) -C (5)	122.3 (2)
C (19) -Tm (1) -C (5)	94.6 (2)	C (1) -Tm (1) -C (5)	30.7 (2)
C (2) -Tm (1) -C (5)	49.4 (2)	N (2) -Tm (1) -C (20)	88.8 (2)
N (1) -Tm (1) -C (20)	107.7 (2)	C (19) -Tm (1) -C (20)	30.8 (2)
C (1) -Tm (1) -C (20)	115.0 (2)	C (2) -Tm (1) -C (20)	133.2 (2)
C (5) -Tm (1) -C (20)	124.2 (2)	N (2) -Tm (1) -C (22)	116.9 (2)
N (1) -Tm (1) -C (22)	79.3 (2)	C (19) -Tm (1) -C (22)	49.7 (2)
C (1) -Tm (1) -C (22)	135.0 (2)	C (2) -Tm (1) -C (22)	163.9 (2)
C (5) -Tm (1) -C (22)	114.7 (2)	C (20) -Tm (1) -C (22)	49.8 (2)
N (2) -Tm (1) -C (18)	138.1 (2)	N (1) -Tm (1) -C (18)	107.0 (2)
C (19) -Tm (1) -C (18)	30.8 (2)	C (1) -Tm (1) -C (18)	105.0 (2)
C (2) -Tm (1) -C (18)	135.0 (2)	C (5) -Tm (1) -C (18)	89.4 (2)
C (20) -Tm (1) -C (18)	50.9 (2)	C (22) -Tm (1) -C (18)	30.2 (2)
N (2) -Tm (1) -C (21)	89.6 (2)	N (1) -Tm (1) -C (21)	79.4 (2)
C (19) -Tm (1) -C (21)	50.2 (2)	C (1) -Tm (1) -C (21)	143.9 (2)
C (2) -Tm (1) -C (21)	161.1 (2)	C (5) -Tm (1) -C (21)	139.6 (2)
C (20) -Tm (1) -C (21)	30.3 (2)	C (22) -Tm (1) -C (21)	29.9 (2)
C (18) -Tm (1) -C (21)	50.3 (2)	N (2) -Tm (1) -C (3)	86.7 (2)
N (1) -Tm (1) -C (3)	86.3 (2)	C (19) -Tm (1) -C (3)	143.0 (2)
C (1) -Tm (1) -C (3)	50.4 (2)	C (2) -Tm (1) -C (3)	29.7 (2)
C (5) -Tm (1) -C (3)	49.6 (2)	C (20) -Tm (1) -C (3)	162.9 (2)
C (22) -Tm (1) -C (3)	145.6 (2)	C (18) -Tm (1) -C (3)	135.2 (2)
C (21) -Tm (1) -C (3)	165.6 (2)	N (2) -Tm (1) -C (4)	116.6 (2)
N (1) -Tm (1) -C (4)	93.3 (2)	C (19) -Tm (1) -C (4)	120.8 (2)
C (1) -Tm (1) -C (4)	50.2 (2)	C (2) -Tm (1) -C (4)	49.1 (2)
C (5) -Tm (1) -C (4)	29.6 (2)	C (20) -Tm (1) -C (4)	151.6 (2)
C (22) -Tm (1) -C (4)	119.3 (2)	C (18) -Tm (1) -C (4)	105.3 (2)
C (21) -Tm (1) -C (4)	149.0 (2)	C (3) -Tm (1) -C (4)	30.1 (2)
C (35) -N (1) -C (46)	118.0 (4)	C (35) -N (1) -Tm (1)	126.4 (3)
C (46) -N (1) -Tm (1)	115.6 (3)	C (45) -N (2) -C (44)	113.4 (4)
C (45) -N (2) -Tm (1)	118.5 (3)	C (44) -N (2) -Tm (1)	126.8 (3)
C (2) -C (1) -C (5)	105.0 (5)	C (2) -C (1) -C (6)	126.3 (5)
C (5) -C (1) -C (6)	124.4 (5)	C (2) -C (1) -Tm (1)	75.0 (3)
C (5) -C (1) -Tm (1)	75.2 (3)	C (6) -C (1) -Tm (1)	133.0 (4)
C (1) -C (2) -C (3)	112.0 (5)	C (1) -C (2) -Tm (1)	74.6 (3)
C (3) -C (2) -Tm (1)	79.6 (3)	C (1) -C (2) -H (2)	124.0
C (3) -C (2) -H (2)	124.0	Tm (1) -C (2) -H (2)	113.5
C (2) -C (3) -C (4)	105.5 (5)	C (2) -C (3) -C (10)	119.9 (5)
C (4) -C (3) -C (10)	132.7 (6)	C (2) -C (3) -Tm (1)	70.7 (3)
C (4) -C (3) -Tm (1)	75.3 (3)	C (10) -C (3) -Tm (1)	130.0 (4)
C (5) -C (4) -C (3)	106.9 (5)	C (5) -C (4) -C (14)	120.2 (5)
C (3) -C (4) -C (14)	131.6 (5)	C (5) -C (4) -Tm (1)	70.7 (3)
C (3) -C (4) -Tm (1)	74.5 (3)	C (14) -C (4) -Tm (1)	129.5 (4)
C (4) -C (5) -C (1)	110.5 (5)	C (4) -C (5) -Tm (1)	79.7 (3)
C (1) -C (5) -Tm (1)	74.1 (3)	C (4) -C (5) -H (5)	124.7
C (1) -C (5) -H (5)	124.7	Tm (1) -C (5) -H (5)	113.4
C (7) -C (6) -C (1)	111.9 (5)	C (7) -C (6) -C (9)	109.4 (6)
C (1) -C (6) -C (9)	113.1 (5)	C (7) -C (6) -C (8)	107.7 (5)

C (1) -C (6) -C (8)	106.4 (5)	C (9) -C (6) -C (8)	108.2 (5)
C (6) -C (7) -H (7A)	109.5	C (6) -C (7) -H (7B)	109.5
H (7A) -C (7) -H (7B)	109.5	C (6) -C (7) -H (7C)	109.5
H (7A) -C (7) -H (7C)	109.5	H (7B) -C (7) -H (7C)	109.5
C (6) -C (8) -H (8A)	109.5	C (6) -C (8) -H (8B)	109.5
H (8A) -C (8) -H (8B)	109.5	C (6) -C (8) -H (8C)	109.5
H (8A) -C (8) -H (8C)	109.5	H (8B) -C (8) -H (8C)	109.5
C (6) -C (9) -H (9A)	109.5	C (6) -C (9) -H (9B)	109.5
H (9A) -C (9) -H (9B)	109.5	C (6) -C (9) -H (9C)	109.5
H (9A) -C (9) -H (9C)	109.5	H (9B) -C (9) -H (9C)	109.5
C (12) -C (10) -C (11)	106.4 (6)	C (12) -C (10) -C (3)	112.9 (6)
C (11) -C (10) -C (3)	108.7 (5)	C (12) -C (10) -C (13)	107.9 (6)
C (11) -C (10) -C (13)	105.0 (7)	C (3) -C (10) -C (13)	115.4 (5)
C (10) -C (11) -H (11A)	109.5	C (10) -C (11) -H (11B)	109.5
H (11A) -C (11) -H (11B)	109.5	C (10) -C (11) -H (11C)	109.5
H (11A) -C (11) -H (11C)	109.5	H (11B) -C (11) -H (11C)	109.5
C (10) -C (12) -H (12A)	109.5	C (10) -C (12) -H (12B)	109.5
H (12A) -C (12) -H (12B)	109.5	C (10) -C (12) -H (12C)	109.5
H (12A) -C (12) -H (12C)	109.5	H (12B) -C (12) -H (12C)	109.5
C (10) -C (13) -H (13A)	109.5	C (10) -C (13) -H (13B)	109.5
H (13A) -C (13) -H (13B)	109.5	C (10) -C (13) -H (13C)	109.5
H (13A) -C (13) -H (13C)	109.5	H (13B) -C (13) -H (13C)	109.5
C (16A) -C (14) -C (15A)	116 (1)	C (17) -C (14) -C (15)	111.0 (8)
C (16A) -C (14) -C (4)	111 (1)	C (17) -C (14) -C (4)	115.2 (6)
C (15A) -C (14) -C (4)	103.2 (8)	C (15) -C (14) -C (4)	116.1 (6)
C (16A) -C (14) -C (17A)	109 (1)	C (15A) -C (14) -C (17A)	105 (1)
C (4) -C (14) -C (17A)	112.3 (8)	C (17) -C (14) -C (16)	102.6 (7)
C (15) -C (14) -C (16)	101.2 (7)	C (4) -C (14) -C (16)	108.8 (6)
C (14) -C (15) -H (15A)	109.5	C (14) -C (15) -H (15B)	109.5
H (15A) -C (15) -H (15B)	109.5	C (14) -C (15) -H (15C)	109.5
H (15A) -C (15) -H (15C)	109.5	H (15B) -C (15) -H (15C)	109.5
C (14) -C (16) -H (16A)	109.5	C (14) -C (16) -H (16B)	109.5
H (16A) -C (16) -H (16B)	109.5	C (14) -C (16) -H (16C)	109.5
H (16A) -C (16) -H (16C)	109.5	H (16B) -C (16) -H (16C)	109.5
C (14) -C (17) -H (17A)	109.5	C (14) -C (17) -H (17B)	109.5
H (17A) -C (17) -H (17B)	109.5	C (14) -C (17) -H (17C)	109.5
H (17A) -C (17) -H (17C)	109.5	H (17B) -C (17) -H (17C)	109.5
C (14) -C (15A) -H (15D)	109.5	C (14) -C (15A) -H (15E)	109.5
H (15D) -C (15A) -H (15E)	109.5	C (14) -C (15A) -H (15F)	109.5
H (15D) -C (15A) -H (15F)	109.5	H (15E) -C (15A) -H (15F)	109.5
C (14) -C (16A) -H (16D)	109.5	C (14) -C (16A) -H (16E)	109.5
H (16D) -C (16A) -H (16E)	109.5	C (14) -C (16A) -H (16F)	109.5
H (16D) -C (16A) -H (16F)	109.5	H (16E) -C (16A) -H (16F)	109.5
C (14) -C (17A) -H (17D)	109.5	C (14) -C (17A) -H (17E)	109.5
H (17D) -C (17A) -H (17E)	109.5	C (14) -C (17A) -H (17F)	109.5
H (17D) -C (17A) -H (17F)	109.5	H (17E) -C (17A) -H (17F)	109.5
C (22) -C (18) -C (19)	104.8 (5)	C (22) -C (18) -C (23)	123.9 (5)
C (19) -C (18) -C (23)	126.7 (5)	C (22) -C (18) -Tm (1)	74.7 (3)
C (19) -C (18) -Tm (1)	71.1 (3)	C (23) -C (18) -Tm (1)	137.7 (4)
C (18) -C (19) -C (20)	110.5 (5)	C (18) -C (19) -Tm (1)	78.2 (3)
C (20) -C (19) -Tm (1)	77.8 (3)	C (18) -C (19) -H (19)	124.7
C (20) -C (19) -H (19)	124.7	Tm (1) -C (19) -H (19)	111.4
C (19) -C (20) -C (21)	106.9 (5)	C (19) -C (20) -C (27)	118.5 (5)
C (21) -C (20) -C (27)	133.6 (5)	C (19) -C (20) -Tm (1)	71.3 (3)
C (21) -C (20) -Tm (1)	77.6 (3)	C (27) -C (20) -Tm (1)	124.3 (4)
C (22) -C (21) -C (20)	106.1 (5)	C (22) -C (21) -C (31)	119.2 (5)
C (20) -C (21) -C (31)	132.4 (5)	C (22) -C (21) -Tm (1)	72.4 (3)
C (20) -C (21) -Tm (1)	72.1 (3)	C (31) -C (21) -Tm (1)	133.2 (4)
C (18) -C (22) -C (21)	111.4 (5)	C (18) -C (22) -Tm (1)	75.2 (3)
C (21) -C (22) -Tm (1)	77.8 (3)	C (18) -C (22) -H (22)	124.3
C (21) -C (22) -H (22)	124.3	Tm (1) -C (22) -H (22)	114.5
C (18) -C (23) -C (25)	105.8 (5)	C (18) -C (23) -C (24)	113.2 (5)
C (25) -C (23) -C (24)	107.1 (5)	C (18) -C (23) -C (26)	112.3 (5)
C (25) -C (23) -C (26)	107.8 (6)	C (24) -C (23) -C (26)	110.3 (6)
C (23) -C (24) -H (24A)	109.5	C (23) -C (24) -H (24B)	109.5
H (24A) -C (24) -H (24B)	109.5	C (23) -C (24) -H (24C)	109.5
H (24A) -C (24) -H (24C)	109.5	H (24B) -C (24) -H (24C)	109.5
C (23) -C (25) -H (25A)	109.5	C (23) -C (25) -H (25B)	109.5

H (25A) -C (25) -H (25B)	109.5	C (23) -C (25) -H (25C)	109.5
H (25A) -C (25) -H (25C)	109.5	H (25B) -C (25) -H (25C)	109.5
C (23) -C (26) -H (26A)	109.5	C (23) -C (26) -H (26B)	109.5
H (26A) -C (26) -H (26B)	109.5	C (23) -C (26) -H (26C)	109.5
H (26A) -C (26) -H (26C)	109.5	H (26B) -C (26) -H (26C)	109.5
C (28) -C (27) -C (20)	115.7 (6)	C (28) -C (27) -C (29)	106.5 (6)
C (20) -C (27) -C (29)	109.5 (5)	C (28) -C (27) -C (30)	108.5 (5)
C (20) -C (27) -C (30)	109.1 (5)	C (29) -C (27) -C (30)	107.3 (6)
C (27) -C (28) -H (28A)	109.5	C (27) -C (28) -H (28B)	109.5
H (28A) -C (28) -H (28B)	109.5	C (27) -C (28) -H (28C)	109.5
H (28A) -C (28) -H (28C)	109.5	H (28B) -C (28) -H (28C)	109.5
C (27) -C (29) -H (29A)	109.5	C (27) -C (29) -H (29B)	109.5
H (29A) -C (29) -H (29B)	109.5	C (27) -C (29) -H (29C)	109.5
H (29A) -C (29) -H (29C)	109.5	H (29B) -C (29) -H (29C)	109.5
C (27) -C (30) -H (30A)	109.5	C (27) -C (30) -H (30B)	109.5
H (30A) -C (30) -H (30B)	109.5	C (27) -C (30) -H (30C)	109.5
H (30A) -C (30) -H (30C)	109.5	H (30B) -C (30) -H (30C)	109.5
C (32) -C (31) -C (34)	110.0 (5)	C (32) -C (31) -C (33)	105.6 (6)
C (34) -C (31) -C (33)	105.1 (6)	C (32) -C (31) -C (21)	117.0 (5)
C (34) -C (31) -C (21)	107.5 (5)	C (33) -C (31) -C (21)	110.9 (5)
C (31) -C (32) -H (32A)	109.5	C (31) -C (32) -H (32B)	109.5
H (32A) -C (32) -H (32B)	109.5	C (31) -C (32) -H (32C)	109.5
H (32A) -C (32) -H (32C)	109.5	H (32B) -C (32) -H (32C)	109.5
C (31) -C (33) -H (33A)	109.5	C (31) -C (33) -H (33B)	109.5
H (33A) -C (33) -H (33B)	109.5	C (31) -C (33) -H (33C)	109.5
H (33A) -C (33) -H (33C)	109.5	H (33B) -C (33) -H (33C)	109.5
C (31) -C (34) -H (34A)	109.5	C (31) -C (34) -H (34B)	109.5
H (34A) -C (34) -H (34B)	109.5	C (31) -C (34) -H (34C)	109.5
H (34A) -C (34) -H (34C)	109.5	H (34B) -C (34) -H (34C)	109.5
N (1) -C (35) -C (36)	123.4 (5)	N (1) -C (35) -H (35)	118.3
C (36) -C (35) -H (35)	118.3	C (37) -C (36) -C (35)	119.2 (5)
C (37) -C (36) -H (36)	120.4	C (35) -C (36) -H (36)	120.4
C (36) -C (37) -C (38)	119.5 (5)	C (36) -C (37) -H (37)	120.3
C (38) -C (37) -H (37)	120.3	C (37) -C (38) -C (46)	118.5 (5)
C (37) -C (38) -C (39)	122.7 (5)	C (46) -C (38) -C (39)	118.8 (5)
C (40) -C (39) -C (38)	119.9 (5)	C (40) -C (39) -H (39)	120.0
C (38) -C (39) -H (39)	120.0	C (39) -C (40) -C (41)	122.4 (5)
C (39) -C (40) -H (40)	118.8	C (41) -C (40) -H (40)	118.8
C (45) -C (41) -C (40)	119.2 (5)	C (45) -C (41) -C (42)	120.2 (5)
C (40) -C (41) -C (42)	120.5 (4)	C (43) -C (42) -C (41)	108.2 (4)
C (43) -C (42) -C (42) #2	113.4 (5)	C (41) -C (42) -C (42) #2	111.4 (5)
C (43) -C (42) -H (42)	107.9	C (41) -C (42) -H (42)	107.9
C (42) #2 -C (42) -H (42)	107.9	C (44) -C (43) -C (42)	120.7 (5)
C (44) -C (43) -H (43)	119.6	C (42) -C (43) -H (43)	119.6
C (43) -C (44) -N (2)	126.7 (5)	C (43) -C (44) -H (44)	116.7
N (2) -C (44) -H (44)	116.7	N (2) -C (45) -C (41)	123.8 (5)
N (2) -C (45) -C (46)	118.0 (4)	C (41) -C (45) -C (46)	118.1 (4)
N (1) -C (46) -C (38)	121.3 (5)	N (1) -C (46) -C (45)	117.3 (4)
C (38) -C (46) -C (45)	121.4 (5)		

5. References

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