Supporting information for the manuscript

Atom economical coupling of benzophenone and N-heterocyclic aromatics with SmI_2

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1. Syntheses.

General considerations.

All reactions were performed using standard Schlenk-line techniques or in argon filled gloveboxes (MBraun). All glassware was dried at 140 °C for at least 12 h prior to use. THF, pyridine, and toluene were dried over sodium, degassed and transferred under reduced pressure in a cold flask. SmI_2 was prepared following the Kagan procedure.[1] Bipyridine, phenanthroline and benzophenone were bought from commercial suppliers and sublimed before use. ^{1}H NMR spectra were recorded in standard tube adapted with J. Young stoppers on Bruker Advance III or II at a Larmor frequency of 300 MHz. UV-Visible measurements were recorded on an Agilent Cary 60 apparatus with 10 mm cuvettes adapted with J. Young stoppers.

Syntheses.

Synthesis of $Sm_2(Ph_2CO)_2(THF)_6I_4$ **(1)**. 5 mL of THF was added at room temperature to a mixture of benzophenone (220 mg, 1.21 mmol) and SmI_2 (500 mg, 1.24 mmol). The blue solution was stirred for 2 h at room temperature while a fine white precipitate started to form. The solution was put at -40 °C overnight. The suspension was filtered and the white microcrystalline powder was dried to form 734 mg of **1** (0.89 mmol, Yield 74%). Pale yellow crystals, suitable for X-ray studies, can be isolated from the mother liquor at -40°C.

Synthesis of $Sm(Ph_2C(O)bipy)I_2(bipy)(py)$ **(2)**. Bipyridine (32 mg, 0.205 mmol) was added to a freshly prepared solution of **1** (183 mg, 0.204 mmol) in pyridine. The dark brown purple solution faded within a few hours and turned yellow after 12 h of stirring at room temperature. After filtration of a slight white precipitate, a layer of pentane was added on top of the pyridine solution, yielding a light brown oil (**2**). The pyridine volatiles were evaporated and the dry residue was dissolved in acetonitrile. The light yellow solution was let stand at room temperature leading to the slow (one week) formation of white crystals. From this batch only few crystals were found suitable for X-ray diffraction (**2b**, 72 mg ; 35 %). The crystal were analyzed as $Sm(Ph_2C(O)bipy)I_2(bipy)(py)$, indicating a conversion rate below 100%. No elemental analysis could be obtained.

Synthesis of $Sm(Ph_2C(O)phen)I_2(py)_3$ **(3)**. Phenanthroline (29.3 mg, 0.163 mmol) was added to a solution of to a freshly prepared solution of **1** (146.4 mg, 0.163 mmol) in pyridine. The black

purple solution faded within a few minutes and turned yellow after 2 h of stirring at room temperature. After filtration of a slight white precipitate, a layer of pentane was added on top of the pyridine solution, and X-ray suitable yellow block crystals were obtained and dried under reduced pressure (162 mg ; 97 %). X-ray suitable yellow crystals can also be obtained from acetonitrile after a few days at –40°C (**3b**). Anal. Calculated for $C_{40}H_{32}N_5OI_2Sm$: C, 47.91; H, 3.22; N, 6.98 Found: C, 48.23; H, 3.25; N, 5.76. The slightly low value for N indicates a possible partial de-coordination of one pyridine upon drying under reduced pressure. Elemental Analysis for **3.pyr-d$_5$** $C_{40}H_{17}D_{15}N_5OI_2Sm$ calcd. C, 47.20; H, 1.68; N, 6.88, found C, 48.81; H, 1.07; N, 6.27.Synthesis of $Sm(Ph_2C(O)pyridine)I_2(py)_3$ **(4)**. Crystals of **1**, prepared previously (159.0 mg 0.177 mmol) were dissolved in pyridine. The black purple solution did not react at room temperature for one week and then was heated and stirred at 100 °C for 12 h. Once cooled, the yellow suspension was filtered and a layer of pentane was added on top of the pyridine solution, yielding X-ray suitable light yellow crystals of **4**. (**2b**, 130 mg ; 80 %). ^{1}H NMR for **4** (δ, 295 K, pyridine-d_5): 9.39 (d, J = 9 Hz, 2H), 8.54 (d, J = 9 Hz, 2H), 7.88 (d, J = 6 Hz, 1H), 7.53 (m, 10H). Elemental analysis for **4**. $C_{33}H_{10}D_{19}N_4OI_2Sm$ calcd. C,43.05; H, 1.09: N, 6.09 found C, 43.10; H, 0.77; N, 6.07.

General procedure for the synthesis of **5-7**.

Pyridine was added to a mixture of benzophenone, phenanthroline or bypyridine (1.25 mmol) and SmI_2 (0.5 g, 1.25 mmol). The solution turned red rapidly red. After stirring for 16 h at room temperature, the yellow solution was put under reduced pressure in order to remove the solvent. For the formation of **5**, similar amounts of benzophenone and SmI_2 were heated for 16 h at 110°C in toluene. The resulting yellow solution was evaporated under reduced pressure.

Outside the glovebox, a 0.1 M HCl solution (5 mL) was added on the residual solids, followed by an extraction with dichloromethane (3x10 mL). The organic phase was washed with water until the washings were no longer acid, and dried over $MgSO_4$. The solvent was removed and the compound was gathered as a yellow powder for 6 and 7 (75 % for **6**, 70 % for **7**) and as a brown oil for **5** (45 % for **5**). Recrystallisation of the powder in EtOH gave colorless crystals suitable for X-ray diffraction analysis for **6** and **7** but not for **5**. The purity of **5** as an oil was difficult to ascertain.

^{1}H NMR for **5** (δ, 295 K, $CDCl_3$): 8.78 (s, 1H), 8.45 (s, 1H), 8.42 (s, 1H), 7.83 (t, J = 7 Hz, 1H), 7.35 (m, 12 H), 7.18 (d, J = 9 Hz, 1H)

^{1}H NMR for **6** (δ, 295 K, $CDCl_3$): 9.15 (d, *J*=8 Hz, 1H), 8.31 (d, *J*=6 Hz, 1H), 8.19 (d, *J*=9 Hz, 1H), 7.83 (s, 2H), 7.67 (dd, *J*=9 Hz, 3 Hz, 1H), 7.52 (d, *J*=9 Hz, 1H), 7.40 (m, 4H), 7.30 (m, 6 H).

^{1}H NMR for **7** (δ, 295 K, $CDCl_3$): 7.40 (m), 7.38 (m), 7.34 (m), 7.31 (m), 7.29 (m), 7.25 (m), relative integration was not possible.

2. ^{1}H NMR Spectroscopy

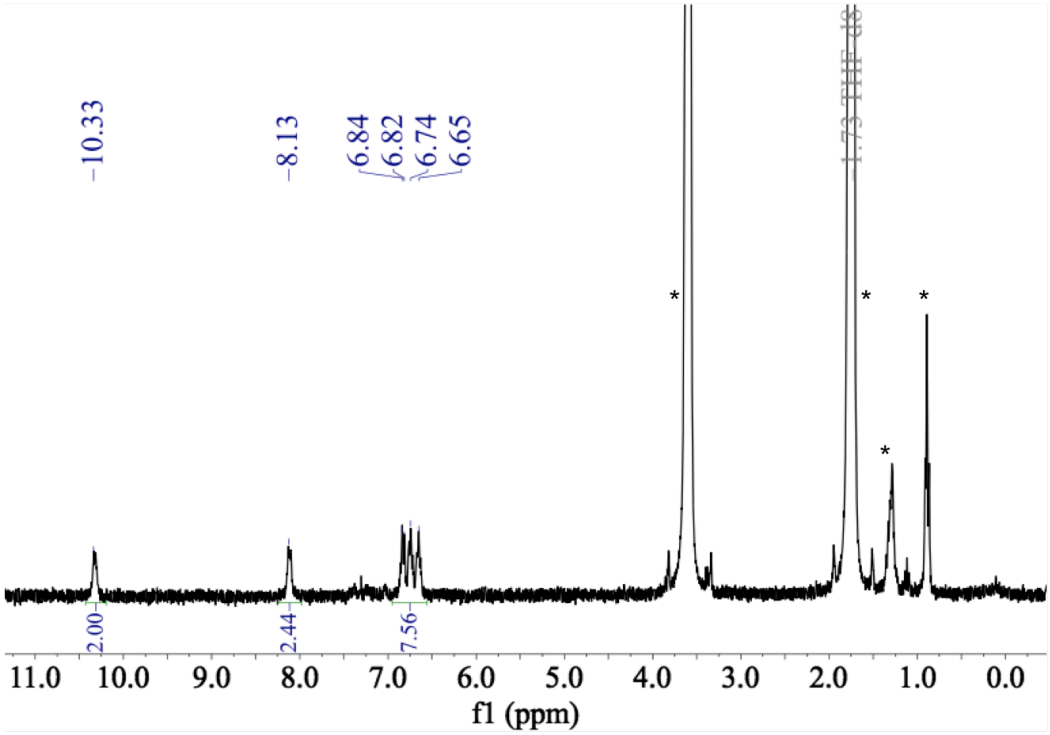

Figure S1. ^{1}H NMR Spectrum of **1** at 293 K in thf-d_8. *are for solvents (pyridine and thf).

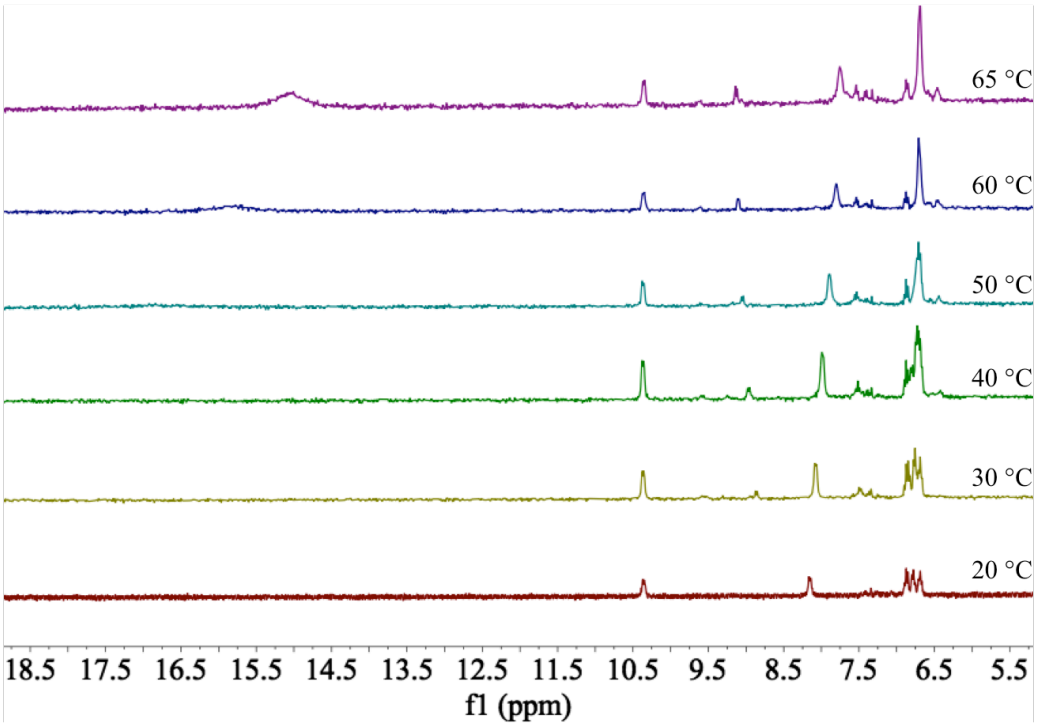

Figure S2. VT ^{1}H NMR Spectra of **1** between 293 K and 338 K in thf-d_8.

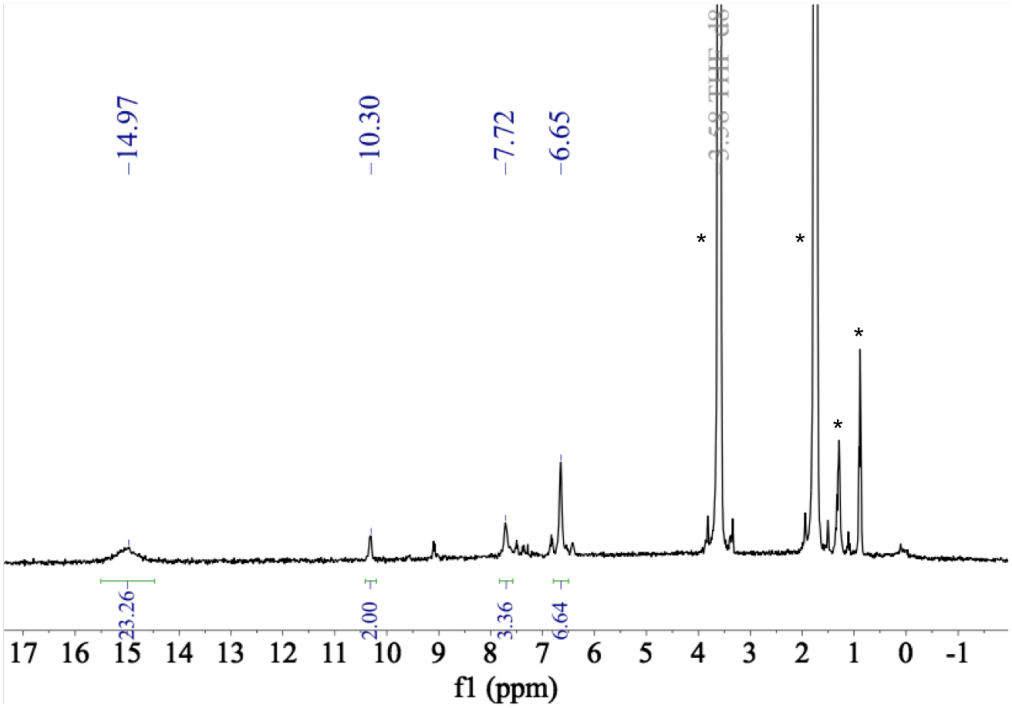

Figure S3. ^{1}H NMR Spectrum of **1** at 338 K in thf-d_8. *are for solvents (pyridine and thf).

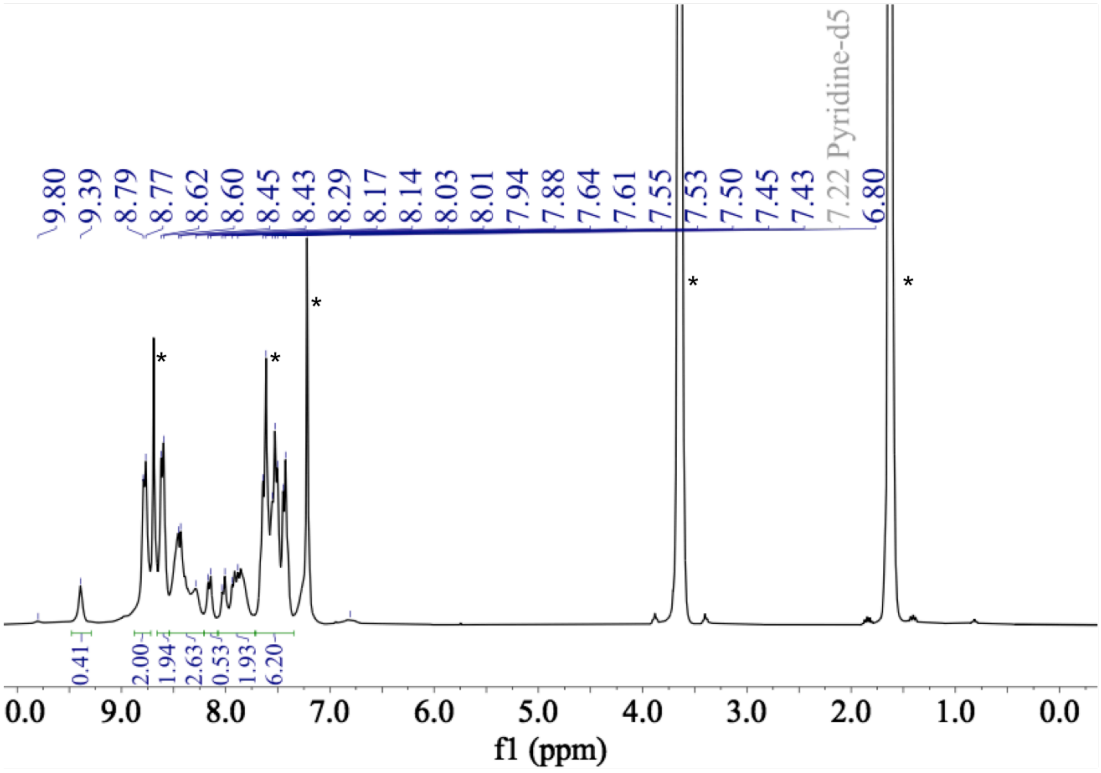

Figure S4. ^{1}H NMR Spectrum of **2** at 293 K in pyridine-d_5. *are for solvents (pyridine and thf).

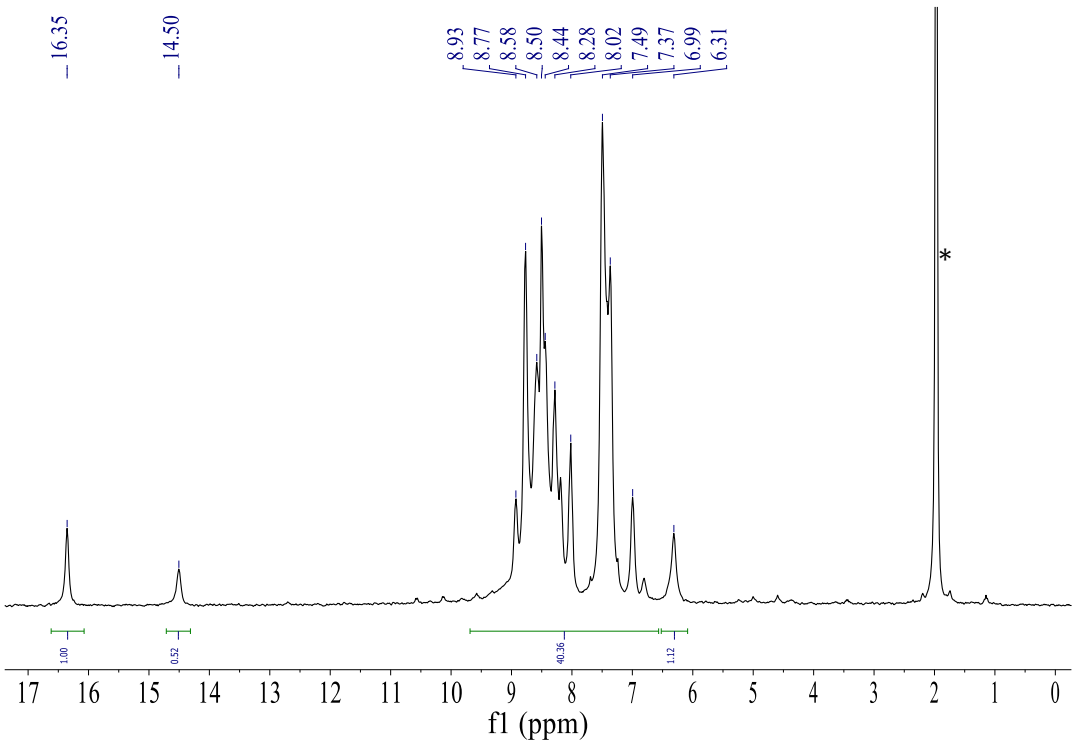

Figure S5. ^{1}H NMR Spectrum of **2** at 293 K in CD_3CN. * is for solvent (CD_3CN).

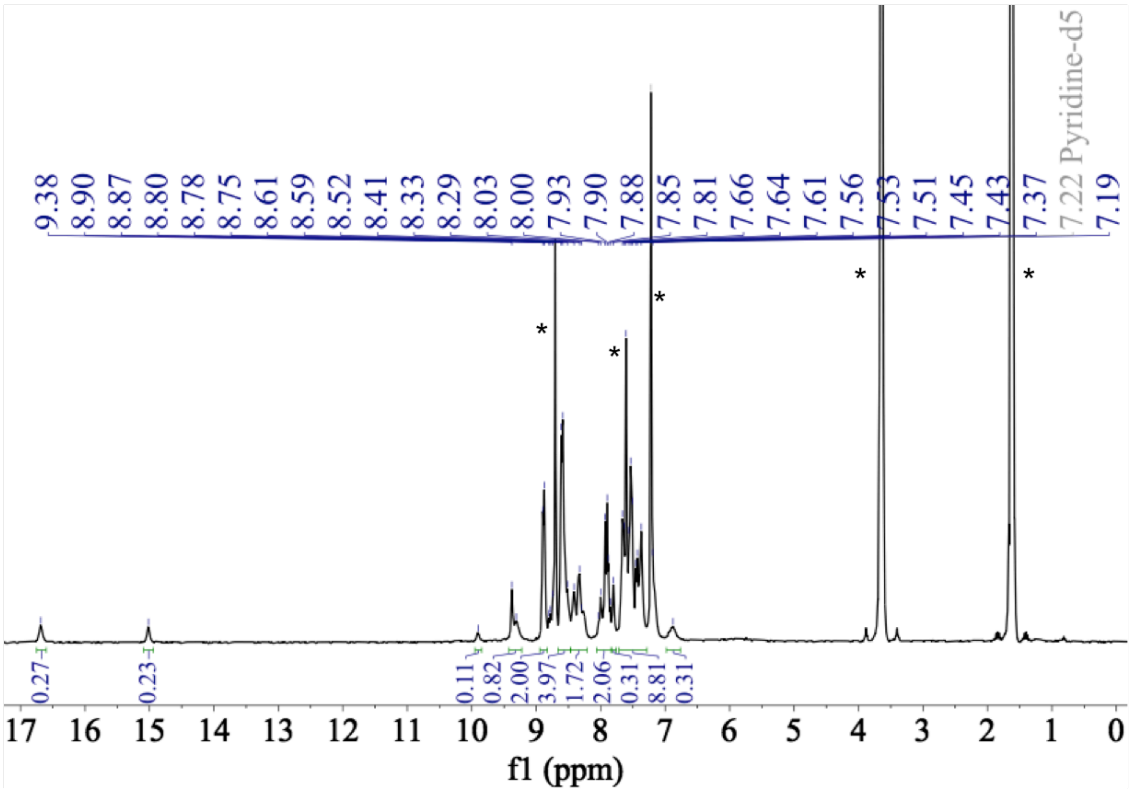

Figure S6. ^{1}H NMR Spectrum of **3** at 293 K in pyridine-d_5. *are for solvents (pyridine and thf).

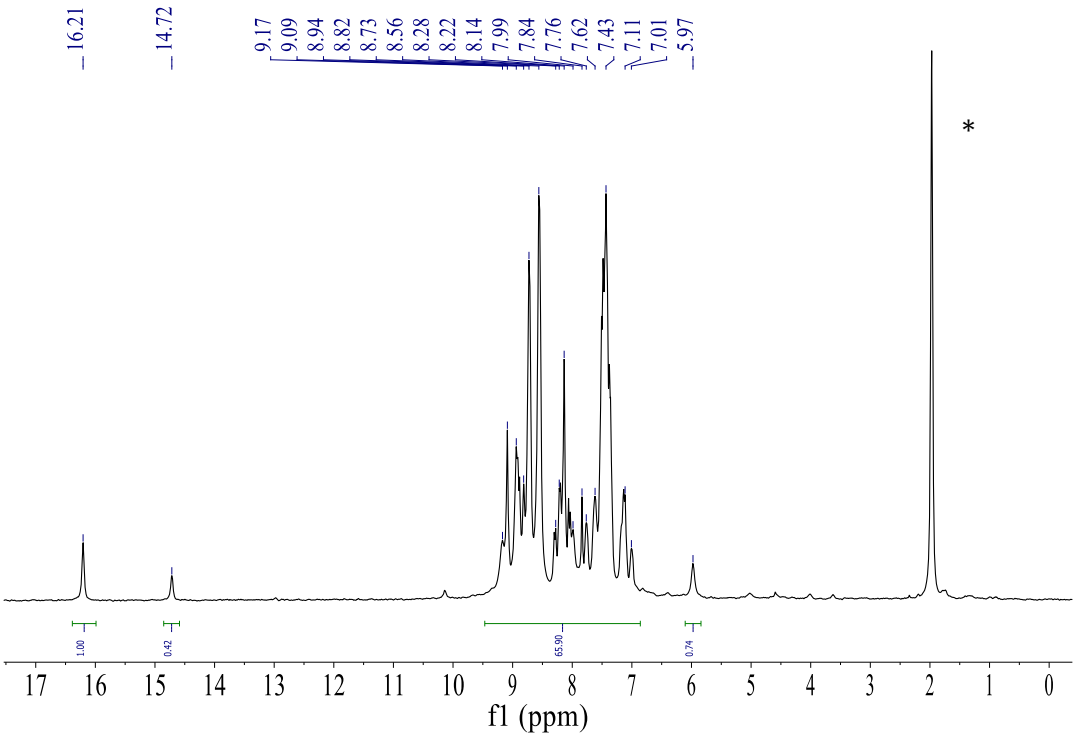

Figure S7. ^{1}H NMR Spectrum of **3** at 293 K in CD_3CN. * is for solvent (CD_3CN).

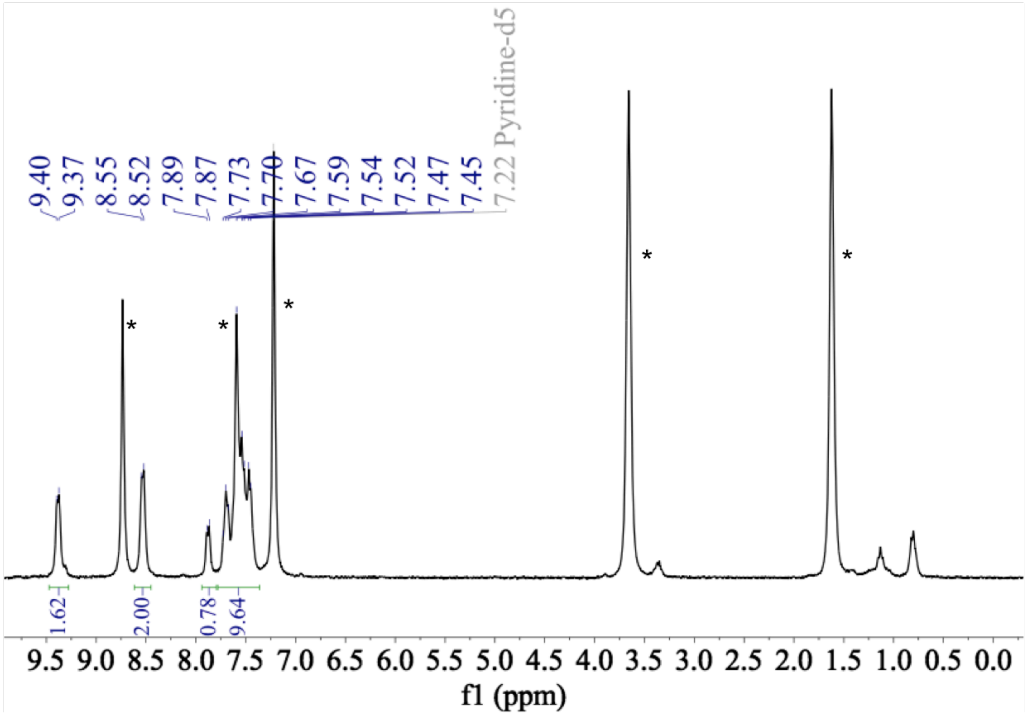

Figure S8. ^{1}H NMR Spectrum of **4** at 293 K in pyridine-d_5. *are for solvents (pyridine and thf).

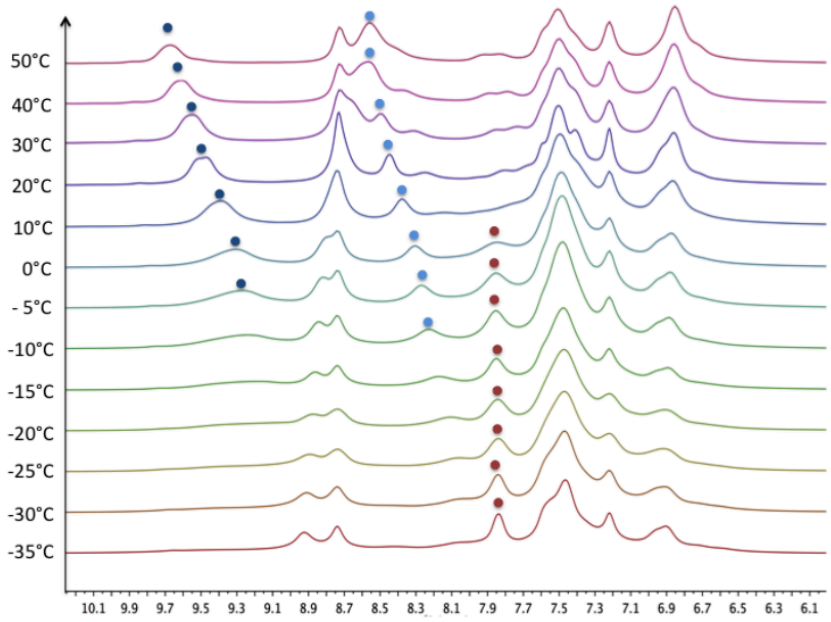

Figure S9. Variable temperature ^{1}H NMR spectra of SmI_2(benzophenone)$(pyr)_x$ in pyridine-d_5. The red dots indicate the disappearance of peaks with increasing temperature and blue dots indicate the appearance of peaks with increasing temperature.

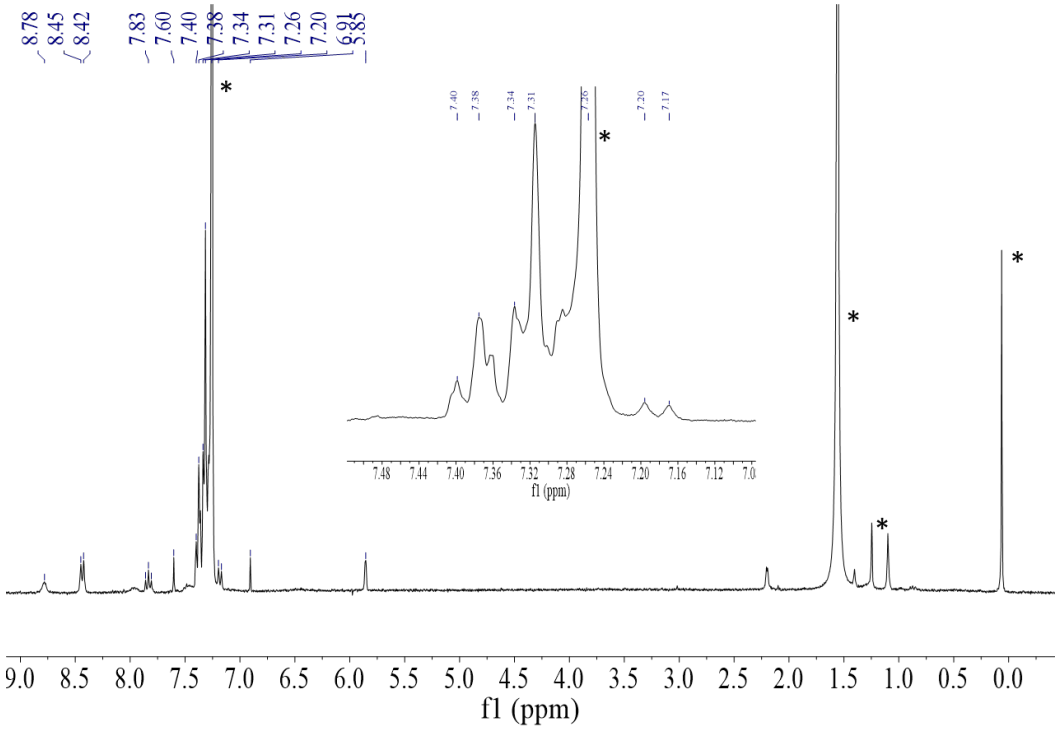

Figure S10. ^{1}H NMR Spectrum of **5** at 293 K in $CDCl_3$. *are for solvents (CD_3Cl) and impurities.

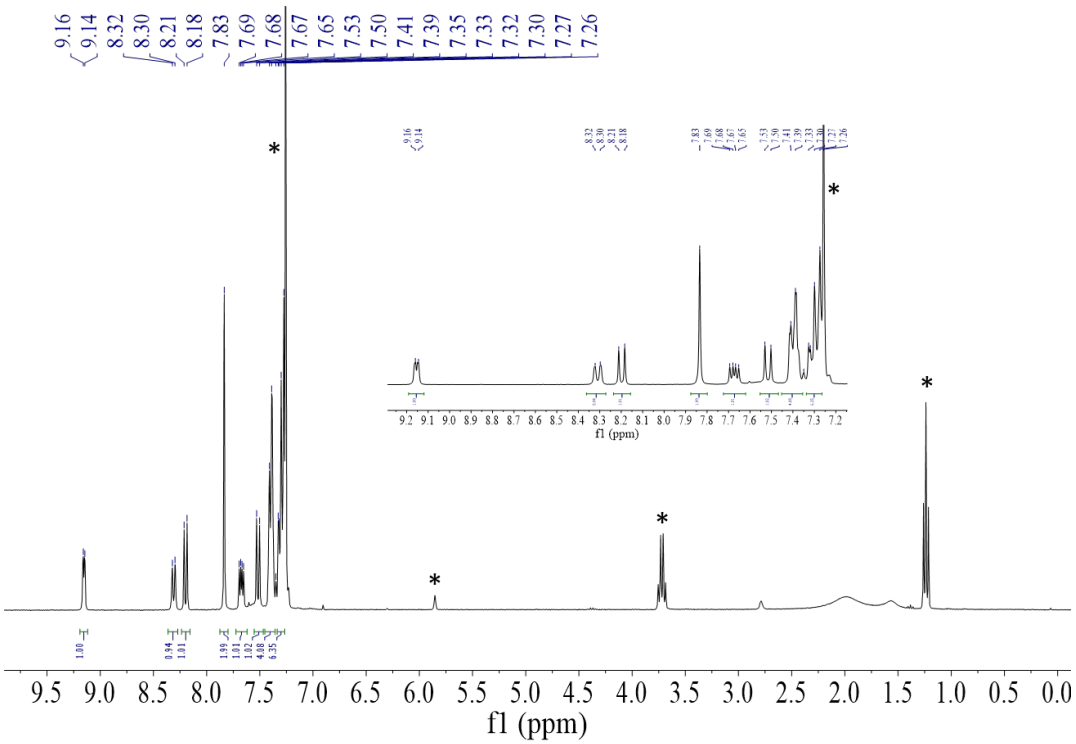

Figure S11. ^{1}H NMR Spectrum of **6** at 293 K in in $CDCl_3$. *are for solvents ($CDCl_3$) and impurities.

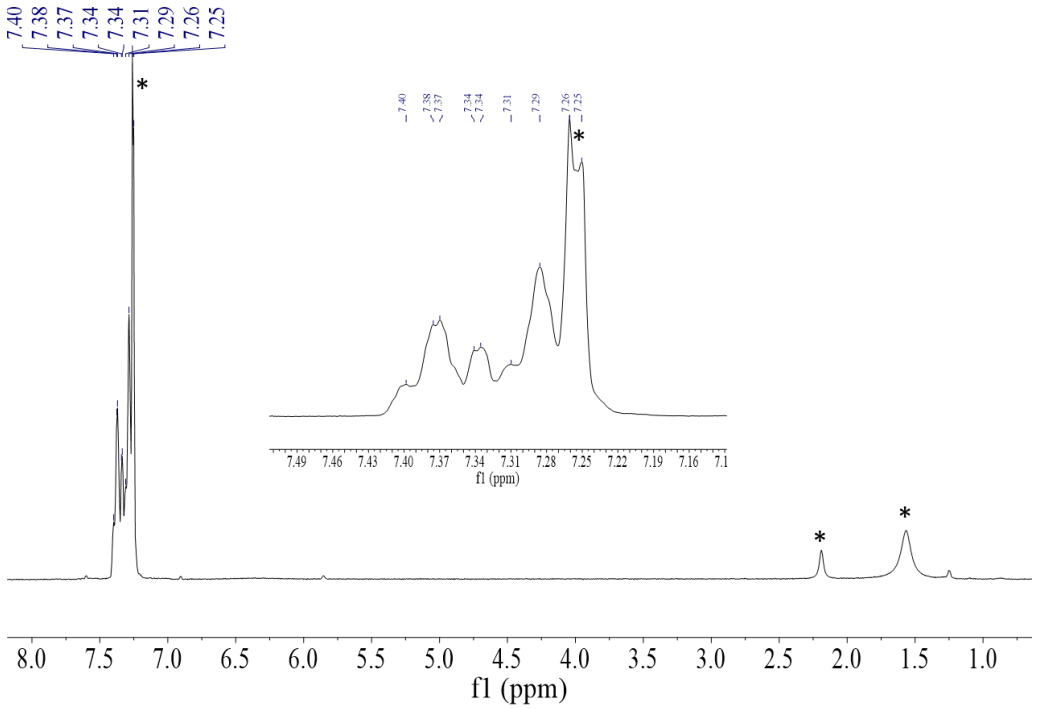

Figure S12. ^{1}H NMR Spectrum of **7** at 293 K in pyridine-d_5. *are for solvents ($CDCl_3$) and impurities.

3. UV-Visible Spectroscopy

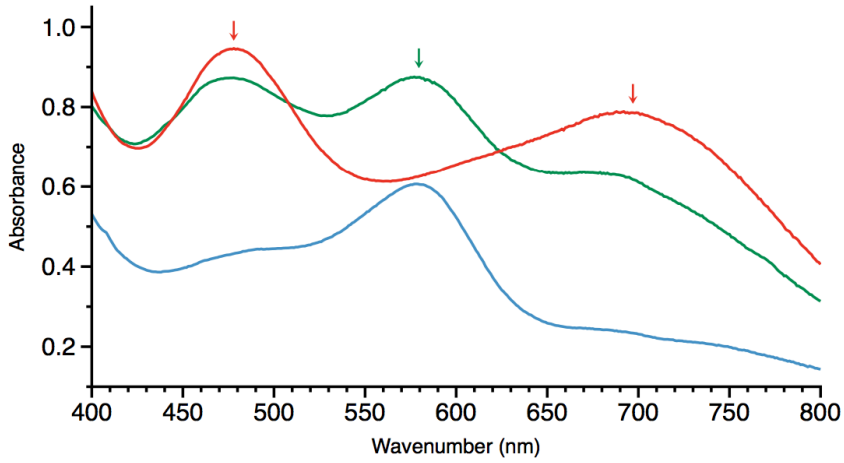

Figure S13. UV-visible spectrum in pyridine of $SmI_2(pyr)_x$ (red) at room temperature, of SmI_2(benzophenone) at room temperature (blue) and of SmI_2(benzophenone) at around 100 °C (green). The green arrow indicates the typical peak of benzophenone ketyl radical while the red arrows indicate the typical peaks of the pyridine radical. Note that the green spectrum shows all features.

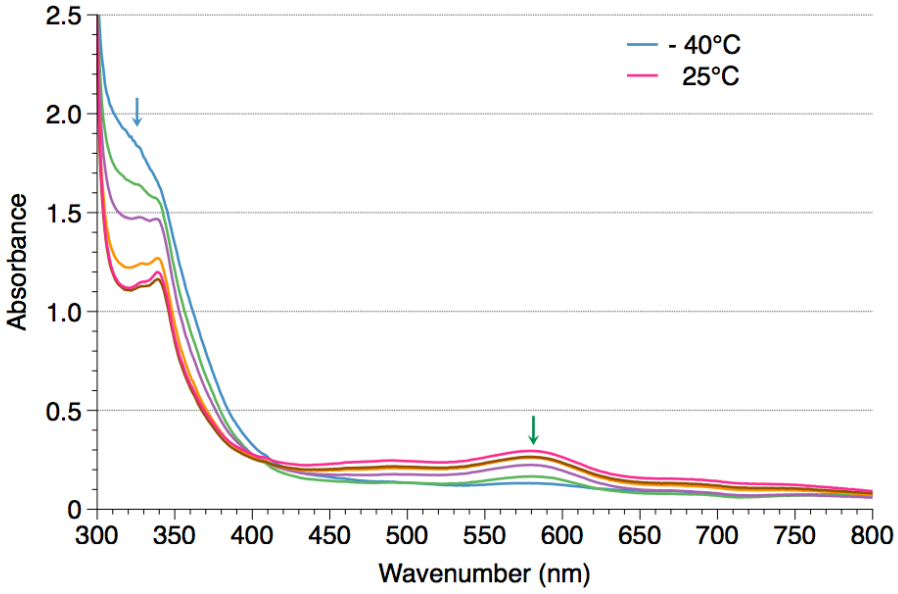

Figure S14. Qualitative variable temperature UV-visible spectrum of SmI_2(benzophenone)$(pyr)_x$ in pyridine between around –40 °C (blue) and around 25 °C (red). The blue arrow indicates the peak of the σ benzophenone dimer (pinacol form) and the green arrow indicates the peak of benzophenone radical.

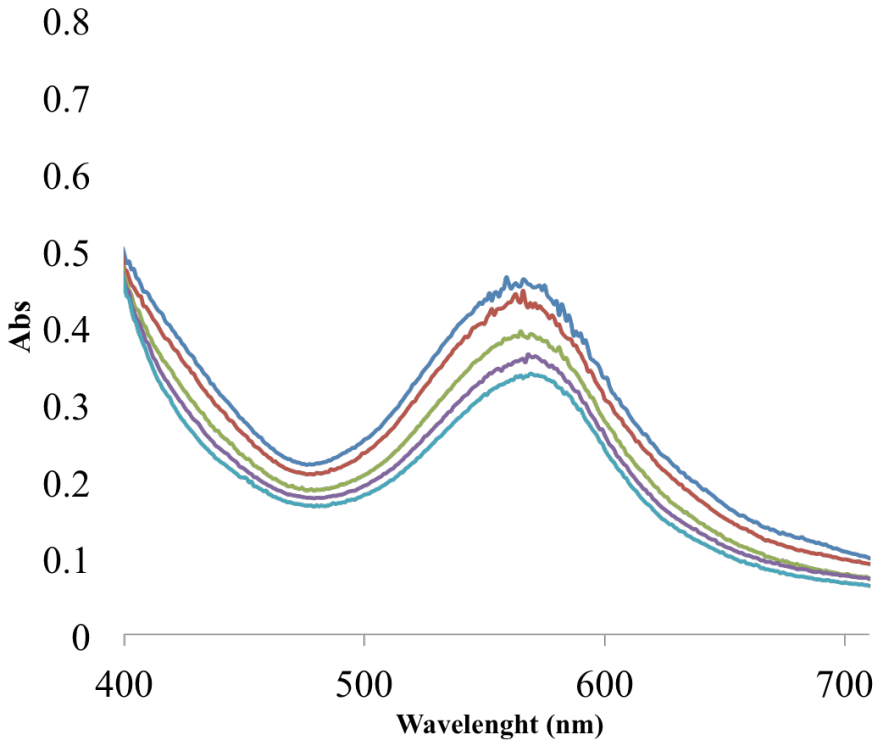

Figure S15. Qualitative variable temperature UV-visible spectrum of SmI_2(benzophenone)$(pyr)_x$ in THF between around 20 °C (light blue) and around 60 °C (dark blue). Note that the concentration is only slightly shifted compared to that in S11.

4. X-ray crystallography

General details. Using Olex2,[2] the structure was solved with the SHELXT[3] structure solution program using Intrinsic Phasing and refined with the SHELXL[4] refinement package using Least Squares minimization. The PLATON software[5] was used to treat cases of twinning and solvent accessible voids. Pictures of the compound structure were obtained using the MERCURY software. During the refinement steps, all atoms, except hydrogen atoms, were refined anisotropically. The positions of the hydrogen atoms were determined geometrically. The crystal structures of **1-7** and **4b** have been deposited in the CCDC with #1861445-1861450.
The structure of compound 3 was refined in P-1, no higher symmetry was found.

A mask was used during the refinement of structure **4**, removing the contribution of 137 electrons from the unit-cell content. This might correspond with just less than 1 molecule of pyridine per formula unit. This disorder could not be treated in another way.

Table S1. Experimental crystallographic parameters for **1-3**.

Compound	**1**	**2**	**3**
Formula	$C_{50}H_{68}I_4O_8Sm_2$, $C_4H_8O_1$	$C_{28}H_{30}I_2N_5OSm$	$C_{40}H_{32}I_2N_5O_1Sm_1$, $3C_5H_5N_1$
Crystal size (mm)	0.300 × 0.200 × 0.050	0.140x0.100x0.080	0.280 x 0.200 x 0.080
Crystal system	orthorhombic	Monoclinic	triclinic
Space group	P 2_1 2_1 2_1	P 2_1/c	P -1
Volume (Å)	5964.1(2)	3507.6(5)	4971.74(18)
a (Å)	16.1373(4)	11.6323(9)	15.8733(3)
b (Å)	17.5042(4)	12.3012(9)	16.1883(3)
c (Å)	21.1140(4)	24.5249(18)	19.8595(5)
α (deg)	90	90	90
β (deg)	90	91.769(2)	103.0300(10)
γ (deg)	90	90	90
Z	4	4	4
Formula weight (g/mol)	1677.44	976.82	1240.15
Density (calcd) (g/cm^{-3})	1.868	1.850	1.657
Absorption coefficient (cm^{-1})	0.407	3.472	2.471
F(000)	3232.0	1876.0	2436.0
Temp (K)	150	150	150
Flack parameter	0.33(3)	-	-
diffractometer	Kappa APEX II CCD	Kappa APEX II CCD	Kappa APEX II CCD
θ range for data collection (deg)	4.654 – 54.968	3.31 – 53.464	3.642-55.386
Absorption correction	Multi-scan	Multi-scan	Multi-scan
Total no. reflections	21322	92555	22156
Unique reflections [R_{int}]	12058 [0.0265]	7525 [0.0950]	22156
Final R indices [I>2σ(I)]	R = 0.0538, R_w = 0.1331	R = 0.0682, R_w = 0.1773	R = 0.0981, R_w = 0.2044
R indices (all data)	R = 0.0573, R_w = 0.1374	R = 0.0901, R_w = 0.1934	R = 0.1155, R_w = 0.2160
Largest diff. peak and hole (e.A^{-3})	3.73 / -2.60	1.91/ -1.39	4.64 / -2.21
GooF	1.048	1.045	1.136

Table S2. Experimental crystallographic parameters for **4** and **6**.

Compound	**4**	**6**
Formula	$2C_{33}H_{29}I_2N_4O_1Sm_1$	$C_{25}H_{18}N_2O$
Crystal size (mm)	0.200x0.060x0.040	0.320×0.300×0.280
Crystal system	monoclinic	monoclinic
Space group	P 2_1/c	C 2/c
Volume (Å)	3470.8(6)	3605.6(4)
a (Å)	9.2854(10)	17.8482(10)
b (Å)	15.4014(14)	18.0365(10)
c (Å)	24.686(3)	12.5808(7)
α (deg)	90	90
β (deg)	100.528(4)	117.094(2)
γ (deg)	90	90
Z	4	8
Formula weight (g/mol)	901.75	362.41
Density (calcd) (g/cm^{-3})	1.726	1.335
Absorption coefficient (cm^{-1})	3.500	0.082
F(000)	1724.0	1520.0
Temp (K)	150	150
diffractometer	Kappa APEX II CCD	Kappa APEX II CCD
θ range for data collection (deg)	5.188 – 26.684	5.128-60.056
Absorption correction	Multi-scan	Multi-scan
Total no. reflections	56938	17987
Unique reflections [R_{int}]	8630 [0.0738]	5253 [0.0386]
Final R indices [I>2σ(I)]	R = 0.0420, R_w = 0.0825	R = 0.0477, R_w = 0.1203
R indices (all data)	R = 0.0594, R_w = 0.0879	R = 0.0625, R_w = 0.1316
Largest diff. peak and hole ($e.A^{-3}$)	2.82 / -1.37	0.43/-0.33
GooF	1.051	1.049

Table S3. Experimental crystallographic parameters for **7** and **3b**.

Compound	**7**	**3b**
Formula	$C_{18}H_{15}NO$	$C_{39}H_{28}I_2N_5OSm$, $C_2H_3N_1$
Crystal size (mm)	0.260x0.160x0.100	0.320×0.300×0.20
Crystal system	monoclinic	triclinic
Space group	P 2_1/c	P -1
Volume (Å)	1368.56(12)	1931.97(16)
a (Å)	8.1307(4)	11.4446(5)
b (Å)	14.6655(8)	11.9484(6)
c (Å)	11.5353(6)	14.6103(7)
α (deg)	90	78.322(2)
β (deg)	95.749(3)	81.9090(10)
γ (deg)	90	84.3380(10)
Z	4	2
Formula weight (g/mol)	261.31	1027.87
Density (calcd) (g/cm^{-3})	1.268	1.767
Absorption coefficient (cm^{-1})	0.078	3.157
F(000)	552.0	990.0
Temp (K)	150	150
diffractometer	Kappa APEX II CCD	Kappa APEX II CCD
θ range for data collection (deg)	4.506-57.386	5.828-55.136
Absorption correction	Multi-scan	Multi-scan
Total no. reflections	8115	27436
Unique reflections [R_{int}]	3462 [0.0359]	8590 [0.0295]
Final R indices [I>2σ(I)]	R = 0.0456, R_w = 0.1093	R = 0.0195, R_w = 0.0472
R indices (all data)	R = 0.0643, R_w = 0.1225	R = 0.0218, R_w = 0.0486
Largest diff. peak and hole ($e.A^{-3}$)	0.270 / -0.200	0.61/-0.31
GooF	1.047	1.031

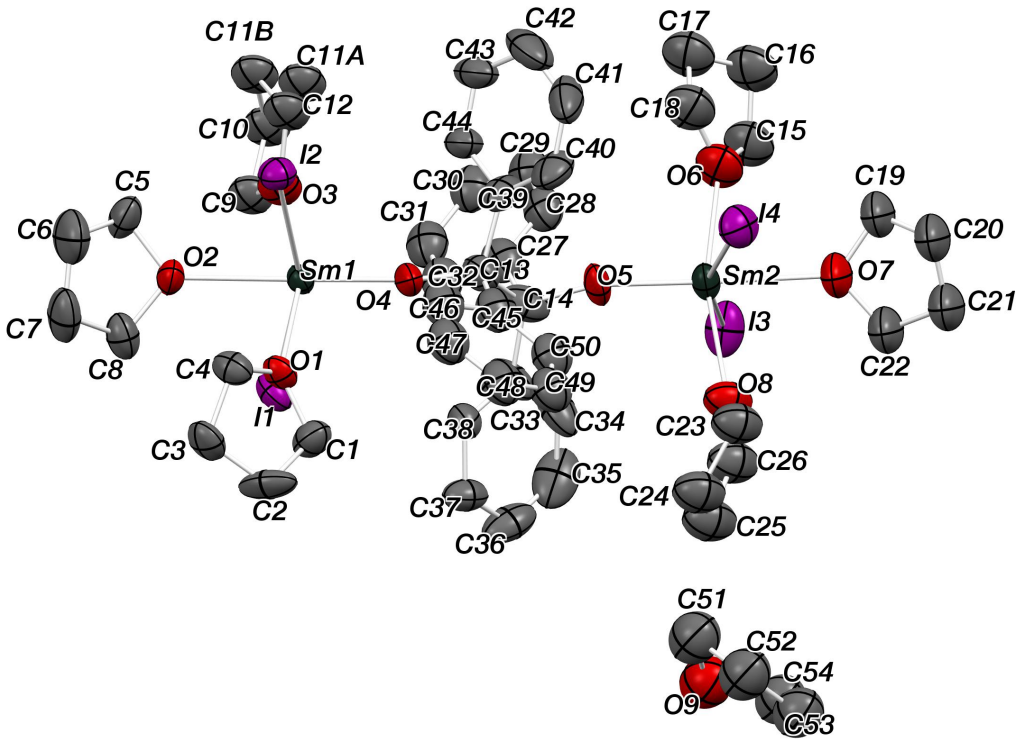

Figure S16. ORTEP of **1**. Thermal ellipsoids are at 50% level. Hydrogen atoms have been omitted for clarity.

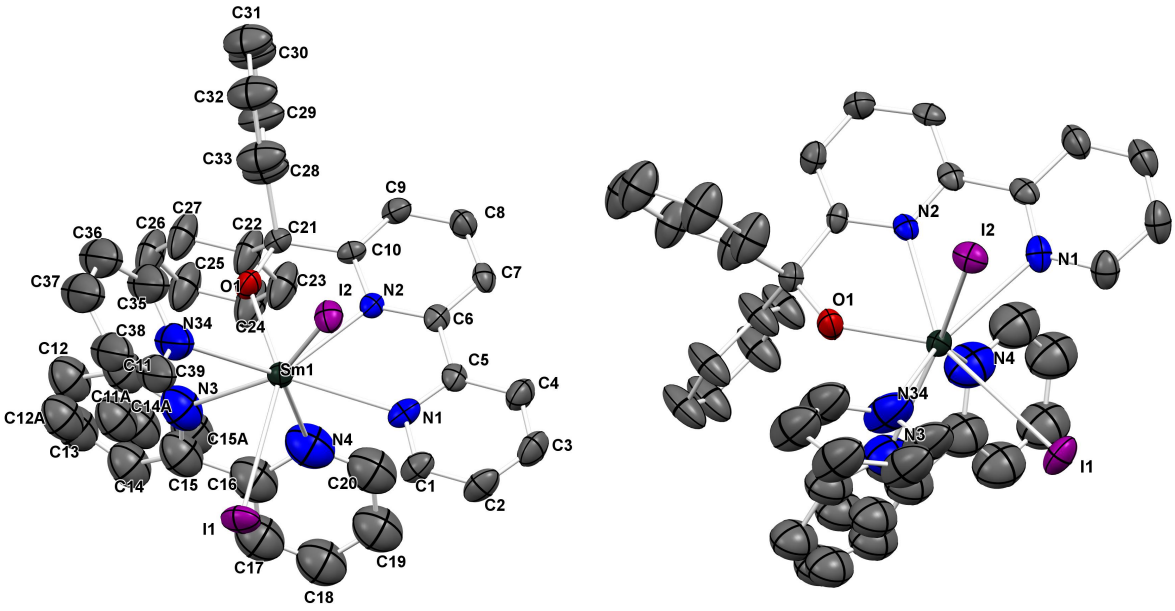

Figure S17. ORTEP of **2**. Thermal ellipsoids are at 50% level.

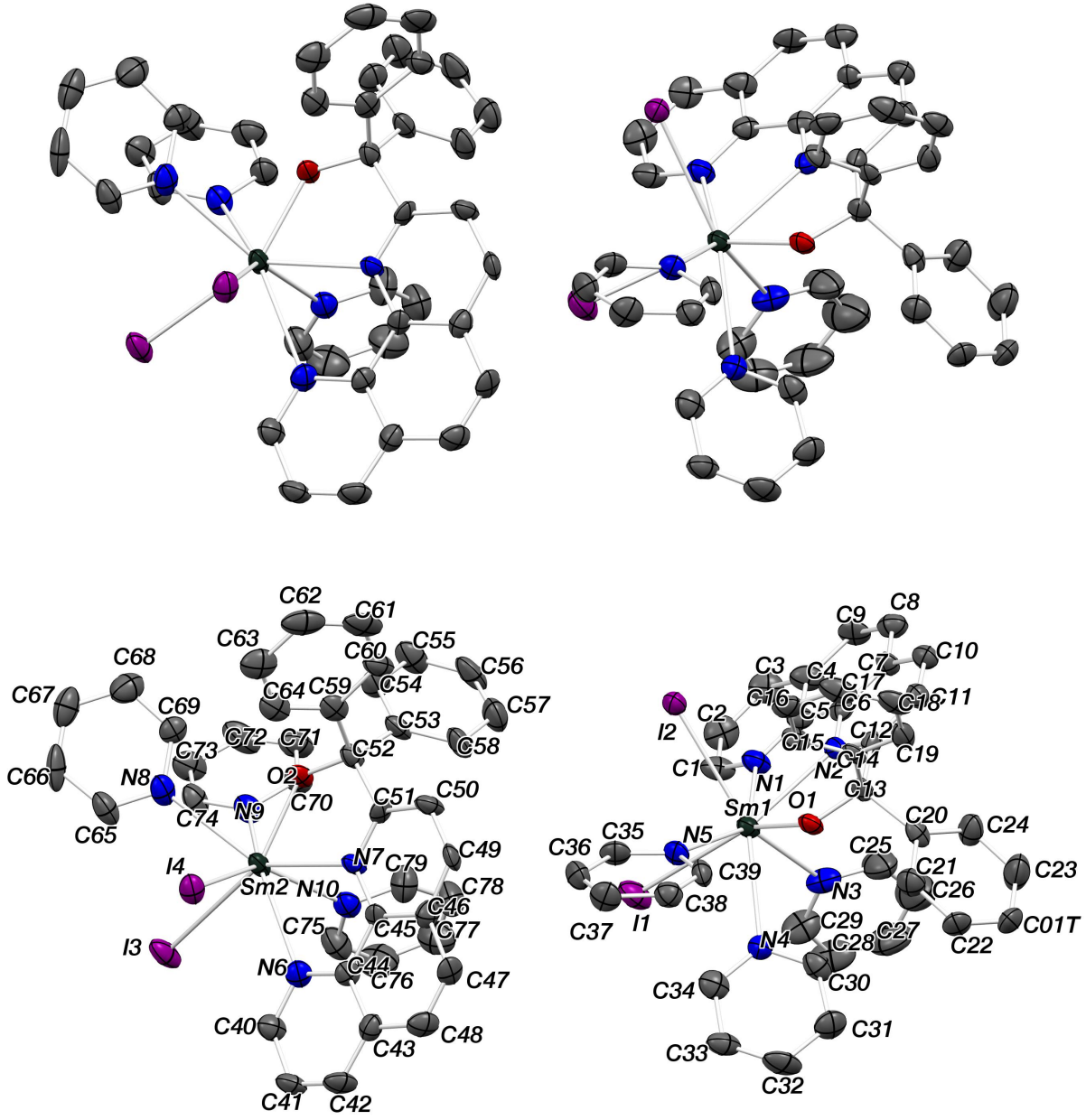

Figure S18. ORTEP of **3**. Thermal ellipsoids are at 50% level. Hydrogen atoms and solvent molecules have been omitted for clarity.

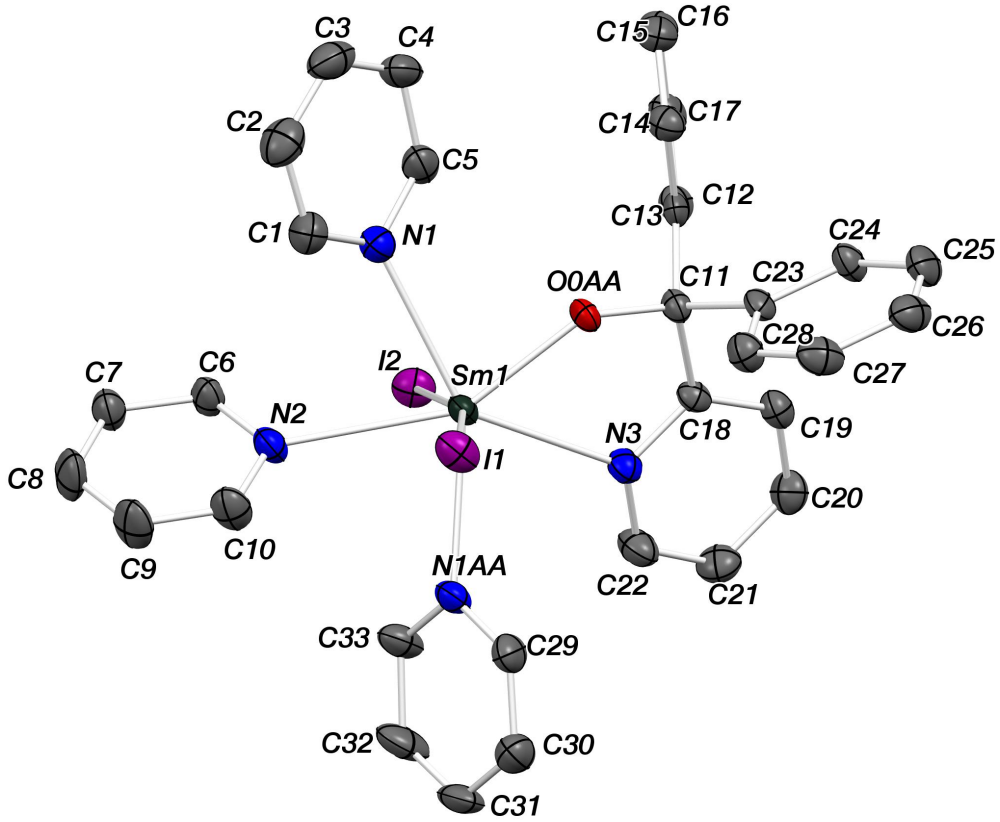

Figure S19. ORTEP of **4**. Thermal ellipsoids are at 50% level. Hydrogen atoms have been omitted for clarity.

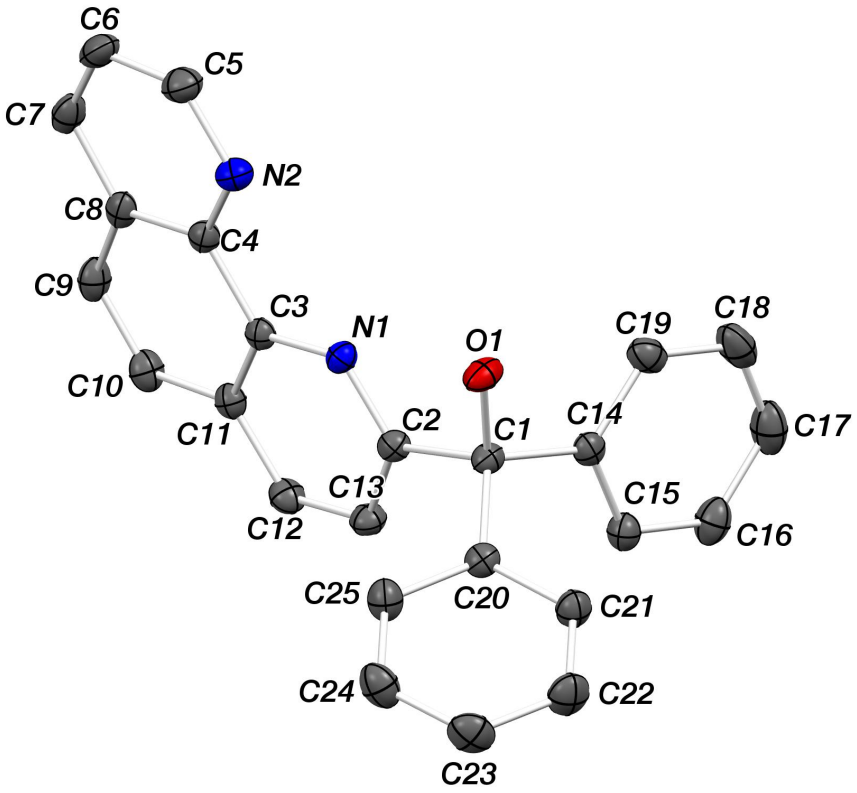

Figure S20. ORTEP of **6**. Thermal ellipsoids are at 50% level. Hydrogen atoms have been omitted for clarity.

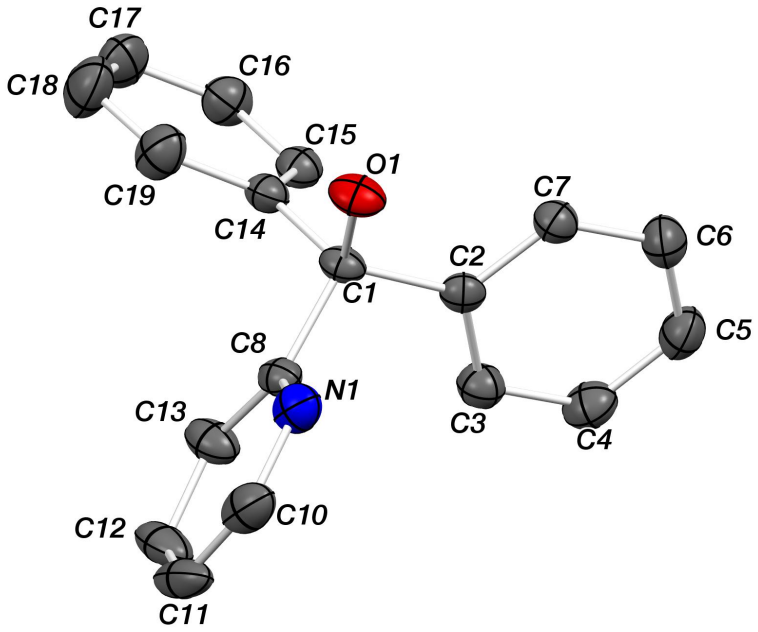

Figure S21. ORTEP of **7**. Thermal ellipsoids are at 50% level. Hydrogen atoms have been omitted for clarity.

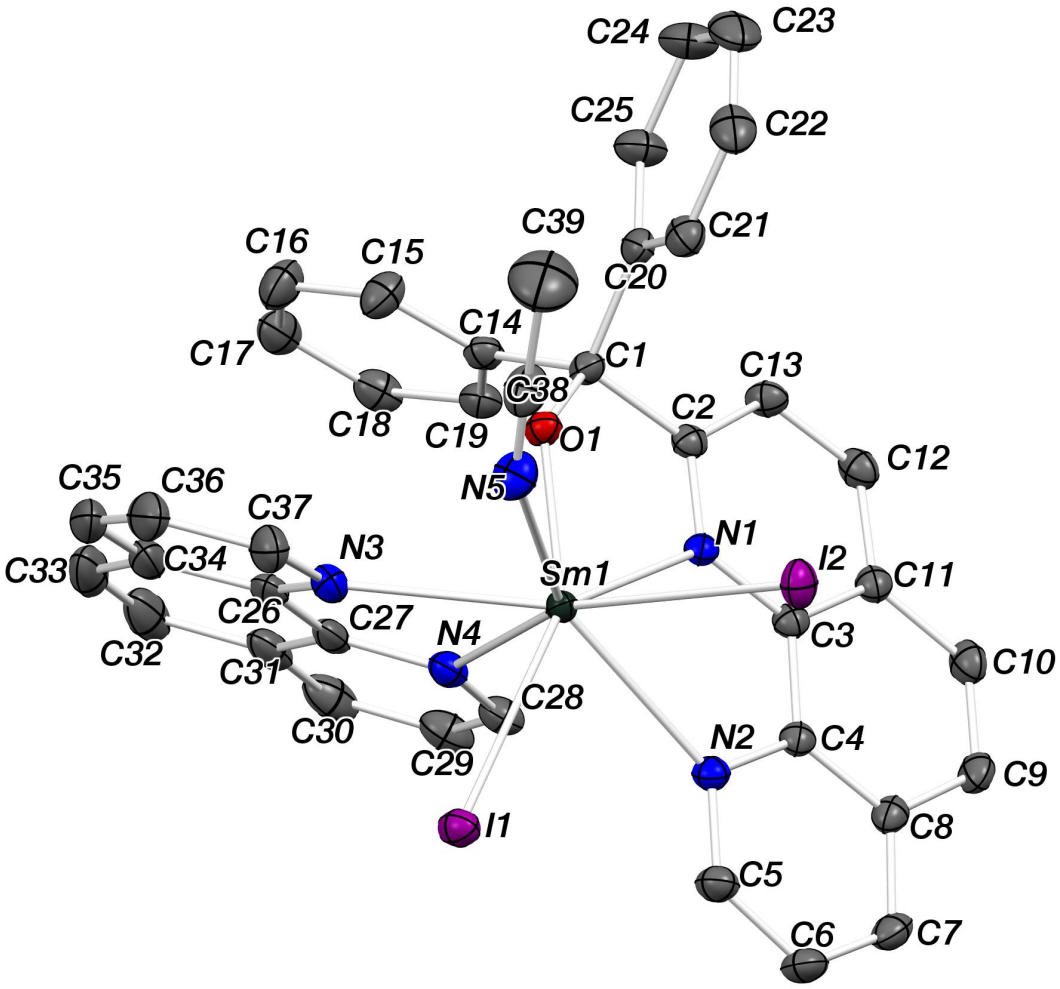

Figure S22. ORTEP of **3b**. Thermal ellipsoids are at 50 % level. Hydrogen atoms and solvents molecules have been omitted for clarity.

Table S4. Bond lengths (Å) for **1**.

Sm1	I1	3.1017(11)	C14	C27	1.64(3)
Sm1	I2	3.0937(11)	C14	C33	1.51(2)
Sm1	O1	2.449(9)	C15	C16	1.45(2)
Sm1	O2	2.487(9)	C16	C17	1.44(2)
Sm1	O3	2.421(11)	C17	C18	1.45(2)
Sm1	O4	2.066(10)	C19	C20	1.45(2)
Sm2	I4	3.0927(14)	C20	C21	1.41(2)
Sm2	O5	2.083(9)	C21	C22	1.44(2)
Sm2	O6	2.394(14)	C23	C24	1.50(2)
Sm2	O7	2.503(12)	C24	C25	1.50(2)
Sm2	O8	2.398(12)	C25	C26	1.50(2)
Sm2	I3	3.1127(14)	C27	C28	1.36(3)
O1	C1	1.409(18)	C27	C32	1.40(3)
O1	C4	1.469(17)	C28	C29	1.42(3)
O2	C5	1.445(18)	C29	C30	1.36(3)
O2	C8	1.447(19)	C30	C31	1.45(3)
O3	C9	1.469(18)	C31	C32	1.34(3)
O3	C12	1.469(18)	C33	C34	1.37(3)
O4	C13	1.46(2)	C33	C38	1.38(2)
O5	C14	1.47(2)	C34	C35	1.35(3)
O6	C15	1.52(3)	C35	C36	1.42(4)
O6	C18	1.37(3)	C36	C37	1.35(3)
O7	C19	1.42(2)	C37	C38	1.44(2)
O7	C22	1.41(2)	C39	C40	1.37(3)
O8	C23	1.50(2)	C39	C44	1.41(2)
O8	C26	1.47(3)	C40	C41	1.38(3)
C1	C2	1.55(2)	C41	C42	1.40(4)
C2	C3	1.47(3)	C42	C43	1.40(3)
C3	C4	1.48(2)	C43	C44	1.37(2)
C5	C6	1.47(3)	C45	C46	1.43(3)
C6	C7	1.51(3)	C45	C50	1.41(3)
C7	C8	1.49(3)	C46	C47	1.33(3)
C9	C10	1.53(2)	C47	C48	1.32(3)
C10	C11A	1.48(4)	C48	C49	1.34(3)
C10	C11B	1.52(3)	C49	C50	1.38(3)
C12	C11A	1.44(4)	O9	C51	1.55(3)
C12	C11B	1.53(3)	O9	C54	1.46(3)
C13	C14	1.56(3)	C51	C52	1.51(4)
C13	C39	1.59(2)	C52	C53	1.50(4)
C13	C45	1.53(3)	C53	C54	1.39(4)

Table S5. Bond angles (deg) for **1**.

I2	Sm1	I1	162.07(3)	O4	C13	C14	103.9(14)
O1	Sm1	I1	86.1(2)	O4	C13	C39	110.9(14)
O1	Sm1	I2	87.6(2)	O4	C13	C45	113.8(14)
O1	Sm1	O2	82.1(3)	C14	C13	C39	108.1(14)
O2	Sm1	I1	80.6(3)	C45	C13	C14	112.9(16)
O2	Sm1	I2	81.9(3)	C45	C13	C39	107.2(16)
O3	Sm1	I1	91.5(3)	O5	C14	C13	105.0(13)
O3	Sm1	I2	89.1(3)	O5	C14	C27	107.5(14)
O3	Sm1	O1	161.4(4)	O5	C14	C33	115.9(18)
O3	Sm1	O2	79.3(4)	C13	C14	C27	107.1(16)
O4	Sm1	I1	99.2(4)	C33	C14	C13	115.2(16)
O4	Sm1	I2	98.3(4)	C33	C14	C27	105.7(15)
O4	Sm1	O1	98.9(4)	C16	C15	O6	101.6(18)
O4	Sm1	O2	179.0(4)	C17	C16	C15	102.3(19)
O4	Sm1	O3	99.7(5)	C16	C17	C18	102(2)
I4	Sm2	I3	161.44(4)	O6	C18	C17	107(2)
O5	Sm2	I4	98.2(3)	O7	C19	C20	104.1(17)
O5	Sm2	O6	99.0(5)	C21	C20	C19	104.3(19)
O5	Sm2	O7	178.2(5)	C20	C21	C22	106.3(18)
O5	Sm2	O8	97.5(5)	O7	C22	C21	107.7(17)
O5	Sm2	I3	100.2(3)	O8	C23	C24	101.7(16)
O6	Sm2	I4	89.6(4)	C25	C24	C23	104.0(18)
O6	Sm2	O7	80.1(5)	C26	C25	C24	109.9(18)
O6	Sm2	O8	162.7(5)	O8	C26	C25	102.4(17)
O6	Sm2	I3	85.1(4)	C28	C27	C14	119.9(18)
O7	Sm2	I4	80.3(4)	C28	C27	C32	119(2)
O7	Sm2	I3	81.3(4)	C32	C27	C14	120.6(17)
O8	Sm2	I4	93.1(3)	C27	C28	C29	124(2)
O8	Sm2	O7	83.5(5)	C30	C29	C28	117.0(19)
O8	Sm2	I3	87.1(3)	C29	C30	C31	118(2)
C1	O1	Sm1	126.7(9)	C32	C31	C30	124(2)
C1	O1	C4	108.0(11)	C31	C32	C27	118(2)
C4	O1	Sm1	125.3(8)	C34	C33	C14	115.9(17)
C5	O2	Sm1	127.9(10)	C34	C33	C38	118.7(18)
C5	O2	C8	103.7(12)	C38	C33	C14	124.5(17)
C8	O2	Sm1	128.2(9)	C35	C34	C33	124(2)
C9	O3	Sm1	125.8(9)	C34	C35	C36	119(2)
C12	O3	Sm1	126.5(10)	C37	C36	C35	119.0(19)
C12	O3	C9	107.5(13)	C36	C37	C38	121.3(19)
C13	O4	Sm1	161.4(12)	C33	C38	C37	118.2(16)
C14	O5	Sm2	159.3(12)	C40	C39	C13	124.3(17)
C15	O6	Sm2	128.2(13)	C40	C39	C44	118.0(17)
C18	O6	Sm2	124.4(12)	C44	C39	C13	117.7(16)
C18	O6	C15	106.6(16)	C39	C40	C41	121(2)
C19	O7	Sm2	125.8(11)	C40	C41	C42	121(2)
C22	O7	Sm2	129.2(12)	C43	C42	C41	118.4(18)
C22	O7	C19	103.8(15)	C44	C43	C42	120(2)
C23	O8	Sm2	122.9(11)	C43	C44	C39	121.6(19)

C26	O8	Sm2	128.4(11)	C46	C45	C13	116.6(18)
C26	O8	C23	108.6(14)	C50	C45	C13	126.1(18)
O1	C1	C2	106.3(13)	C50	C45	C46	117(2)
C3	C2	C1	104.2(12)	C47	C46	C45	120(2)
C2	C3	C4	104.3(13)	C48	C47	C46	124(2)
O1	C4	C3	103.2(12)	C47	C48	C49	117(2)
O2	C5	C6	104.2(16)	C48	C49	C50	125(2)
C5	C6	C7	105.1(19)	C49	C50	C45	117(2)
C8	C7	C6	104.3(16)	C12	C11A	C10	109(2)
O2	C8	C7	106.5(16)	C10	C11B	C12	102(2)
O3	C9	C10	105.6(14)	C54	O9	C51	103(2)
C11A	C10	C9	104.1(17)	C52	C51	O9	99(2)
C11B	C10	C9	100.5(19)	C53	C52	C51	109(2)
O3	C12	C11B	106.3(18)	C54	C53	C52	105(2)
C11A	C12	O3	103(2)	C53	C54	O9	109(2)

Table S6. Bond lengths (Å) for **2**.

Sm1	I2	3.2049(10)	C30	C31	1.3900
Sm1	I1	3.2129(10)	C31	C32	1.3900
Sm1	O1	2.145(8)	C32	C33	1.3900
Sm1	N1	2.653(10)	C22	C27	1.3900
Sm1	N2	2.556(9)	C22	C23	1.3900
Sm1	N3	2.633(16)	C27	C26	1.3900
Sm1	N34	2.703(15)	C26	C25	1.3900
Sm1	N4	2.662(11)	C25	C24	1.3900
O1	C21	1.381(14)	C24	C23	1.3900
N1	C5	1.342(15)	N34	C39	1.31(3)
N1	C1	1.356(16)	N34	C35	1.30(3)
N2	C6	1.352(14)	C39	C38	1.39(3)
N2	C10	1.352(13)	C3	C2	1.38(2)
C21	C10	1.519(16)	N4	C20	1.3900
C21	C28	1.551(13)	N4	C16	1.3900
C21	C22	1.533(13)	C20	C19	1.3900
C6	C5	1.485(16)	C19	C18	1.3900
C6	C7	1.387(16)	C18	C17	1.3900
C5	C4	1.402(17)	C17	C16	1.3900
C10	C9	1.385(16)	C36	C37	1.40(3)
C4	C3	1.38(2)	C36	C35	1.35(3)
N3	C15	1.24(3)	C37	C38	1.36(3)
N3	C11	1.41(3)	C13	C14	1.30(3)
N3	C15A	1.26(3)	C13	C12	1.44(3)
N3	C11A	1.41(3)	C13	C14A	1.31(4)
C8	C7	1.382(17)	C13	C12A	1.43(4)
C8	C9	1.389(17)	C14	C15	1.44(3)
C1	C2	1.39(2)	C12	C11	1.35(3)
C28	C29	1.3900	C14A	C15A	1.44(3)
C28	C33	1.3900	C11A	C12A	1.35(4)
C29	C30	1.3900			

Table S7. Bond angles (deg) for **2**.

I2	Sm1	I1	97.56(3)	C11	N3	Sm1	117.7(15)
O1	Sm1	I2	98.4(3)	C15A	N3	Sm1	121(2)
O1	Sm1	I1	147.1(2)	C15A	N3	C11A	113(3)
O1	Sm1	N1	126.4(3)	C11A	N3	Sm1	124.2(19)
O1	Sm1	N2	65.1(3)	C7	C8	C9	119.8(11)
O1	Sm1	N3	74.8(5)	N1	C1	C2	121.8(13)
O1	Sm1	N34	77.0(5)	C29	C28	C21	121.3(7)
O1	Sm1	N4	101.1(4)	C29	C28	C33	120.0
N1	Sm1	I2	72.5(2)	C33	C28	C21	118.7(7)
N1	Sm1	I1	85.8(2)	C28	C29	C30	120.0
N1	Sm1	N34	138.9(5)	C31	C30	C29	120.0
N1	Sm1	N4	74.7(4)	C30	C31	C32	120.0
N2	Sm1	I2	86.21(19)	C31	C32	C33	120.0
N2	Sm1	I1	144.7(2)	C32	C33	C28	120.0
N2	Sm1	N1	61.8(3)	C8	C7	C6	118.7(11)
N2	Sm1	N3	116.9(4)	C27	C22	C21	117.2(7)
N2	Sm1	N34	132.0(4)	C27	C22	C23	120.0
N2	Sm1	N4	78.6(4)	C23	C22	C21	122.2(7)
N3	Sm1	I2	148.1(4)	C26	C27	C22	120.0
N3	Sm1	I1	76.4(4)	C27	C26	C25	120.0
N3	Sm1	N1	136.7(5)	C24	C25	C26	120.0
N3	Sm1	N34	77.4(6)	C25	C24	C23	120.0
N3	Sm1	N4	63.4(5)	C24	C23	C22	120.0
N34	Sm1	I2	70.7(4)	C10	C9	C8	119.2(11)
N34	Sm1	I1	81.4(3)	C39	N34	Sm1	123.5(14)
N4	Sm1	I2	147.3(3)	C39	N34	C35	115.9(18)
N4	Sm1	I1	79.7(3)	C35	N34	Sm1	118.7(13)
N4	Sm1	N34	139.5(5)	N34	C39	C38	126(2)
C21	O1	Sm1	133.2(7)	C4	C3	C2	119.9(13)
C5	N1	Sm1	121.1(7)	C3	C2	C1	119.0(13)
C5	N1	C1	118.7(11)	C20	N4	Sm1	125.9(7)
C1	N1	Sm1	120.1(9)	C20	N4	C16	120.0
C6	N2	Sm1	124.6(7)	C16	N4	Sm1	108.4(7)
C10	N2	Sm1	115.5(7)	C19	C20	N4	120.0
C10	N2	C6	119.9(10)	C18	C19	C20	120.0
O1	C21	C10	108.5(9)	C19	C18	C17	120.0
O1	C21	C28	109.8(9)	C16	C17	C18	120.0
O1	C21	C22	107.6(10)	C17	C16	N4	120.0
C10	C21	C28	107.4(9)	C35	C36	C37	119(2)
C10	C21	C22	111.9(9)	C36	C37	C38	119(2)
C22	C21	C28	111.6(9)	C14	C13	C12	121(2)
N2	C6	C5	115.9(10)	C14A	C13	C12A	118(3)
N2	C6	C7	121.5(10)	C13	C14	C15	119(3)
C7	C6	C5	122.6(10)	C37	C38	C39	115(2)
N1	C5	C6	116.5(10)	N3	C15	C14	123(3)
N1	C5	C4	122.1(12)	C11	C12	C13	114(3)
C4	C5	C6	121.4(11)	N34	C35	C36	124(2)
N2	C10	C21	115.7(9)	C12	C11	N3	125(3)

N2	C10	C9	120.9(10)	C13	C14A	C15A	121(3)
C9	C10	C21	123.3(10)	N3	C15A	C14A	116(3)
C3	C4	C5	118.4(14)	C12A	C11A	N3	125(3)
C15	N3	Sm1	125.8(17)	C11A	C12A	C13	113(3)
C15	N3	C11	117(2)				

Table S8. Bond lengths for **3**.

Sm1	I1	3.2739(12)	N10	C79	1.33(2)
Sm1	I2	3.1747(11)	C40	C41	1.413(19)
Sm1	O1	2.134(9)	C41	C42	1.36(2)
Sm1	N1	2.712(11)	C42	C43	1.40(2)
Sm1	N2	2.571(10)	C43	C44	1.411(17)
Sm1	N3	2.615(12)	C43	C48	1.435(19)
Sm1	N4	2.722(11)	C44	C45	1.432(18)
Sm1	N5	2.669(11)	C45	C46	1.407(18)
O1	C13	1.390(15)	C46	C47	1.441(17)
N1	C1	1.333(18)	C46	C49	1.392(19)
N1	C5	1.356(17)	C47	C48	1.33(2)
N2	C6	1.364(16)	C49	C50	1.356(18)
N2	C12	1.311(16)	C50	C51	1.391(18)
N3	C25	1.29(2)	C51	C52	1.540(17)
N3	C29	1.35(2)	C52	C53	1.56(2)
N4	C30	1.324(19)	C52	C59	1.55(2)
N4	C34	1.343(19)	C53	C54	1.392(18)
N5	C35	1.337(18)	C53	C58	1.38(2)
N5	C39	1.329(17)	C54	C55	1.38(2)
C1	C2	1.40(2)	C55	C56	1.35(2)
C01T	C22	1.39(2)	C56	C57	1.35(2)
C01T	C23	1.40(2)	C57	C58	1.38(2)
C2	C3	1.39(2)	C59	C60	1.433(19)
C3	C4	1.41(2)	C59	C64	1.39(2)
C4	C5	1.428(18)	C60	C61	1.35(2)
C4	C9	1.43(2)	C61	C62	1.39(3)
C5	C6	1.450(18)	C62	C63	1.40(2)
C6	C7	1.429(17)	C63	C64	1.40(2)
C7	C8	1.430(18)	C65	C66	1.40(2)
C7	C10	1.386(19)	C66	C67	1.35(3)
C8	C9	1.32(2)	C67	C68	1.38(2)
C10	C11	1.376(18)	C68	C69	1.36(2)
C11	C12	1.423(18)	C70	C71	1.40(2)
C12	C13	1.540(17)	C71	C72	1.35(2)
C13	C14	1.555(19)	C72	C73	1.38(2)
C13	C20	1.538(19)	C73	C74	1.397(19)
C14	C15	1.379(19)	C75	C76	1.34(3)
C14	C19	1.366(18)	C76	C77	1.37(3)
C15	C16	1.41(2)	C77	C78	1.35(3)
C16	C17	1.38(2)	C78	C79	1.39(2)
C17	C18	1.35(2)	N14	C95	1.39(3)
C18	C19	1.38(2)	N14	C99	1.36(3)
C20	C21	1.400(19)	C95	C96	1.37(3)
C20	C24	1.39(2)	C96	C97	1.34(4)
C21	C22	1.36(2)	C97	C98	1.24(3)
C23	C24	1.37(2)	C98	C99	1.36(3)
C25	C26	1.39(3)	N15	C100	1.42(4)
C26	C27	1.38(3)	N15	C104	1.37(3)

C27	C28	1.33(3)	C100	C101	1.32(4)
C28	C29	1.34(2)	C101	C102	1.29(4)
C30	C31	1.39(2)	C102	C103	1.43(4)
C31	C32	1.37(2)	C103	C104	1.39(4)
C32	C33	1.35(2)	N13	C90	1.36(3)
C33	C34	1.40(2)	N13	C94	1.35(3)
C35	C36	1.40(2)	C90	C91	1.38(3)
C36	C37	1.37(2)	C91	C92	1.38(3)
C37	C38	1.38(2)	C92	C93	1.39(3)
C38	C39	1.403(19)	C93	C94	1.29(3)
Sm2	I3	3.2693(11)	N11	C80	1.37(3)
Sm2	I4	3.2104(11)	N11	C84	1.33(3)
Sm2	O2	2.159(9)	C80	C81	1.32(3)
Sm2	N6	2.682(11)	C81	C82	1.32(3)
Sm2	N7	2.548(10)	C82	C83	1.37(3)
Sm2	N8	2.663(12)	C83	C84	1.33(3)
Sm2	N9	2.727(11)	N16	C105	1.37(3)
Sm2	N10	2.651(12)	N16	C109	1.33(3)
O2	C52	1.400(14)	C105	C106	1.41(3)
N6	C40	1.334(18)	C106	C107	1.38(3)
N6	C44	1.365(16)	C107	C108	1.37(3)
N7	C45	1.354(15)	C108	C109	1.33(3)
N7	C51	1.327(17)	N12	C85	1.39(3)
N8	C65	1.308(18)	N12	C89	1.35(3)
N8	C69	1.338(18)	C85	C86	1.37(3)
N9	C70	1.358(18)	C86	C87	1.27(3)
N9	C74	1.326(17)	C87	C88	1.29(3)
N10	C75	1.33(2)	C88	C89	1.38(3)

Table S9. Bond angles (Å) for **3**.

I2	Sm1	I1	93.81(3)	N8	Sm2	I4	75.0(2)
O1	Sm1	I1	149.4(2)	N8	Sm2	N6	142.7(4)
O1	Sm1	I2	100.8(2)	N8	Sm2	N9	69.6(4)
O1	Sm1	N1	126.6(3)	N9	Sm2	I3	76.0(2)
O1	Sm1	N2	64.7(3)	N9	Sm2	I4	144.0(3)
O1	Sm1	N3	96.0(4)	N10	Sm2	I3	87.4(3)
O1	Sm1	N4	76.8(3)	N10	Sm2	I4	143.9(2)
O1	Sm1	N5	77.3(3)	N10	Sm2	N6	71.5(3)
N1	Sm1	I1	83.3(2)	N10	Sm2	N8	140.5(3)
N1	Sm1	I2	73.0(3)	N10	Sm2	N9	70.9(4)
N1	Sm1	N4	135.7(4)	C52	O2	Sm2	133.8(7)
N2	Sm1	I1	145.2(2)	C40	N6	Sm2	125.3(9)
N2	Sm1	I2	79.3(2)	C40	N6	C44	117.7(11)
N2	Sm1	N1	62.0(3)	C44	N6	Sm2	116.8(9)
N2	Sm1	N3	77.5(4)	C45	N7	Sm2	122.3(8)
N2	Sm1	N4	126.6(3)	C51	N7	Sm2	119.0(8)
N2	Sm1	N5	129.7(4)	C51	N7	C45	118.6(11)
N3	Sm1	I1	88.5(3)	C65	N8	Sm2	124.4(11)
N3	Sm1	I2	142.0(3)	C65	N8	C69	117.7(14)
N3	Sm1	N1	69.6(4)	C69	N8	Sm2	117.8(9)
N3	Sm1	N4	71.1(4)	C70	N9	Sm2	118.2(9)
N3	Sm1	N5	140.7(4)	C74	N9	Sm2	124.8(9)
N4	Sm1	I1	76.2(3)	C74	N9	C70	116.3(12)
N4	Sm1	I2	146.0(3)	C75	N10	Sm2	122.5(10)
N5	Sm1	I1	80.2(3)	C75	N10	C79	115.6(14)
N5	Sm1	I2	76.6(2)	C79	N10	Sm2	121.8(11)
N5	Sm1	N1	144.2(4)	N6	C40	C41	124.3(13)
N5	Sm1	N4	69.7(4)	C42	C41	C40	117.2(13)
C13	O1	Sm1	134.9(7)	C41	C42	C43	121.0(12)
C1	N1	Sm1	124.0(9)	C42	C43	C44	117.7(13)
C1	N1	C5	117.2(12)	C42	C43	C48	122.8(12)
C5	N1	Sm1	118.8(8)	C44	C43	C48	119.5(13)
C6	N2	Sm1	123.2(8)	N6	C44	C43	122.1(13)
C12	N2	Sm1	116.3(8)	N6	C44	C45	119.1(11)
C12	N2	C6	120.4(11)	C43	C44	C45	118.9(12)
C25	N3	Sm1	127.0(12)	N7	C45	C44	118.5(11)
C25	N3	C29	115.2(16)	N7	C45	C46	121.2(12)
C29	N3	Sm1	117.6(12)	C46	C45	C44	120.3(11)
C30	N4	Sm1	115.6(9)	C45	C46	C47	118.7(13)
C30	N4	C34	118.4(13)	C49	C46	C45	117.9(12)
C34	N4	Sm1	125.2(10)	C49	C46	C47	123.3(12)
C35	N5	Sm1	125.0(9)	C48	C47	C46	121.3(12)
C39	N5	Sm1	119.1(9)	C47	C48	C43	121.3(12)
C39	N5	C35	115.7(11)	C50	C49	C46	120.5(12)
N1	C1	C2	123.0(15)	C49	C50	C51	118.1(12)
C22	C01T	C23	118.9(14)	N7	C51	C50	123.4(11)
C3	C2	C1	120.1(15)	N7	C51	C52	113.7(11)
C2	C3	C4	119.1(14)	C50	C51	C52	122.8(12)

C3	C4	C5	116.1(14)	O2	C52	C51	108.9(10)
C3	C4	C9	124.5(13)	O2	C52	C53	107.8(11)
C5	C4	C9	119.4(13)	O2	C52	C59	110.7(11)
N1	C5	C4	124.5(12)	C51	C52	C53	111.4(11)
N1	C5	C6	117.7(11)	C51	C52	C59	107.6(11)
C4	C5	C6	117.8(12)	C59	C52	C53	110.5(11)
N2	C6	C5	118.2(11)	C54	C53	C52	117.9(13)
N2	C6	C7	121.7(12)	C58	C53	C52	126.2(12)
C7	C6	C5	120.1(11)	C58	C53	C54	115.9(14)
C6	C7	C8	118.9(12)	C55	C54	C53	122.9(15)
C10	C7	C6	117.6(11)	C56	C55	C54	118.8(15)
C10	C7	C8	123.4(12)	C55	C56	C57	120.3(15)
C9	C8	C7	121.1(14)	C56	C57	C58	121.5(16)
C8	C9	C4	122.7(13)	C57	C58	C53	120.6(14)
C11	C10	C7	119.2(13)	C60	C59	C52	120.1(13)
C10	C11	C12	120.7(13)	C64	C59	C52	120.4(12)
N2	C12	C11	120.3(12)	C64	C59	C60	119.4(15)
N2	C12	C13	116.1(11)	C61	C60	C59	119.5(17)
C11	C12	C13	123.6(11)	C60	C61	C62	121.5(17)
O1	C13	C12	107.6(10)	C61	C62	C63	120.2(17)
O1	C13	C14	111.7(10)	C64	C63	C62	119.0(18)
O1	C13	C20	108.5(10)	C59	C64	C63	120.3(15)
C12	C13	C14	108.4(10)	N8	C65	C66	122.5(16)
C20	C13	C12	111.5(10)	C67	C66	C65	119.7(15)
C20	C13	C14	109.2(10)	C66	C67	C68	117.4(16)
C15	C14	C13	119.2(10)	C69	C68	C67	120.0(17)
C19	C14	C13	122.4(12)	N8	C69	C68	122.6(15)
C19	C14	C15	118.4(13)	N9	C70	C71	123.3(14)
C14	C15	C16	120.0(12)	C72	C71	C70	118.3(16)
C17	C16	C15	120.0(15)	C71	C72	C73	120.2(14)
C18	C17	C16	118.9(15)	C72	C73	C74	117.7(14)
C17	C18	C19	121.1(14)	N9	C74	C73	124.1(14)
C14	C19	C18	121.2(14)	N10	C75	C76	124.6(17)
C21	C20	C13	116.4(12)	C75	C76	C77	119.5(19)
C24	C20	C13	125.3(12)	C78	C77	C76	117.8(19)
C24	C20	C21	118.2(14)	C77	C78	C79	119.1(18)
C22	C21	C20	120.6(15)	N10	C79	C78	123.3(17)
C21	C22	C01T	121.1(13)	C99	N14	C95	115(2)
C24	C23	C01T	119.6(16)	C96	C95	N14	118(2)
C23	C24	C20	121.6(15)	C97	C96	C95	126(2)
N3	C25	C26	124(2)	C98	C97	C96	113(2)
C27	C26	C25	117(2)	C97	C98	C99	127(2)
C28	C27	C26	120(2)	C98	C99	N14	121(2)
C27	C28	C29	118(2)	C104	N15	C100	117(3)
C28	C29	N3	125(2)	C101	C100	N15	123(3)
N4	C30	C31	122.2(14)	C102	C101	C100	119(3)
C32	C31	C30	118.4(15)	C101	C102	C103	123(3)
C33	C32	C31	120.8(14)	C104	C103	C102	117(3)
C32	C33	C34	117.5(15)	N15	C104	C103	120(3)
N4	C34	C33	122.5(15)	C94	N13	C90	115(2)

N5	C35	C36	124.7(14)	N13	C90	C91	125(2)
C37	C36	C35	118.1(14)	C92	C91	C90	117(2)
C36	C37	C38	118.9(13)	C91	C92	C93	117.5(18)
C37	C38	C39	118.6(13)	C94	C93	C92	122(2)
N5	C39	C38	124.0(12)	C93	C94	N13	124(2)
I4	Sm2	I3	93.24(3)	C84	N11	C80	119(2)
O2	Sm2	I3	150.4(2)	C81	C80	N11	120(2)
O2	Sm2	I4	101.7(3)	C82	C81	C80	122(2)
O2	Sm2	N6	127.5(3)	C81	C82	C83	118(2)
O2	Sm2	N7	64.4(3)	C84	C83	C82	121(2)
O2	Sm2	N8	77.4(4)	C83	C84	N11	121(2)
O2	Sm2	N9	76.9(3)	C109	N16	C105	112.4(19)
O2	Sm2	N10	95.0(4)	N16	C105	C106	126(2)
N6	Sm2	I3	81.2(3)	C107	C106	C105	116(2)
N6	Sm2	I4	73.0(3)	C108	C107	C106	118(2)
N6	Sm2	N9	136.5(4)	C109	C108	C107	120(2)
N7	Sm2	I3	143.9(2)	C108	C109	N16	127(2)
N7	Sm2	I4	81.9(3)	C89	N12	C85	117.6(18)
N7	Sm2	N6	63.1(3)	C86	C85	N12	119.0(19)
N7	Sm2	N8	129.8(4)	C87	C86	C85	123(2)
N7	Sm2	N9	126.3(3)	C86	C87	C88	118.1(19)
N7	Sm2	N10	76.7(4)	C87	C88	C89	125(2)
N8	Sm2	I3	82.1(3)	N12	C89	C88	117.0(19)

Table S10. Bond lengths (Å) for **4**.

Sm1	I1	3.1337(5)	C11	C12	1.545(7)
Sm1	I2	3.1057(5)	C11	C18	1.544(7)
Sm1	O1	2.128(3)	C11	C23	1.548(7)
Sm1	N1	2.612(4)	C12	C13	1.385(7)
Sm1	N4	2.569(4)	C12	C17	1.391(7)
Sm1	N2	2.680(4)	C13	C14	1.398(7)
Sm1	N3	2.632(4)	C14	C15	1.382(8)
O1	C11	1.395(6)	C15	C16	1.376(8)
N1	C1	1.345(7)	C16	C17	1.379(7)
N1	C5	1.329(7)	C18	C19	1.394(7)
N4	C29	1.333(7)	C19	C20	1.358(7)
N4	C33	1.338(7)	C20	C21	1.375(8)
N2	C6	1.340(7)	C21	C22	1.371(8)
N2	C10	1.350(7)	C23	C24	1.379(7)
N3	C18	1.341(6)	C23	C28	1.402(7)
N3	C22	1.347(7)	C24	C25	1.391(7)
C1	C2	1.381(8)	C25	C26	1.380(8)
C2	C3	1.388(9)	C26	C27	1.380(8)
C3	C4	1.366(9)	C27	C28	1.379(8)
C4	C5	1.387(8)	C29	C30	1.381(8)
C6	C7	1.365(7)	C30	C31	1.378(8)
C7	C8	1.380(8)	C31	C32	1.373(9)
C8	C9	1.367(8)	C32	C33	1.399(8)
C9	C10	1.360(8)			

Table S11. Bond angles (deg) for **4**.

I2	Sm1	I1	165.289(13)	N2	C6	C7	123.4(5)
O1	Sm1	I1	90.84(9)	C6	C7	C8	118.6(5)
O1	Sm1	I2	103.00(9)	C9	C8	C7	118.9(5)
O1	Sm1	N1	78.45(13)	C10	C9	C8	119.4(5)
O1	Sm1	N4	130.65(13)	N2	C10	C9	122.9(5)
O1	Sm1	N2	151.16(13)	O1	C11	C12	107.8(4)
O1	Sm1	N3	64.55(13)	O1	C11	C18	108.7(4)
N1	Sm1	I1	86.12(10)	O1	C11	C23	111.2(4)
N1	Sm1	I2	91.74(10)	C12	C11	C23	110.2(4)
N1	Sm1	N2	72.90(13)	C18	C11	C12	112.7(4)
N1	Sm1	N3	136.85(13)	C18	C11	C23	106.2(4)
N4	Sm1	I1	81.19(10)	C13	C12	C11	124.6(4)
N4	Sm1	I2	93.23(10)	C13	C12	C17	118.2(5)
N4	Sm1	N1	148.03(14)	C17	C12	C11	117.0(4)
N4	Sm1	N2	76.68(13)	C12	C13	C14	120.4(5)
N4	Sm1	N3	74.86(13)	C15	C14	C13	120.0(5)
N2	Sm1	I1	84.10(9)	C16	C15	C14	120.1(5)
N2	Sm1	I2	81.36(10)	C15	C16	C17	119.5(5)
N3	Sm1	I1	114.53(9)	C16	C17	C12	121.8(5)
N3	Sm1	I2	76.61(9)	N3	C18	C11	115.7(4)
N3	Sm1	N2	142.63(13)	N3	C18	C19	120.7(4)

C11	O1	Sm1	134.8(3)	C19	C18	C11	123.6(4)
C1	N1	Sm1	124.6(4)	C20	C19	C18	120.3(5)
C5	N1	Sm1	115.9(4)	C19	C20	C21	119.5(5)
C5	N1	C1	117.9(5)	C22	C21	C20	117.8(5)
C29	N4	Sm1	121.9(3)	N3	C22	C21	123.8(5)
C29	N4	C33	117.6(5)	C24	C23	C11	122.2(5)
C33	N4	Sm1	120.0(3)	C24	C23	C28	118.9(5)
C6	N2	Sm1	120.8(3)	C28	C23	C11	118.9(4)
C6	N2	C10	116.8(5)	C23	C24	C25	120.5(5)
C10	N2	Sm1	122.4(3)	C26	C25	C24	120.4(5)
C18	N3	Sm1	113.9(3)	C25	C26	C27	119.4(5)
C18	N3	C22	117.9(5)	C28	C27	C26	120.7(5)
C22	N3	Sm1	127.2(3)	C27	C28	C23	120.2(5)
N1	C1	C2	122.3(6)	N4	C29	C30	123.5(5)
C1	C2	C3	118.7(6)	C31	C30	C29	118.8(5)
C4	C3	C2	119.4(6)	C32	C31	C30	118.7(5)
C3	C4	C5	118.3(6)	C31	C32	C33	119.1(5)
N1	C5	C4	123.4(6)	N4	C33	C32	122.3(5)

Table S12. Bond lengths (Å) for **6**.

C1	C2	1.5438(15)	C9	C10	1.3518(18)
C1	C14	1.5362(16)	C10	C11	1.4303(16)
C1	C20	1.5278(16)	C11	C12	1.4102(16)
C1	O1	1.4236(13)	C12	C13	1.3689(17)
C2	C13	1.4108(15)	C14	C15	1.3931(16)
C2	N1	1.3190(14)	C14	C19	1.3957(16)
C3	C4	1.4435(15)	C15	C16	1.3864(17)
C3	C11	1.4118(15)	C16	C17	1.386(2)
C3	N1	1.3538(14)	C17	C18	1.376(2)
C4	C8	1.4123(16)	C18	C19	1.3924(19)
C4	N2	1.3600(14)	C20	C21	1.3914(17)
C5	C6	1.3971(19)	C20	C25	1.3947(16)
C5	N2	1.3240(16)	C21	C22	1.3914(17)
C6	C7	1.3682(19)	C22	C23	1.3866(19)
C7	C8	1.4113(17)	C23	C24	1.382(2)
C8	C9	1.4297(17)	C24	C25	1.3876(18)

Table S12. Bond angles (deg) for **6**.

C14	C1	C2	107.44(9)	C3	C11	C10	119.52(10)
C20	C1	C2	112.53(9)	C12	C11	C3	117.29(10)
C20	C1	C14	113.10(9)	C12	C11	C10	123.19(10)
O1	C1	C2	107.78(9)	C13	C12	C11	120.14(10)
O1	C1	C14	109.67(9)	C12	C13	C2	118.50(11)
O1	C1	C20	106.19(8)	C15	C14	C1	121.07(10)
C13	C2	C1	124.01(10)	C15	C14	C19	118.49(11)
N1	C2	C1	113.34(9)	C19	C14	C1	120.42(10)
N1	C2	C13	122.61(10)	C16	C15	C14	120.89(12)
C11	C3	C4	119.71(10)	C15	C16	C17	120.07(13)
N1	C3	C4	118.35(9)	C18	C17	C16	119.67(12)
N1	C3	C11	121.93(10)	C17	C18	C19	120.61(12)
C8	C4	C3	118.96(10)	C18	C19	C14	120.26(12)
N2	C4	C3	117.99(10)	C21	C20	C1	120.80(10)
N2	C4	C8	123.06(10)	C21	C20	C25	118.38(11)
N2	C5	C6	124.87(12)	C25	C20	C1	120.40(10)
C7	C6	C5	118.48(11)	C20	C21	C22	120.89(11)
C6	C7	C8	119.33(12)	C23	C22	C21	119.96(12)
C4	C8	C9	119.69(11)	C24	C23	C22	119.71(12)
C7	C8	C4	117.54(11)	C23	C24	C25	120.26(12)
C7	C8	C9	122.77(11)	C24	C25	C20	120.79(12)
C10	C9	C8	121.29(11)	C2	N1	C3	119.49(9)
C9	C10	C11	120.82(11)	C5	N2	C4	116.72(11)

Table S13. Bond lengths (Å) for **7**.

C1	C2	1.5342(17)	C8	N1	1.3426(17)
C1	C8	1.5344(16)	C10	C11	1.373(2)
C1	C14	1.5292(17)	C10	N1	1.3448(18)
C1	O1	1.4265(14)	C11	C12	1.382(2)
C2	C3	1.3947(18)	C12	C13	1.385(2)
C2	C7	1.3780(18)	C14	C15	1.3858(18)
C3	C4	1.3859(19)	C14	C19	1.3904(19)
C4	C5	1.382(2)	C15	C16	1.3915(19)
C5	C6	1.378(2)	C16	C17	1.374(2)
C6	C7	1.3790(19)	C17	C18	1.384(2)
C8	C13	1.3815(19)	C18	C19	1.383(2)

Table S14. Bond angles (deg) for **7**.

C2	C1	C8	110.09(10)	N1	C8	C1	114.22(11)
C14	C1	C2	112.53(10)	N1	C8	C13	122.45(12)
C14	C1	C8	110.56(10)	N1	C10	C11	123.07(14)
O1	C1	C2	109.23(10)	C10	C11	C12	118.74(13)
O1	C1	C8	107.89(9)	C11	C12	C13	118.95(15)
O1	C1	C14	106.37(10)	C8	C13	C12	118.87(14)
C3	C2	C1	122.50(11)	C15	C14	C1	123.39(11)
C7	C2	C1	118.99(11)	C15	C14	C19	118.57(12)
C7	C2	C3	118.48(12)	C19	C14	C1	118.04(12)
C4	C3	C2	120.57(13)	C14	C15	C16	120.82(13)
C5	C4	C3	120.15(13)	C17	C16	C15	120.00(13)
C6	C5	C4	119.23(13)	C16	C17	C18	119.72(14)
C5	C6	C7	120.69(13)	C19	C18	C17	120.35(15)
C2	C7	C6	120.88(13)	C18	C19	C14	120.53(14)
C13	C8	C1	123.32(12)	C8	N1	C10	117.86(13)

Table S15. Bond lengths (Å) for **3b**.

Sm1	I1	3.2828(2)	C10	C11	1.434(3)
Sm1	I2	3.1819(2)	C11	C12	1.416(3)
Sm1	O1	2.1289(14)	C12	C13	1.370(3)
Sm1	N1	2.5442(18)	C14	C15	1.404(3)
Sm1	N2	2.6816(17)	C14	C19	1.377(3)
Sm1	N3	2.6216(18)	C15	C16	1.386(3)
Sm1	N4	2.6066(19)	C16	C17	1.380(4)
Sm1	N5	2.610(2)	C17	C18	1.380(4)
O1	C1	1.391(3)	C18	C19	1.398(3)
N1	C2	1.327(3)	C20	C21	1.395(3)
N1	C3	1.365(3)	C20	C25	1.390(3)
N2	C4	1.369(3)	C21	C22	1.387(3)
N2	C5	1.328(3)	C22	C23	1.381(4)
N3	C26	1.364(3)	C23	C24	1.378(4)
N3	C37	1.327(3)	C24	C25	1.394(3)
N4	C27	1.371(3)	C26	C27	1.433(4)
N4	C28	1.322(3)	C26	C34	1.416(3)
N5	C38	1.137(3)	C27	C31	1.418(3)
C1	C2	1.536(3)	C28	C29	1.406(3)
C1	C14	1.542(3)	C29	C30	1.367(4)
C1	C20	1.540(3)	C30	C31	1.391(4)
C2	C13	1.413(3)	C31	C32	1.436(4)
C3	C4	1.436(3)	C32	C33	1.335(4)
C3	C11	1.403(3)	C33	C34	1.439(4)
C4	C8	1.408(3)	C34	C35	1.402(4)
C5	C6	1.397(3)	C35	C36	1.361(4)
C6	C7	1.362(3)	C36	C37	1.404(3)
C7	C8	1.410(3)	C38	C39	1.453(4)
C8	C9	1.429(3)	N6	C40	1.135(5)
C9	C10	1.358(3)	C40	C41	1.450(5)

Table S16. Bond angles (deg) for **3b**.

I2	Sm1	I1	93.365(5)	N2	C4	C3	117.88(18)
O1	Sm1	I1	149.36(4)	N2	C4	C8	123.23(19)
O1	Sm1	I2	100.78(4)	C8	C4	C3	118.9(2)
O1	Sm1	N1	64.90(5)	N2	C5	C6	123.9(2)
O1	Sm1	N2	127.05(5)	C7	C6	C5	119.7(2)
O1	Sm1	N3	79.32(6)	C6	C7	C8	119.0(2)
O1	Sm1	N4	85.98(6)	C4	C8	C7	117.6(2)
O1	Sm1	N5	73.78(6)	C4	C8	C9	119.99(19)
N1	Sm1	I1	144.73(4)	C7	C8	C9	122.39(19)
N1	Sm1	I2	82.17(4)	C10	C9	C8	121.0(2)
N1	Sm1	N2	62.17(5)	C9	C10	C11	120.3(2)
N1	Sm1	N3	126.75(6)	C3	C11	C10	119.83(19)
N1	Sm1	N4	75.69(6)	C3	C11	C12	117.14(19)
N1	Sm1	N5	125.45(6)	C12	C11	C10	123.0(2)
N2	Sm1	I1	82.95(4)	C13	C12	C11	119.4(2)

N2	Sm1	I2	73.48(4)	C12	C13	C2	119.87(19)
N3	Sm1	I1	73.69(4)	C15	C14	C1	115.8(2)
N3	Sm1	I2	145.14(5)	C19	C14	C1	125.33(19)
N3	Sm1	N2	134.09(6)	C19	C14	C15	118.7(2)
N4	Sm1	I1	94.44(4)	C16	C15	C14	120.5(2)
N4	Sm1	I2	151.49(4)	C17	C16	C15	120.1(2)
N4	Sm1	N2	80.33(6)	C16	C17	C18	119.9(2)
N4	Sm1	N3	63.19(6)	C17	C18	C19	120.2(2)
N4	Sm1	N5	136.00(6)	C14	C19	C18	120.6(2)
N5	Sm1	I1	85.21(5)	C21	C20	C1	118.60(19)
N5	Sm1	I2	71.99(5)	C25	C20	C1	122.9(2)
N5	Sm1	N2	142.63(6)	C25	C20	C21	118.5(2)
N5	Sm1	N3	74.72(6)	C22	C21	C20	120.6(2)
C1	O1	Sm1	133.75(12)	C23	C22	C21	120.3(2)
C2	N1	Sm1	117.26(13)	C24	C23	C22	119.7(2)
C2	N1	C3	118.96(18)	C23	C24	C25	120.3(2)
C3	N1	Sm1	123.67(13)	C20	C25	C24	120.5(2)
C4	N2	Sm1	117.99(12)	N3	C26	C27	118.1(2)
C5	N2	Sm1	124.81(15)	N3	C26	C34	122.1(2)
C5	N2	C4	116.64(18)	C34	C26	C27	119.7(2)
C26	N3	Sm1	118.46(15)	N4	C27	C26	118.9(2)
C37	N3	Sm1	123.14(16)	N4	C27	C31	121.7(2)
C37	N3	C26	117.7(2)	C31	C27	C26	119.4(2)
C27	N4	Sm1	118.47(15)	N4	C28	C29	124.3(2)
C28	N4	Sm1	123.20(15)	C30	C29	C28	118.1(2)
C28	N4	C27	117.5(2)	C29	C30	C31	120.1(2)
C38	N5	Sm1	151.2(2)	C27	C31	C32	118.9(3)
O1	C1	C2	108.13(15)	C30	C31	C27	118.3(2)
O1	C1	C14	107.59(17)	C30	C31	C32	122.9(2)
O1	C1	C20	109.92(17)	C33	C32	C31	122.1(3)
C2	C1	C14	111.58(18)	C32	C33	C34	120.5(2)
C2	C1	C20	107.99(17)	C26	C34	C33	119.4(3)
C20	C1	C14	111.58(16)	C35	C34	C26	117.9(2)
N1	C2	C1	114.60(18)	C35	C34	C33	122.6(2)
N1	C2	C13	121.67(19)	C36	C35	C34	119.6(2)
C13	C2	C1	123.72(18)	C35	C36	C37	118.9(3)
N1	C3	C4	117.18(19)	N3	C37	C36	123.7(3)
N1	C3	C11	122.88(19)	N5	C38	C39	178.4(3)
C11	C3	C4	119.95(19)	N6	C40	C41	179.5(4)

5. Theoretical calculations

All calculations conducted at B3PW91 level of theory by using GAUSSIAN09 code.[6] The equilibrium and transition structures were fully optimized at the Becke's 3-parameter hybrid functional[7] combined with the non-local correlation functional provided by Perdew/Wang.[8] Two different Stuttgart-Dresden effective core potentials were used for samarium atoms; the small core ECP was used in combination with its adapted basis set to study the change of oxidation state from +II to +III,[9, 10] while the 4f-in-large-core ECP (augmented by a *f* polarization function, α = 1.0) was also used for the reactions, in which the samarium's oxidation state is +III.[11, 12] Iodine atoms were represented by means of a Stuttgart-Dresden effective core potentials in association with its basis set,[13] augmented by a d-polarization function (α = 0,730).[14] For the rest of non-metal atoms the 6-31G(d,p) basis set was used.[15-17] Enthalpies were obtained at T=298.15K within the harmonic approximation.

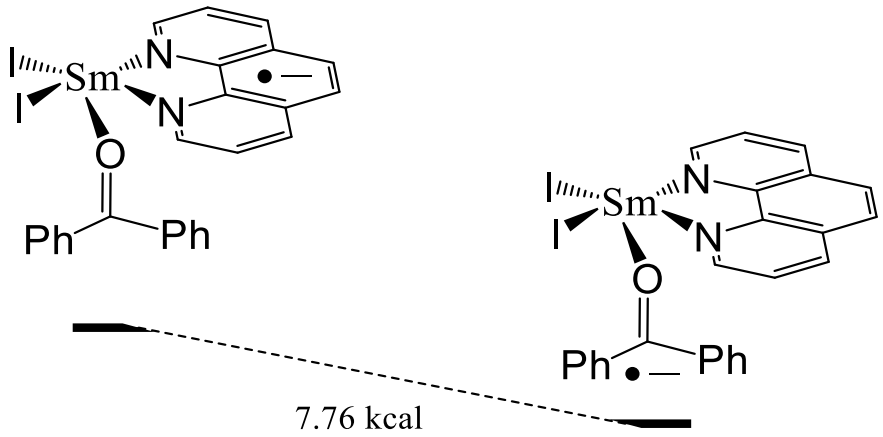

Figure S23. Computed enthalpy for the equilibrium ketyl-bipyridyl.

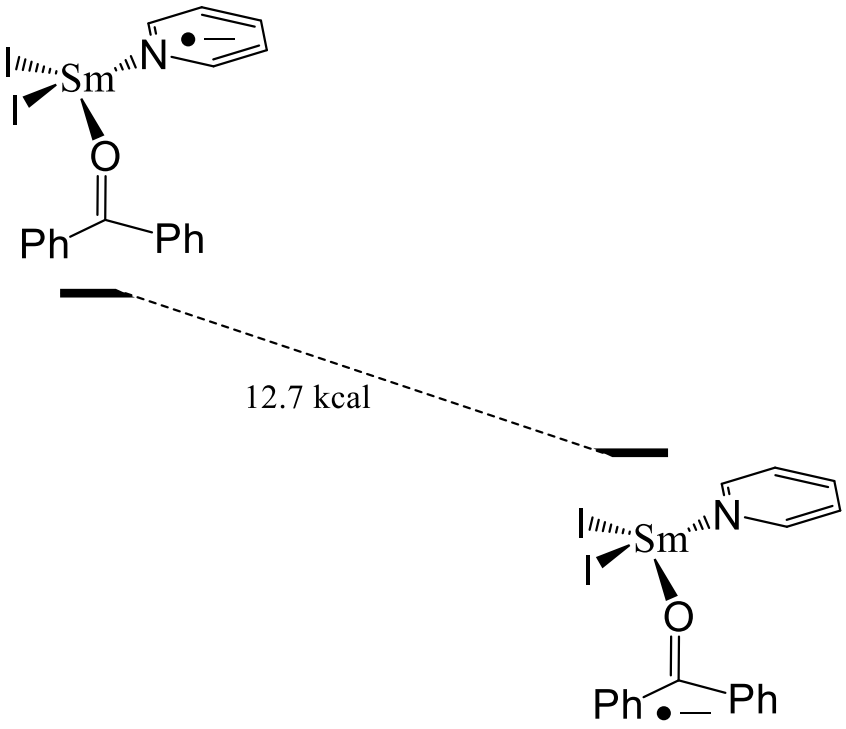

Figure S24. Computed enthalpy for the equilibrium ketyl-pyridyl.

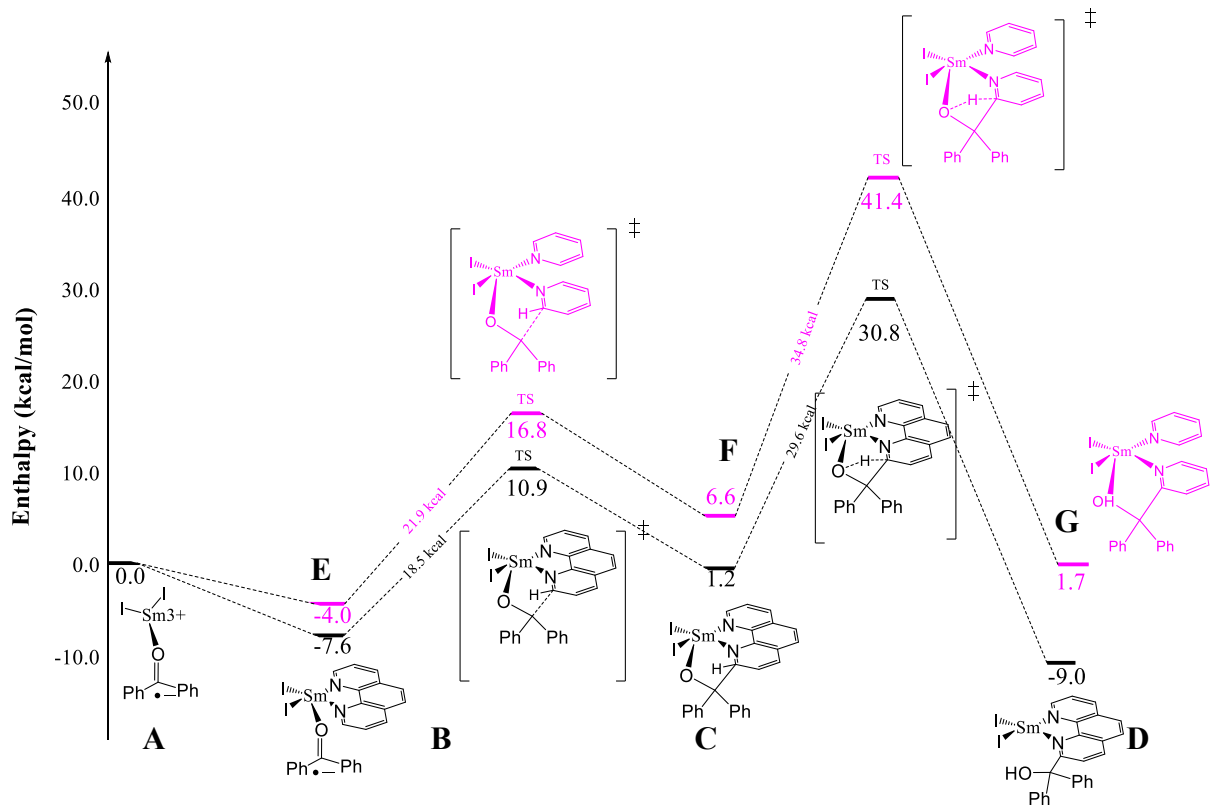

Figure S25. Computed enthalpy profile for the formation of **D** (black) and **G** (pink).

Cartesian coordinates of all optimized structures

a

C	-5.82012000	2.10140000	-0.18340500
C	-4.46573900	1.85629100	0.01488300
C	-3.56784400	2.91082300	0.29167300
C	-4.09315400	4.22149400	0.33801300
C	-5.44920400	4.45880500	0.14334900
C	-6.32475100	3.40173900	-0.11591300
H	-6.48592400	1.27095500	-0.40536100
H	-4.08716200	0.84287500	-0.07767000
H	-3.42557500	5.05260400	0.54731100
H	-5.82383200	5.47750500	0.20306800
H	-7.38446100	3.58849600	-0.26625500
C	-2.13208600	2.70165300	0.46993500
O	-1.32455000	3.66799600	0.04723400
C	-1.54512500	1.54654900	1.11681600
C	-0.14530100	1.32824800	1.04949300

C	-2.30278400	0.63398100	1.89608800
C	0.44692900	0.24396900	1.68300400
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C	-1.70085400	-0.44746100	2.52291400
H	-3.36505400	0.80276700	2.03618100
C	-0.32313800	-0.66174100	2.41627100
H	1.52280600	0.10980900	1.60617500
H	-2.31059900	-1.12298900	3.11801300
H	0.14290200	-1.50934500	2.91065600
Sm	0.06287000	5.16578600	-0.67195600
I	2.97541600	4.36241200	0.36364600
I	-1.78923200	7.75953800	-0.43988600
C	2.86698100	6.87638300	-2.40654900
C	3.58570100	7.76862900	-3.19635500
C	2.89198600	8.72347500	-3.93333700
C	1.50305000	8.74763000	-3.84599900
C	0.86428400	7.81863400	-3.03130700
N	1.52424400	6.88555000	-2.32009300
H	3.42227900	9.43869300	-4.55613400
H	3.37481300	6.13214100	-1.79729700
H	4.66916300	7.71169500	-3.21779400
H	0.91274600	9.47872100	-4.38863900
H	-0.21555200	7.83077800	-2.91515400
C	-2.69802200	5.03126100	-2.87670600
C	-3.53322200	4.95507200	-3.98741400
C	-2.96866900	5.00685100	-5.25769900
C	-1.58489500	5.12099900	-5.36749900
C	-0.82718500	5.17572000	-4.20324400
N	-1.36317500	5.13979600	-2.97367800
H	-3.59299300	4.95796400	-6.14546500
H	-3.11085000	5.00419200	-1.87346500
H	-4.60424700	4.86139900	-3.84334100
H	-1.09453100	5.16334200	-6.33465100
H	0.25497600	5.25033300	-4.25284300
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C	2.27699300	1.97057400	-3.78538100
C	1.35397200	0.94088200	-3.94715100
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C	-0.10330700	2.12762500	-2.46212300
N	0.78209300	3.12342800	-2.29828700
H	1.57845600	0.08983400	-4.58400100
H	2.66464400	3.83202800	-2.76682800
H	3.24042200	1.95186600	-4.28418000
H	-0.60640600	0.23957800	-3.35096900
H	-1.03511300	2.22386800	-1.91447900
C	0.53679700	6.97407000	2.34528000
C	0.66537700	7.26919200	3.69671600
C	0.34671600	6.28578600	4.62951800
C	-0.08522400	5.04596900	4.16975600

C	-0.17648600	4.83431800	2.79805100
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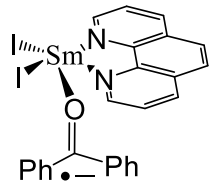
H	0.75452500	7.72496400	1.59162300
H	1.00400000	8.25326000	4.00320500
H	-0.34691300	4.24597400	4.85417500
H	-0.50131800	3.87744200	2.40301900



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C	-2.66129700	4.59337500	3.46015100
C	-3.65187700	5.08302300	2.57672500
C	-4.98605200	4.72694500	2.72494800
C	-5.38112900	3.85562300	3.74284000
H	-4.70008700	2.63531700	5.38597600
H	-2.33657700	3.24858200	5.12614800
H	-3.36359200	5.76342500	1.78100600
H	-5.72474800	5.13671500	2.04066500
H	-6.42521400	3.57703200	3.85582700
C	-1.26912600	4.97585600	3.27098000
C	-0.26622500	4.98311400	4.32456000
C	1.10705000	4.94347900	3.98669000
C	-0.59546200	5.10131400	5.69655300
C	2.08925600	4.98644100	4.96750000
H	1.39027100	4.84555800	2.94389400
C	0.39401500	5.14735200	6.67008300
H	-1.63548600	5.19559200	5.99194600
C	1.74463800	5.08400300	6.31767900
H	3.13483000	4.93467000	4.67417900
H	0.10922300	5.24804300	7.71467800
H	2.51525100	5.11607100	7.08294700
Sm	-0.32839200	6.05202000	0.09151300
I	2.08831700	4.01161400	-0.04691000
I	-2.75862400	7.91033100	-0.75921500
C	-0.45792200	6.82577300	-3.49585200
C	-0.41701800	6.71070100	-4.88188900
C	-0.09543800	5.47806000	-5.44304100
C	0.17788100	4.41088900	-4.59240600
C	0.12197500	4.61798200	-3.21734300
N	-0.19221700	5.80263000	-2.66597600
H	-0.05920700	5.35170900	-6.52161100
H	-0.73352500	7.76489700	-3.02487500
H	-0.64214900	7.57389700	-5.49970500
H	0.43588300	3.42989000	-4.97769800
H	0.35358900	3.81608800	-2.52216900

C	-1.73768400	2.87630500	0.10195300
C	-2.53426500	1.75474600	-0.10275300
C	-3.56267800	1.82560700	-1.03745000
C	-3.75491900	3.01699000	-1.73187200
C	-2.90998700	4.08911100	-1.46739000
N	-1.91282300	4.02574900	-0.57040300
H	-4.20658900	0.96929700	-1.21782000
H	-0.92638900	2.86207100	0.82309800
H	-2.34824700	0.85192200	0.46904700
H	-4.54867700	3.12464700	-2.46382500
H	-3.03649300	5.04262700	-1.97250600
C	-0.76235100	9.57682600	3.37991000
C	0.16092000	10.55064500	3.06748800
C	1.03209100	10.35540500	1.97625300
C	0.90494400	9.14910100	1.24457900
C	-0.81124400	8.41232100	2.59822200
C	2.02279000	11.31601200	1.59506900
C	1.77648900	8.90544700	0.12317900
C	2.75619500	9.87326100	-0.21563200
C	2.85264700	11.08387000	0.54275900
C	3.60913200	9.58716000	-1.30011200
H	4.37173600	10.30740000	-1.58507600
C	3.47092300	8.39354200	-1.97504000
C	2.47038300	7.49796000	-1.56786300
H	2.10085400	12.23530100	2.16900600
H	-1.44645200	9.68980700	4.21367000
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H	-1.52266800	7.62403200	2.81870300
H	3.60708100	11.81298600	0.26046600
H	4.11932100	8.13132400	-2.80401500
H	2.35232700	6.54080600	-2.06573100
N	1.63673200	7.74196900	-0.56197700
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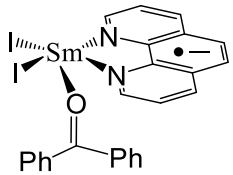
O	-0.89863000	5.36511400	2.06244100



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C	0.13960300	7.77185600	-6.19677300
C	0.48170200	6.42356200	-6.14720900
C	0.33881000	5.73950500	-4.94423900
N	-0.12418500	6.32402000	-3.82584400
H	0.24194700	8.33583700	-7.11966300
H	-0.84373900	8.06244000	-2.96643100

H	-0.61757600	9.43215900	-5.02768300
H	0.85976700	5.90164700	-7.01997700
H	0.61735500	4.69290400	-4.85461800
C	-1.48918900	2.00682500	-3.19270300
C	-2.11968000	1.07732000	-4.01347200
C	-2.98438300	1.53446700	-5.00316000
C	-3.19175900	2.90548100	-5.12595400
C	-2.52984400	3.76295100	-4.25387300
N	-1.68400600	3.33119300	-3.30422500
H	-3.49014000	0.83569000	-5.66379600
H	-0.79890100	1.68768700	-2.41908900
H	-1.92726600	0.01895900	-3.87284100
H	-3.86250000	3.31299300	-5.87521600
H	-2.69526800	4.83526800	-4.29250100
C	-1.61906300	6.02600800	2.90573700
C	-0.63704800	6.89738800	3.37582100
C	0.39268500	7.29239600	2.51390800
C	0.40222300	6.77249600	1.18847500
C	-1.53428100	5.55378800	1.60236400
C	1.42982000	8.20115600	2.90727900
C	1.41261400	7.16940400	0.27741500
C	2.43294400	8.07235400	0.69499500
C	2.40577000	8.57428100	2.03771500
C	3.42383000	8.42922600	-0.22549000
H	4.21184300	9.11648800	0.07032400
C	3.38788000	7.88413100	-1.50861800
C	2.36182400	7.00729000	-1.83958400
H	1.41667400	8.58887500	3.92268500
H	-2.44412600	5.71118100	3.53519700
H	-0.66517100	7.27851100	4.39291800
H	-2.29218100	4.88094900	1.21581200
H	3.18817500	9.26293300	2.34611700
H	4.14728500	8.12052300	-2.24589100
H	2.33370500	6.55179600	-2.82412800
N	1.37693400	6.64932500	-0.99854600
N	-0.55323800	5.88773200	0.74723900
C	-3.84388300	-0.31705500	2.06365600
C	-2.61158000	0.30860000	1.90543400
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H	-1.71573000	-0.16000000	2.29985700
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H	-5.95971400	-0.23243800	1.65734300
C	-1.21982900	2.19718800	0.95608600
O	-1.10553500	2.91727700	-0.06924100

C	-0.07272500	2.03352600	1.86789600
C	1.22575200	2.21046000	1.35529100
C	-0.22796300	1.77775800	3.24414500
C	2.33367600	2.10548100	2.18775700
H	1.35654600	2.40874400	0.29550000
C	0.88373100	1.68648900	4.07344400
H	-1.22330200	1.68836800	3.66772600
C	2.16853500	1.84156800	3.54827400
H	3.32876200	2.23064900	1.77033400
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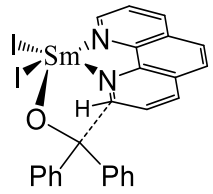

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C	1.00025000	4.86622400	3.39033500
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H	1.30767000	6.81376200	6.71729700
H	3.18987700	5.37887800	5.94670400
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C	-0.45854300	6.96922400	-3.70619500
C	-0.28111600	7.09728100	-5.08019000
C	0.25356900	6.02520400	-5.78949500
C	0.59545000	4.86971200	-5.09283600
C	0.39623800	4.83271400	-3.71568000
N	-0.12438800	5.86068000	-3.02335300
H	0.39953400	6.08883700	-6.86432300

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H	-0.56815100	8.01879900	-5.57596700
H	1.01598000	4.00625800	-5.59798100
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C	-3.45879300	1.32525300	-1.41476000
C	-3.41313000	2.36139500	-2.34395200
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N	-1.99347600	3.63762400	-0.89054800
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H	-1.50063300	2.80212700	0.92939500
H	-2.77645800	0.69280200	0.54099800
H	-3.94611000	2.30068800	-3.28708100
H	-2.63219200	4.33893500	-2.72517900
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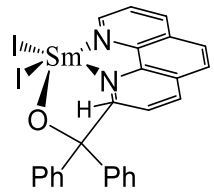

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H	-5.93832100	5.28932100	2.83395300
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C	0.93815800	4.73226800	3.42356300
C	0.11621100	6.30225100	5.04221300
C	2.08552400	4.53986900	4.19319700
H	0.81554400	4.18621600	2.49551500
C	1.25854800	6.10892400	5.81570600
H	-0.64596500	6.98697300	5.40011100
C	2.25285500	5.22769100	5.39171900
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H	1.36996300	6.64957000	6.75221700
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I	-2.99811900	7.43068200	-1.10852700
C	-0.41048600	6.90173300	-3.73787800
C	-0.23585700	6.99934900	-5.11504300
C	0.30650300	5.91581100	-5.80052600
C	0.65872000	4.77990000	-5.07733000
C	0.46086700	4.77345500	-3.69942900
N	-0.06764700	5.81214800	-3.02927400
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H	-0.53088200	7.90706900	-5.63132900
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C	-3.50937100	1.39209400	-1.38058400
C	-3.42765400	2.41686600	-2.32002100
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H	-1.52791600	2.83970400	0.96370900
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H	-3.95762900	2.36263700	-3.26524100
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C	-1.42392300	8.45177700	3.52242500
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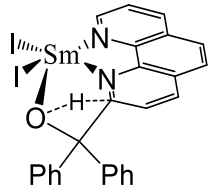

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C	0.89401100	5.24664800	3.28519700
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C	2.03922300	5.96343400	3.64331900
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H	0.08011200	3.29024300	2.91897700
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H	1.99175400	7.04443200	3.73584600
C	3.31374900	3.91471200	3.76979300
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H	4.25236100	3.39912500	3.95201200
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N	1.51975000	8.15355200	-0.74688900
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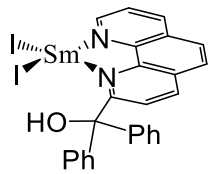

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H	-0.24391700	3.26834400	3.06146200
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C	-1.04831600	6.85385700	-3.57184600
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C	0.33838900	4.96506400	-4.97554500
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H	-0.66617000	5.70536800	-6.73746400
H	-1.59253200	7.58050100	-2.97559200
H	-1.93477200	7.44104200	-5.43519000
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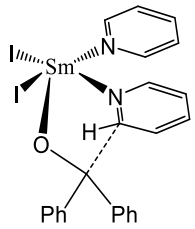

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Sm	-0.06459200	5.99074700	-0.36110200
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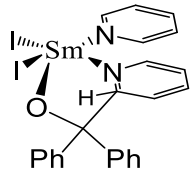

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H	-2.93201500	5.99096600	2.28137900
H	-4.92540800	5.81895600	3.74886800
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C	-0.32267000	5.97665500	2.94084900
C	0.90092500	5.22433100	3.48449300
C	0.92774000	3.83884400	3.26656300
C	1.95268600	5.79820900	4.20098600
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H	1.96801700	6.86513300	4.38961400
C	3.01707200	3.64158700	4.46341100
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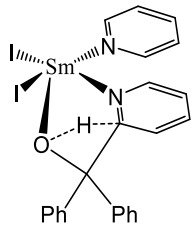

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C	2.67571400	3.26564100	3.49541200
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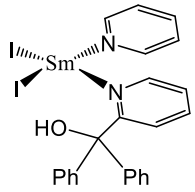

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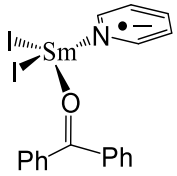

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H	1.64901000	0.66063000	-2.61994100
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N	1.97913900	4.41233000	-3.17150400
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H	3.27759300	4.81069800	-1.59839000
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H	-3.24924900	0.62959500	5.16768600
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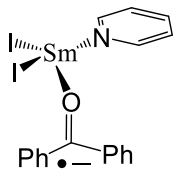

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H	-2.51143100	0.18636600	1.64318900
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H	-0.86234600	4.12152900	2.23252800
C	-1.10724100	1.53826600	4.42538700
H	-1.96968800	-0.38516500	3.97106000
H	-0.29250600	3.53177100	4.54828800
H	-0.85766000	1.27970400	5.45061200
Sm	0.12336200	4.94377600	-0.93416700
I	2.87198500	3.98455100	0.06094100
I	-0.82356200	7.36019200	0.72597100
C	2.72132100	6.45794000	-2.91146200
C	3.50759400	7.41819700	-3.53935800
C	2.98153100	8.69242800	-3.73349100
C	1.68855400	8.95698900	-3.29047000
C	0.97087300	7.93737000	-2.67468500
N	1.46735600	6.70109900	-2.49030700
H	3.57273400	9.46853900	-4.21130300
H	3.11044400	5.46377800	-2.70744000
H	4.51588600	7.16760900	-3.85177100
H	1.24007200	9.93834500	-3.40347400
H	-0.02913700	8.11452300	-2.28809700
C	-3.03250100	5.60283300	-2.09379200
C	-4.17475500	5.94472500	-2.81058200
C	-4.04026900	6.35170200	-4.13369700
C	-2.76512600	6.40028700	-4.69293700
C	-1.67997500	6.04271400	-3.90242700
N	-1.79875400	5.65172300	-2.62434500
H	-4.91236900	6.62637900	-4.72011200

H	-3.10046300	5.27981800	-1.06004800
H	-5.14532300	5.88526400	-2.33055700
H	-2.60859100	6.71123200	-5.72064000
H	-0.67041400	6.07969400	-4.30087000
C	1.06145600	3.46376300	-4.14933200
C	1.42889800	2.45915000	-5.03652000
C	1.33696000	1.13410300	-4.61712600
C	0.88095000	0.87082200	-3.32936400
C	0.53369700	1.93919800	-2.50938700
N	0.61881000	3.22015900	-2.90694500
H	1.61878000	0.32260300	-5.28178900
H	1.13582400	4.50858000	-4.43787400
H	1.78263400	2.71513700	-6.02983700
H	0.79385800	-0.14328500	-2.95472900
H	0.17525000	1.77551200	-1.49756400

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