Table S1. Crystallographic Experimental Details for

$[Sm\{C(Ph_2P{=}NSiMe_3)_2\text{-}\kappa^3C,N,N'\}(NCy_2)(THF)]\cdot 0.5PhMe$

A. Crystal Data	
formula	$C_{50.5}H_{72}N_3OP_2Si_2Sm$
formula weight	1005.58
crystal dimensions (mm)	0.30 × 0.23 × 0.20
crystal system	triclinic
space group	$P\bar{1}$ (No. 2)
unit cell parameters[a]	
a (Å)	10.7169 (6)
b (Å)	11.3464 (6)
c (Å)	21.6988 (12)
α (deg)	81.0950 (10)
β (deg)	82.1520 (10)
γ (deg)	84.7740 (10)
V (Å^3)	2575.7 (2)
Z	2
ρ_{calcd} (g cm^{-3})	1.297
μ (mm^{-1})	1.286
B. Data Collection and Refinement Conditions	
diffractometer	Bruker P4/RA/SMART 1000 CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–80
scan type	ϕ rotations (0.3°) / ω scans (0.3°) (20 s exposures)
data collection 2θ limit (deg)	51.48

(continued)

Table S1. Crystallographic Experimental Details for

$[Sm\{C(Ph_2P{=}NSiMe_3)_2\text{-}\kappa^3C,N,N'\}(NCy_2)(THF)]\cdot 0.5PhMe$ (continued)

total data collected	16418 ($-12 \le h \le 13$, $-12 \le k \le 13$, $-26 \le l \le 26$)
independent reflections	9731
number of observations (*NO*)	8085 [$F_o^2 \ge 2\sigma(F_o^2)$]
structure solution method	direct methods/fragment search (*DIRDIF–96*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–93*[d])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	0.7918–0.6991
data/restraints/parameters	9731 [$F_o^2 \ge -3\sigma(F_o^2)$] / 16[e]/ 539
goodness-of-fit (*S*)[f]	1.007 [$F_o^2 \ge -3\sigma(F_o^2)$]
final *R* indices[g]	
R_1 [$F_o^2 \ge 2\sigma(F_o^2)$]	0.0457
wR_2 [$F_o^2 \ge -3\sigma(F_o^2)$]	0.1220
largest difference peak and hole	1.671 and –1.988 e Å^{-3}

[a]Obtained from least-squares refinement of 8192 centered reflections.

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

[c]Beurskens, P. T.; Beurskens, G.; Bosman, W. P.; de Gelder, R.; Garcia Granda, S.; Gould, R. O.; Israel, R.; Smits, J. M. M. (1996). The *DIRDIF-96* program system. Crystallography Laboratory, University of Nijmegen, The Netherlands.

(continued)

Table S1. Crystallographic Experimental Details for
$[Sm\{C(Ph_2P{=}NSiMe_3)_2\text{-}\kappa^3C,N,N'\}(NCy_2)(THF)]\cdot 0.5PhMe$ (continued)

[d]Sheldrick, G. M. *SHELXL-93*. Program for crystal structure determination. University of Göttingen, Germany, 1993. Refinement on F_o^2 for all reflections (all of these having $F_o^2 \geq -3\sigma(F_o^2)$). Weighted R-factors wR_2 and all goodnesses of fit S are based on F_o^2; conventional R-factors R_1 are based on F_o, with F_o set to zero for negative F_o^2. The observed criterion of $F_o^2 > 2\sigma(F_o^2)$ is used only for calculating R_1, and is not relevant to the choice of reflections for refinement. R-factors based on F_o^2 are statistically about twice as large as those based on F_o, and R-factors based on ALL data will be even larger.

[e]Restraints were applied to impose an idealized geometry upon the inversion-disordered solvent toluene molecule: d(C90–C91) = d(C91–C92) = d(C91–C92') = d(C92–C93) = d(C93–C90') = d(C90'–C94) = d(C94–C92') = 1.42 Å; d(C90···C92) = d(C90···C92') = d(C91···C93) = d(C91···C94) = d(C92···C92') = d(C93···C94) = 2.46 Å; d(C91···C90') = d(C92···C94) = d(C93···C92') = 2.84 Å (primed atoms are related to unprimed ones via the crystallographic inversion center (0, 0, 0)).

[f]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n-p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0758P)^2]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

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

Table S2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for [Sm{C(Ph_2P=N$SiMe_3$)$_2$-κ^3*C,N,N'*}(NCy_2)(THF)]•0.5PhMe

(a) atoms of [Sm{C(Ph_2P=N$SiMe_3$)$_2$-κ^3C,N,N'}(NCy_2)(THF)]•0.5PhMe

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Sm	0.13339(2)	0.414878(18)	0.276022(10)	0.02440(9)*
P(1)	0.33851(10)	0.21990(9)	0.29835(5)	0.0231(2)*
P(2)	0.36153(10)	0.40845(9)	0.17742(5)	0.0250(2)*
Si(1)	0.12375(12)	0.16045(11)	0.40617(6)	0.0325(3)*
Si(2)	0.15505(12)	0.56011(12)	0.10748(6)	0.0322(3)*
O	-0.0615(3)	0.3314(3)	0.25703(18)	0.0432(9)*
N(1)	0.1958(3)	0.2267(3)	0.33571(17)	0.0271(8)*
N(2)	0.2206(4)	0.4657(3)	0.16568(18)	0.0317(8)*
N(3)	0.0959(3)	0.5658(3)	0.33127(18)	0.0315(9)*
C(1)	0.3592(4)	0.3515(3)	0.2530(2)	0.0241(9)*
C(2)	-0.0345(5)	0.2420(6)	0.4204(3)	0.0513(14)*
C(3)	0.2078(5)	0.1696(6)	0.4751(2)	0.0520(14)*
C(4)	0.1012(7)	-0.0003(5)	0.4062(3)	0.068(2)*
C(5)	0.2002(6)	0.7179(5)	0.1000(3)	0.0500(14)*
C(6)	0.1911(6)	0.5092(5)	0.0284(2)	0.0508(14)*
C(7)	-0.0201(5)	0.5637(6)	0.1285(3)	0.0545(15)*
C(11)	0.3635(4)	0.0903(4)	0.2569(2)	0.0267(9)*
C(12)	0.4840(4)	0.0516(4)	0.2316(2)	0.0339(10)*
C(13)	0.5019(5)	-0.0438(4)	0.1978(3)	0.0411(12)*
C(14)	0.3991(5)	-0.1011(4)	0.1873(3)	0.0435(13)*
C(15)	0.2792(5)	-0.0623(4)	0.2109(3)	0.0419(12)*
C(16)	0.2616(4)	0.0317(4)	0.2460(2)	0.0311(10)*
C(21)	0.4540(4)	0.1862(4)	0.3548(2)	0.0279(9)*

Table S2. Atomic Coordinates and Displacement Parameters for [Sm{C(Ph_2P=N$SiMe_3$)$_2$-κ^3*C,N,N'*}(NCy_2)(THF)]•0.5PhMe (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C(22)	0.5041(5)	0.2805(5)	0.3745(2)	0.0379(11)*
C(23)	0.5877(5)	0.2598(5)	0.4186(3)	0.0485(14)*
C(24)	0.6226(5)	0.1450(6)	0.4435(3)	0.0531(15)*
C(25)	0.5740(5)	0.0487(5)	0.4238(2)	0.0462(13)*
C(26)	0.4893(5)	0.0696(4)	0.3802(2)	0.0365(11)*
C(31)	0.4753(4)	0.5241(4)	0.1570(2)	0.0297(10)*
C(32)	0.5337(4)	0.5575(4)	0.2044(2)	0.0352(11)*
C(33)	0.6194(5)	0.6457(4)	0.1898(3)	0.0441(13)*
C(34)	0.6513(5)	0.6956(5)	0.1291(3)	0.0523(16)*
C(35)	0.5950(5)	0.6642(5)	0.0820(3)	0.0520(16)*
C(36)	0.5069(5)	0.5779(5)	0.0959(2)	0.0425(12)*
C(41)	0.4214(4)	0.3034(4)	0.1220(2)	0.0304(10)*
C(42)	0.3416(5)	0.2257(4)	0.1061(2)	0.0371(11)*
C(43)	0.3901(6)	0.1372(5)	0.0705(2)	0.0473(13)*
C(44)	0.5184(6)	0.1249(5)	0.0492(3)	0.0539(15)*
C(45)	0.5976(6)	0.2019(5)	0.0641(3)	0.0514(14)*
C(46)	0.5510(5)	0.2894(4)	0.1007(2)	0.0390(11)*
C(51)	0.1736(4)	0.6144(4)	0.3711(2)	0.0370(11)*
C(52)	0.2086(6)	0.5201(6)	0.4244(3)	0.0558(16)*
C(53)	0.2961(6)	0.5625(7)	0.4660(3)	0.0676(19)*
C(54)	0.4131(5)	0.6116(5)	0.4273(3)	0.0525(15)*
C(55)	0.3787(6)	0.7086(6)	0.3741(3)	0.0641(18)*
C(56)	0.2921(5)	0.6637(5)	0.3339(3)	0.0505(14)*
C(61)	-0.0226(4)	0.6332(4)	0.3195(2)	0.0337(10)*

Table S2. Atomic Coordinates and Displacement Parameters for [Sm{C(Ph_2P=NSiMe_3)$_2$-κ^3*C,N,N'*}(NCy_2)(THF)]•0.5PhMe (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C(62)	-0.0096(5)	0.7609(4)	0.2841(3)	0.0435(12)*
C(63)	-0.1355(6)	0.8244(5)	0.2689(3)	0.0557(15)*
C(64)	-0.2298(6)	0.8253(6)	0.3279(3)	0.0687(19)*
C(65)	-0.2464(5)	0.7036(6)	0.3627(3)	0.0619(17)*
C(66)	-0.1199(5)	0.6367(5)	0.3784(3)	0.0460(13)*
C(71)	-0.1935(5)	0.3729(5)	0.2684(3)	0.0463(13)*
C(72)	-0.2639(6)	0.2852(8)	0.2446(4)	0.082(3)*
C(73a)[a]	-0.1997(14)	0.1859(13)	0.2457(11)	0.087(6)*
C(74a)[a]	-0.060(2)	0.212(2)	0.2443(11)	0.057(6)*
C(73b)[a]	-0.1731(11)	0.2288(14)	0.1971(7)	0.056(4)*
C(74b)[a]	-0.045(3)	0.238(3)	0.2146(11)	0.076(9)*

(b) solvent toluene atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C(90)[b]	0.0103(12)	0.1061(10)	0.0717(5)	0.163(3)
C(91)[a,b]	0.0060(11)	0.0332(10)	0.0246(3)	0.163(3)
C(92)[b]	-0.0818(8)	-0.0566(8)	0.0344(3)	0.163(3)
C(93)[a,b]	-0.0859(15)	-0.1296(11)	-0.0127(7)	0.163(3)
C(94)[a,b]	0.0705(16)	-0.0105(15)	-0.0833(3)	0.163(3)

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

Table S3. Selected Interatomic Distances (Å) for

[Sm{C(Ph_2P=N$SiMe_3$)$_2$-κ^3*C,N,N'*}(NCy_2)(THF)]•0.5PhMe

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
Sm	O	2.479(3)	N(3)	C(51)	1.474(6)
Sm	N(1)	2.409(4)	N(3)	C(61)	1.454(6)
Sm	N(2)	2.449(4)	C(11)	C(12)	1.392(6)
Sm	N(3)	2.216(4)	C(11)	C(16)	1.394(6)
Sm	C(1)	2.467(4)	C(12)	C(13)	1.384(6)
P(1)	N(1)	1.632(4)	C(13)	C(14)	1.390(7)
P(1)	C(1)	1.671(4)	C(14)	C(15)	1.376(7)
P(1)	C(11)	1.821(4)	C(15)	C(16)	1.390(6)
P(1)	C(21)	1.833(4)	C(21)	C(22)	1.388(6)
P(2)	N(2)	1.626(4)	C(21)	C(26)	1.391(6)
P(2)	C(1)	1.666(4)	C(22)	C(23)	1.379(7)
P(2)	C(31)	1.836(4)	C(23)	C(24)	1.370(8)
P(2)	C(41)	1.836(4)	C(24)	C(25)	1.399(8)
Si(1)	N(1)	1.711(4)	C(25)	C(26)	1.379(7)
Si(1)	C(2)	1.867(5)	C(31)	C(32)	1.391(7)
Si(1)	C(3)	1.869(6)	C(31)	C(36)	1.382(7)
Si(1)	C(4)	1.861(6)	C(32)	C(33)	1.392(6)
Si(2)	N(2)	1.709(4)	C(33)	C(34)	1.361(8)
Si(2)	C(5)	1.874(5)	C(34)	C(35)	1.363(9)
Si(2)	C(6)	1.875(5)	C(35)	C(36)	1.392(7)
Si(2)	C(7)	1.868(5)	C(41)	C(42)	1.393(6)
O	C(71)	1.449(6)	C(41)	C(46)	1.406(7)
O	C(74a)	1.42(3)	C(42)	C(43)	1.382(7)
O	C(74b)	1.50(3)	C(43)	C(44)	1.390(8)

Table S3. Selected Interatomic Distances for

[Sm{C(Ph_2P=N$SiMe_3$)$_2$-κ^3*C,N,N'*}(NCy_2)(THF)]•0.5PhMe (continued)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
C(44)	C(45)	1.373(8)	C(62)	C(63)	1.523(8)
C(45)	C(46)	1.382(7)	C(63)	C(64)	1.519(9)
C(51)	C(52)	1.512(8)	C(64)	C(65)	1.482(9)
C(51)	C(56)	1.512(7)	C(65)	C(66)	1.546(8)
C(52)	C(53)	1.540(7)	C(71)	C(72)	1.493(8)
C(53)	C(54)	1.511(8)	C(72)	C(73a)	1.264(15)
C(54)	C(55)	1.526(9)	C(72)	C(73b)	1.495(14)
C(55)	C(56)	1.525(8)	C(73a)	C(74a)	1.55(3)
C(61)	C(62)	1.539(7)	C(73b)	C(74b)	1.49(3)
C(61)	C(66)	1.538(7)			

Table S4. Selected Interatomic Angles (deg) for

[Sm{C(Ph_2P=N$SiMe_3$)$_2$-κ^3*C,N,N'*}(NCy_2)(THF)]•0.5PhMe

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
O	Sm	N(1)	90.20(12)	N(1)	Si(1)	C(4)	112.6(2)
O	Sm	N(2)	97.17(12)	C(2)	Si(1)	C(3)	106.6(3)
O	Sm	N(3)	113.28(13)	C(2)	Si(1)	C(4)	108.7(3)
O	Sm	C(1)	132.29(12)	C(3)	Si(1)	C(4)	107.2(3)
N(1)	Sm	N(2)	120.58(12)	N(2)	Si(2)	C(5)	113.4(2)
N(1)	Sm	N(3)	114.39(13)	N(2)	Si(2)	C(6)	113.5(2)
N(1)	Sm	C(1)	66.22(13)	N(2)	Si(2)	C(7)	107.3(2)
N(2)	Sm	N(3)	115.97(13)	C(5)	Si(2)	C(6)	108.5(3)
N(2)	Sm	C(1)	65.84(13)	C(5)	Si(2)	C(7)	106.9(3)
N(3)	Sm	C(1)	114.20(13)	C(6)	Si(2)	C(7)	106.9(3)
N(1)	P(1)	C(1)	107.5(2)	Sm	O	C(71)	131.5(3)
N(1)	P(1)	C(11)	110.16(19)	Sm	O	C(74a)	121.0(10)
N(1)	P(1)	C(21)	109.95(19)	Sm	O	C(74b)	116.6(12)
C(1)	P(1)	C(11)	115.1(2)	C(71)	O	C(74a)	106.2(10)
C(1)	P(1)	C(21)	111.6(2)	C(71)	O	C(74b)	110.5(12)
C(11)	P(1)	C(21)	102.4(2)	C(74a)	O	C(74b)	26.4(15)
N(2)	P(2)	C(1)	108.5(2)	Sm	N(1)	P(1)	94.15(16)
N(2)	P(2)	C(31)	110.2(2)	Sm	N(1)	Si(1)	127.71(19)
N(2)	P(2)	C(41)	111.3(2)	P(1)	N(1)	Si(1)	135.2(2)
C(1)	P(2)	C(31)	109.6(2)	Sm	N(2)	P(2)	93.64(17)
C(1)	P(2)	C(41)	114.9(2)	Sm	N(2)	Si(2)	128.4(2)
C(31)	P(2)	C(41)	102.1(2)	P(2)	N(2)	Si(2)	136.2(2)
N(1)	Si(1)	C(2)	107.0(2)	Sm	N(3)	C(51)	131.8(3)
N(1)	Si(1)	C(3)	114.5(2)	Sm	N(3)	C(61)	111.3(3)

Table S4. Selected Interatomic Angles for

[Sm{C(Ph_2P=N$SiMe_3$)$_2$-κ^3*C,N,N'*}(NCy_2)(THF)]•0.5PhMe (continued)

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C(51)	N(3)	C(61)	116.6(4)	C(32)	C(33)	C(34)	120.7(5)
Sm	C(1)	P(1)	91.09(17)	C(33)	C(34)	C(35)	120.5(5)
Sm	C(1)	P(2)	92.00(18)	C(34)	C(35)	C(36)	119.6(5)
P(1)	C(1)	P(2)	138.0(3)	C(31)	C(36)	C(35)	120.9(5)
P(1)	C(11)	C(12)	121.1(3)	P(2)	C(41)	C(42)	120.5(4)
P(1)	C(11)	C(16)	120.8(3)	P(2)	C(41)	C(46)	120.8(3)
C(12)	C(11)	C(16)	118.0(4)	C(42)	C(41)	C(46)	118.3(4)
C(11)	C(12)	C(13)	120.9(4)	C(41)	C(42)	C(43)	120.2(5)
C(12)	C(13)	C(14)	120.4(5)	C(42)	C(43)	C(44)	121.0(5)
C(13)	C(14)	C(15)	119.5(4)	C(43)	C(44)	C(45)	119.2(5)
C(14)	C(15)	C(16)	120.1(4)	C(44)	C(45)	C(46)	120.6(5)
C(11)	C(16)	C(15)	121.2(4)	C(41)	C(46)	C(45)	120.7(5)
P(1)	C(21)	C(22)	118.7(4)	N(3)	C(51)	C(52)	110.9(4)
P(1)	C(21)	C(26)	122.2(3)	N(3)	C(51)	C(56)	112.1(4)
C(22)	C(21)	C(26)	119.1(4)	C(52)	C(51)	C(56)	109.6(4)
C(21)	C(22)	C(23)	120.8(5)	C(51)	C(52)	C(53)	113.8(5)
C(22)	C(23)	C(24)	120.1(5)	C(52)	C(53)	C(54)	111.5(5)
C(23)	C(24)	C(25)	119.9(5)	C(53)	C(54)	C(55)	111.0(5)
C(24)	C(25)	C(26)	119.9(5)	C(54)	C(55)	C(56)	111.3(5)
C(21)	C(26)	C(25)	120.2(5)	C(51)	C(56)	C(55)	113.7(5)
P(2)	C(31)	C(32)	119.0(3)	N(3)	C(61)	C(62)	115.1(4)
P(2)	C(31)	C(36)	122.4(4)	N(3)	C(61)	C(66)	114.2(4)
C(32)	C(31)	C(36)	118.6(4)	C(62)	C(61)	C(66)	109.5(4)
C(31)	C(32)	C(33)	119.6(5)	C(61)	C(62)	C(63)	113.0(4)

Table S4. Selected Interatomic Angles for

[Sm{C(Ph_2P=N$SiMe_3$)$_2$-κ^3*C,N,N'*}(NCy_2)(THF)]•0.5PhMe (continued)

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C(62)	C(63)	C(64)	111.1(5)	C(71)	C(72)	C(73b)	106.6(7)
C(63)	C(64)	C(65)	112.3(5)	C(73a)	C(72)	C(73b)	46.2(10)
C(64)	C(65)	C(66)	112.5(5)	C(72)	C(73a)	C(74a)	107.0(14)
C(61)	C(66)	C(65)	112.0(5)	O	C(74a)	C(73a)	106.0(15)
O	C(71)	C(72)	105.2(4)	C(72)	C(73b)	C(74b)	106.0(13)
C(71)	C(72)	C(73a)	109.8(8)	O	C(74b)	C(73b)	105.2(19)

Table S5. Torsional Angles (deg)for

[Sm{C(Ph_2P=NSiMe_3)$_2$-κ^3*C,N,N'*}(NCy_2)(THF)]•0.5PhMe

Atom 1	Atom 2	Atom 3	Atom 4	Angle	Atom 1	Atom 2	Atom 3	Atom 4	Angle
N(1)	Sm	O	C(71)	125.9(4)	N(3)	Sm	N(2)	P(2)	105.70(17)
N(1)	Sm	O	C(74a)	-39.4(11)	N(3)	Sm	N(2)	Si(2)	-60.8(3)
N(1)	Sm	O	C(74b)	-69.2(13)	C(1)	Sm	N(2)	P(2)	-0.63(14)
N(2)	Sm	O	C(71)	-113.2(4)	C(1)	Sm	N(2)	Si(2)	-167.2(3)
N(2)	Sm	O	C(74a)	81.5(11)	O	Sm	N(3)	C(51)	156.0(4)
N(2)	Sm	O	C(74b)	51.6(13)	O	Sm	N(3)	C(61)	-30.9(3)
N(3)	Sm	O	C(71)	9.1(5)	N(1)	Sm	N(3)	C(51)	54.6(4)
N(3)	Sm	O	C(74a)	-156.2(11)	N(1)	Sm	N(3)	C(61)	-132.4(3)
N(3)	Sm	O	C(74b)	174.0(13)	N(2)	Sm	N(3)	C(51)	-92.8(4)
C(1)	Sm	O	C(71)	-176.9(4)	N(2)	Sm	N(3)	C(61)	80.2(3)
C(1)	Sm	O	C(74a)	17.8(12)	C(1)	Sm	N(3)	C(51)	-19.1(4)
C(1)	Sm	O	C(74b)	-12.0(13)	C(1)	Sm	N(3)	C(61)	153.9(3)
O	Sm	N(1)	P(1)	130.78(16)	O	Sm	C(1)	P(1)	-60.4(2)
O	Sm	N(1)	Si(1)	-66.4(2)	O	Sm	C(1)	P(2)	77.7(2)
N(2)	Sm	N(1)	P(1)	32.3(2)	N(1)	Sm	C(1)	P(1)	6.25(14)
N(2)	Sm	N(1)	Si(1)	-164.8(2)	N(1)	Sm	C(1)	P(2)	144.41(19)
N(3)	Sm	N(1)	P(1)	-113.40(16)	N(2)	Sm	C(1)	P(1)	-137.5(2)
N(3)	Sm	N(1)	Si(1)	49.4(3)	N(2)	Sm	C(1)	P(2)	0.61(14)
C(1)	Sm	N(1)	P(1)	-6.42(14)	N(3)	Sm	C(1)	P(1)	113.52(17)
C(1)	Sm	N(1)	Si(1)	156.4(3)	N(3)	Sm	C(1)	P(2)	-108.33(17)
O	Sm	N(2)	P(2)	-134.01(15)	C(1)	P(1)	N(1)	Sm	9.1(2)
O	Sm	N(2)	Si(2)	59.5(2)	C(1)	P(1)	N(1)	Si(1)	-151.5(3)
N(1)	Sm	N(2)	P(2)	-39.5(2)	C(11)	P(1)	N(1)	Sm	-117.09(17)
N(1)	Sm	N(2)	Si(2)	154.0(2)	C(11)	P(1)	N(1)	Si(1)	82.3(3)

Table S5. Torsional Angles for

[Sm{C(Ph_2P=NSiMe_3)$_2$-κ^3*C,N,N'*}(NCy_2)(THF)]•0.5PhMe (continued)

Atom 1	Atom 2	Atom 3	Atom 4	Angle	Atom 1	Atom 2	Atom 3	Atom 4	Angle
C(21)	P(1)	N(1)	Sm	130.82(17)	C(41)	P(2)	N(2)	Sm	128.29(17)
C(21)	P(1)	N(1)	Si(1)	-29.8(4)	C(41)	P(2)	N(2)	Si(2)	-67.0(4)
N(1)	P(1)	C(1)	Sm	-8.9(2)	N(2)	P(2)	C(1)	Sm	-0.9(2)
N(1)	P(1)	C(1)	P(2)	-103.1(4)	N(2)	P(2)	C(1)	P(1)	93.0(4)
C(11)	P(1)	C(1)	Sm	114.33(19)	C(31)	P(2)	C(1)	Sm	119.56(17)
C(11)	P(1)	C(1)	P(2)	20.1(5)	C(31)	P(2)	C(1)	P(1)	-146.6(4)
C(21)	P(1)	C(1)	Sm	-129.55(17)	C(41)	P(2)	C(1)	Sm	-126.16(18)
C(21)	P(1)	C(1)	P(2)	136.3(4)	C(41)	P(2)	C(1)	P(1)	-32.3(5)
N(1)	P(1)	C(11)	C(12)	-167.5(4)	N(2)	P(2)	C(31)	C(32)	113.6(4)
N(1)	P(1)	C(11)	C(16)	16.7(4)	N(2)	P(2)	C(31)	C(36)	-67.6(4)
C(1)	P(1)	C(11)	C(12)	70.6(4)	C(1)	P(2)	C(31)	C(32)	-5.8(4)
C(1)	P(1)	C(11)	C(16)	-105.1(4)	C(1)	P(2)	C(31)	C(36)	173.0(4)
C(21)	P(1)	C(11)	C(12)	-50.6(4)	C(41)	P(2)	C(31)	C(32)	-128.1(4)
C(21)	P(1)	C(11)	C(16)	133.6(4)	C(41)	P(2)	C(31)	C(36)	50.7(4)
N(1)	P(1)	C(21)	C(22)	-91.7(4)	N(2)	P(2)	C(41)	C(42)	-39.9(4)
N(1)	P(1)	C(21)	C(26)	85.7(4)	N(2)	P(2)	C(41)	C(46)	147.8(4)
C(1)	P(1)	C(21)	C(22)	27.5(4)	C(1)	P(2)	C(41)	C(42)	83.9(4)
C(1)	P(1)	C(21)	C(26)	-155.0(4)	C(1)	P(2)	C(41)	C(46)	-88.3(4)
C(11)	P(1)	C(21)	C(22)	151.2(4)	C(31)	P(2)	C(41)	C(42)	-157.5(4)
C(11)	P(1)	C(21)	C(26)	-31.3(4)	C(31)	P(2)	C(41)	C(46)	30.3(4)
C(1)	P(2)	N(2)	Sm	0.9(2)	C(2)	Si(1)	N(1)	Sm	13.1(3)
C(1)	P(2)	N(2)	Si(2)	165.6(3)	C(2)	Si(1)	N(1)	P(1)	168.4(3)
C(31)	P(2)	N(2)	Sm	-119.19(18)	C(3)	Si(1)	N(1)	Sm	-104.8(3)
C(31)	P(2)	N(2)	Si(2)	45.5(4)	C(3)	Si(1)	N(1)	P(1)	50.5(4)

Table S5. Torsional Angles for

[Sm{C(Ph_2P=N$SiMe_3$)$_2$-κ^3*C,N,N'*}(NCy_2)(THF)]•0.5PhMe (continued)

Atom 1	Atom 2	Atom 3	Atom 4	Angle	Atom 1	Atom 2	Atom 3	Atom 4	Angle
C(4)	Si(1)	N(1)	Sm	132.4(3)	C(51)	N(3)	C(61)	C(66)	-65.7(5)
C(4)	Si(1)	N(1)	P(1)	-72.3(4)	P(1)	C(11)	C(12)	C(13)	-177.2(4)
C(5)	Si(2)	N(2)	Sm	91.1(3)	C(16)	C(11)	C(12)	C(13)	-1.4(7)
C(5)	Si(2)	N(2)	P(2)	-69.3(4)	P(1)	C(11)	C(16)	C(15)	175.8(4)
C(6)	Si(2)	N(2)	Sm	-144.5(3)	C(12)	C(11)	C(16)	C(15)	-0.1(7)
C(6)	Si(2)	N(2)	P(2)	55.1(4)	C(11)	C(12)	C(13)	C(14)	1.5(8)
C(7)	Si(2)	N(2)	Sm	-26.6(3)	C(12)	C(13)	C(14)	C(15)	-0.1(8)
C(7)	Si(2)	N(2)	P(2)	173.0(4)	C(13)	C(14)	C(15)	C(16)	-1.4(8)
Sm	O	C(71)	C(72)	178.0(5)	C(14)	C(15)	C(16)	C(11)	1.5(8)
C(74a)	O	C(71)	C(72)	-15.1(12)	P(1)	C(21)	C(22)	C(23)	177.6(4)
C(74b)	O	C(71)	C(72)	12.5(13)	C(26)	C(21)	C(22)	C(23)	0.1(7)
Sm	O	C(74a)	C(73a)	171.2(11)	P(1)	C(21)	C(26)	C(25)	-178.2(4)
C(71)	O	C(74a)	C(73a)	2.6(18)	C(22)	C(21)	C(26)	C(25)	-0.8(7)
C(74b)	O	C(74a)	C(73a)	-101(5)	C(21)	C(22)	C(23)	C(24)	0.1(8)
Sm	O	C(74b)	C(73b)	-164.6(11)	C(22)	C(23)	C(24)	C(25)	0.4(9)
C(71)	O	C(74b)	C(73b)	3(2)	C(23)	C(24)	C(25)	C(26)	-1.2(8)
C(74a)	O	C(74b)	C(73b)	89(5)	C(24)	C(25)	C(26)	C(21)	1.3(8)
Sm	N(3)	C(51)	C(52)	-59.5(6)	P(2)	C(31)	C(32)	C(33)	-179.5(4)
Sm	N(3)	C(51)	C(56)	63.3(6)	C(36)	C(31)	C(32)	C(33)	1.6(7)
C(61)	N(3)	C(51)	C(52)	127.7(5)	P(2)	C(31)	C(36)	C(35)	-179.1(4)
C(61)	N(3)	C(51)	C(56)	-109.4(5)	C(32)	C(31)	C(36)	C(35)	-0.3(7)
Sm	N(3)	C(61)	C(62)	-112.0(4)	C(31)	C(32)	C(33)	C(34)	-3.2(7)
Sm	N(3)	C(61)	C(66)	120.1(4)	C(32)	C(33)	C(34)	C(35)	3.3(8)
C(51)	N(3)	C(61)	C(62)	62.2(5)	C(33)	C(34)	C(35)	C(36)	-1.9(8)

Table S5. Torsional Angles for

[Sm{C(Ph_2P=NSiMe_3)$_2$-κ^3*C,N,N'*}(NCy_2)(THF)]•0.5PhMe (continued)

Atom 1	Atom 2	Atom 3	Atom 4	Angle
C(34)	C(35)	C(36)	C(31)	0.4(8)
P(2)	C(41)	C(42)	C(43)	-172.1(4)
C(46)	C(41)	C(42)	C(43)	0.3(7)
P(2)	C(41)	C(46)	C(45)	173.4(4)
C(42)	C(41)	C(46)	C(45)	1.0(7)
C(41)	C(42)	C(43)	C(44)	-0.9(8)
C(42)	C(43)	C(44)	C(45)	0.2(9)
C(43)	C(44)	C(45)	C(46)	1.1(9)
C(44)	C(45)	C(46)	C(41)	-1.7(9)
N(3)	C(51)	C(52)	C(53)	176.8(5)
C(56)	C(51)	C(52)	C(53)	52.5(7)
N(3)	C(51)	C(56)	C(55)	-176.8(5)
C(52)	C(51)	C(56)	C(55)	-53.2(6)
C(51)	C(52)	C(53)	C(54)	-54.0(8)
C(52)	C(53)	C(54)	C(55)	53.5(8)
C(53)	C(54)	C(55)	C(56)	-54.2(7)
C(54)	C(55)	C(56)	C(51)	55.1(7)
N(3)	C(61)	C(62)	C(63)	175.9(4)
C(66)	C(61)	C(62)	C(63)	-53.9(6)
N(3)	C(61)	C(66)	C(65)	-176.9(4)
C(62)	C(61)	C(66)	C(65)	52.4(6)
C(61)	C(62)	C(63)	C(64)	54.9(7)
C(62)	C(63)	C(64)	C(65)	-54.5(7)
C(63)	C(64)	C(65)	C(66)	54.3(8)
C(64)	C(65)	C(66)	C(61)	-54.0(7)
O	C(71)	C(72)	C(73a)	25.1(15)
O	C(71)	C(72)	C(73b)	-23.6(10)
C(71)	C(72)	C(73a)	C(74a)	-23(2)
C(73b)	C(72)	C(73a)	C(74a)	71.3(17)
C(71)	C(72)	C(73b)	C(74b)	26.0(18)
C(73a)	C(72)	C(73b)	C(74b)	-75.8(18)
C(72)	C(73a)	C(74a)	O	13(2)
C(72)	C(73b)	C(74b)	O	-18(2)

Table S6. Least-Squares Planes for

[Sm{C(Ph_2P=NSiMe_3)$_2$-κ^3*C,N,N'*}(NCy_2)(THF)]•0.5PhMe

Plane	Coefficients[a]			Defining Atoms with Deviations (Å)[b]			
1	4.181(14)	6.723(11)	18.45(2)	8.4765(12)			
				Sm	-0.0373(8)	N(1)	0.0595(13)
				P(1)	-0.0788(18)	C(1)	0.0566(13)
				Si(1)	0.613(6)		
2	3.781(13)	10.708(7)	8.01(3)	7.153(7)			
				Sm	0.0036(8)	N(2)	-0.0058(13)
				P(2)	0.0077(17)	C(1)	-0.0056(12)
				Si(2)	0.291(6)		

Dihedral angle between planes 1 and 2: 37.69(13)°

[a]Coefficients are for the form $ax+by+cz = d$ where x, y and z are crystallographic coordinates.

[b]Underlined atoms were not included in the definition of the plane.

Table S7. Anisotropic Displacement Parameters (U_{ij}, Å^2) for

[Sm{C(Ph_2P=N$SiMe_3$)$_2$-κ^3*C,N,N'*}(NCy_2)(THF)]•0.5PhMe

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sm	0.02058(13)	0.02311(12)	0.03043(14)	-0.00646(9)	-0.00225(9)	-0.00334(8)
P(1)	0.0200(6)	0.0224(5)	0.0280(6)	-0.0055(4)	-0.0028(4)	-0.0033(4)
P(2)	0.0220(6)	0.0262(5)	0.0275(6)	-0.0049(4)	-0.0021(4)	-0.0045(4)
Si(1)	0.0307(7)	0.0303(6)	0.0337(7)	-0.0004(5)	0.0039(5)	-0.0052(5)
Si(2)	0.0303(7)	0.0372(7)	0.0288(7)	-0.0039(5)	-0.0062(5)	0.0010(6)
O	0.0268(18)	0.0397(18)	0.068(2)	-0.0152(17)	-0.0139(17)	-0.0042(15)
N(1)	0.0224(19)	0.0286(18)	0.031(2)	-0.0032(15)	-0.0030(15)	-0.0068(15)
N(2)	0.028(2)	0.0344(19)	0.034(2)	-0.0061(16)	-0.0050(16)	-0.0034(16)
N(3)	0.026(2)	0.0314(19)	0.039(2)	-0.0116(17)	-0.0003(17)	-0.0040(16)
C(1)	0.022(2)	0.0216(19)	0.029(2)	-0.0043(17)	-0.0036(17)	-0.0032(17)
C(2)	0.031(3)	0.068(4)	0.047(3)	0.002(3)	0.007(2)	0.002(3)
C(3)	0.047(3)	0.069(4)	0.035(3)	0.001(3)	-0.002(3)	0.001(3)
C(4)	0.096(5)	0.040(3)	0.060(4)	-0.002(3)	0.025(4)	-0.023(3)
C(5)	0.054(4)	0.037(3)	0.057(4)	-0.003(2)	-0.007(3)	0.000(3)
C(6)	0.060(4)	0.061(3)	0.034(3)	-0.013(3)	-0.013(3)	0.003(3)
C(7)	0.035(3)	0.073(4)	0.051(3)	0.004(3)	-0.010(3)	0.006(3)
C(11)	0.030(2)	0.0221(19)	0.028(2)	-0.0017(17)	-0.0056(18)	-0.0036(18)
C(12)	0.027(2)	0.033(2)	0.043(3)	-0.011(2)	-0.004(2)	-0.004(2)
C(13)	0.034(3)	0.038(3)	0.053(3)	-0.017(2)	-0.003(2)	0.002(2)
C(14)	0.047(3)	0.034(2)	0.051(3)	-0.020(2)	-0.001(3)	-0.001(2)
C(15)	0.044(3)	0.033(2)	0.053(3)	-0.013(2)	-0.009(2)	-0.015(2)
C(16)	0.024(2)	0.032(2)	0.037(3)	-0.008(2)	0.0007(19)	-0.0041(19)
C(21)	0.021(2)	0.036(2)	0.027(2)	-0.0043(18)	-0.0033(18)	-0.0011(18)
C(22)	0.036(3)	0.043(3)	0.036(3)	-0.008(2)	-0.004(2)	-0.008(2)

Table S7. Anisotropic Displacement Parameters for

[Sm{C(Ph_2P=N$SiMe_3$)$_2$-κ^3*C,N,N'*}(NCy_2)(THF)]•0.5PhMe (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(23)	0.044(3)	0.064(3)	0.045(3)	-0.014(3)	-0.015(3)	-0.014(3)
C(24)	0.039(3)	0.087(4)	0.033(3)	-0.002(3)	-0.016(2)	0.006(3)
C(25)	0.039(3)	0.055(3)	0.040(3)	0.002(3)	-0.006(2)	0.005(3)
C(26)	0.033(3)	0.040(3)	0.033(3)	0.001(2)	-0.004(2)	0.001(2)
C(31)	0.024(2)	0.026(2)	0.038(3)	-0.0043(19)	0.0007(19)	-0.0002(18)
C(32)	0.029(3)	0.028(2)	0.048(3)	-0.003(2)	-0.002(2)	-0.0041(19)
C(33)	0.027(3)	0.033(2)	0.076(4)	-0.014(3)	-0.008(3)	-0.010(2)
C(34)	0.033(3)	0.031(3)	0.089(5)	-0.009(3)	0.012(3)	-0.008(2)
C(35)	0.046(3)	0.037(3)	0.060(4)	0.008(3)	0.022(3)	-0.001(2)
C(36)	0.041(3)	0.043(3)	0.039(3)	-0.001(2)	0.006(2)	-0.002(2)
C(41)	0.033(3)	0.035(2)	0.024(2)	-0.0051(19)	-0.0028(19)	-0.002(2)
C(42)	0.038(3)	0.038(2)	0.035(3)	-0.005(2)	-0.006(2)	-0.003(2)
C(43)	0.062(4)	0.045(3)	0.041(3)	-0.016(2)	-0.012(3)	-0.008(3)
C(44)	0.073(4)	0.050(3)	0.040(3)	-0.021(3)	-0.001(3)	0.004(3)
C(45)	0.048(3)	0.058(3)	0.046(3)	-0.020(3)	0.007(3)	0.005(3)
C(46)	0.036(3)	0.044(3)	0.037(3)	-0.009(2)	0.000(2)	-0.002(2)
C(51)	0.027(3)	0.037(2)	0.051(3)	-0.019(2)	-0.007(2)	-0.002(2)
C(52)	0.049(3)	0.080(4)	0.043(3)	-0.007(3)	-0.008(3)	-0.031(3)
C(53)	0.054(4)	0.110(6)	0.047(4)	-0.017(4)	-0.015(3)	-0.028(4)
C(54)	0.037(3)	0.066(4)	0.062(4)	-0.026(3)	-0.011(3)	-0.008(3)
C(55)	0.041(3)	0.059(4)	0.097(5)	-0.010(4)	-0.017(3)	-0.022(3)
C(56)	0.042(3)	0.051(3)	0.059(4)	0.005(3)	-0.010(3)	-0.021(3)
C(61)	0.028(2)	0.034(2)	0.041(3)	-0.011(2)	-0.002(2)	-0.006(2)
C(62)	0.043(3)	0.033(2)	0.056(3)	-0.010(2)	-0.004(3)	-0.005(2)

Table S7. Anisotropic Displacement Parameters for [Sm{C(Ph_2P=N$SiMe_3$)$_2$-κ^3*C,N,N'*}(NCy_2)(THF)]•0.5PhMe (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(63)	0.058(4)	0.044(3)	0.066(4)	-0.003(3)	-0.024(3)	0.007(3)
C(64)	0.046(4)	0.074(4)	0.087(5)	-0.023(4)	-0.017(3)	0.027(3)
C(65)	0.030(3)	0.087(5)	0.066(4)	-0.019(4)	0.003(3)	0.009(3)
C(66)	0.034(3)	0.059(3)	0.045(3)	-0.012(3)	0.002(2)	-0.003(3)
C(71)	0.025(3)	0.047(3)	0.069(4)	-0.015(3)	-0.006(2)	-0.004(2)
C(72)	0.035(4)	0.113(6)	0.118(6)	-0.073(5)	-0.010(4)	-0.009(4)
C(73a)	0.044(9)	0.057(9)	0.18(2)	-0.044(11)	-0.047(11)	-0.004(7)
C(74a)	0.025(9)	0.046(9)	0.11(2)	-0.038(12)	-0.028(11)	0.009(7)
C(73b)	0.033(7)	0.075(9)	0.070(9)	-0.039(8)	-0.005(6)	-0.012(6)
C(74b)	0.050(10)	0.09(2)	0.11(2)	-0.067(17)	-0.010(14)	-0.008(11)

The form of the anisotropic displacement parameter is:

$$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$$

Table S8. Derived Atomic Coordinates and Displacement Parameters for Hydrogen Atoms for [Sm{C(Ph_2P=N$SiMe_3$)$_2$-κ^3*C,N,N'*}(NCy_2)(THF)]•0.5PhMe

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H(2A)	-0.0238	0.3267	0.4209	0.062
H(2B)	-0.0782	0.2076	0.4609	0.062
H(2C)	-0.0845	0.2344	0.3868	0.062
H(3A)	0.2208	0.2533	0.4768	0.062
H(3B)	0.2897	0.1237	0.4709	0.062
H(3C)	0.1569	0.1364	0.5139	0.062
H(4A)	0.1837	-0.0441	0.3987	0.082
H(4B)	0.0505	-0.0079	0.3729	0.082
H(4C)	0.0575	-0.0335	0.4470	0.082
H(5A)	0.2918	0.7200	0.0887	0.060
H(5B)	0.1754	0.7481	0.1402	0.060
H(5C)	0.1571	0.7681	0.0672	0.060
H(6A)	0.2824	0.5066	0.0154	0.061
H(6B)	0.1482	0.5652	-0.0024	0.061
H(6C)	0.1614	0.4293	0.0307	0.061
H(7A)	-0.0477	0.4825	0.1328	0.065
H(7B)	-0.0609	0.6151	0.0953	0.065
H(7C)	-0.0434	0.5954	0.1683	0.065
H(12)	0.5548	0.0912	0.2376	0.041
H(13)	0.5849	-0.0703	0.1817	0.049
H(14)	0.4115	-0.1665	0.1641	0.052
H(15)	0.2084	-0.0999	0.2031	0.050
H(16)	0.1785	0.0566	0.2629	0.037
H(22)	0.4804	0.3604	0.3574	0.045

Table S8. Derived Parameters for Hydrogen Atoms for $[Sm\{C(Ph_2P{=}NSiMe_3)_2\text{-}\kappa^3C,N,N'\}(NCy_2)(THF)]\bullet 0.5PhMe$ (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H(23)	0.6212	0.3252	0.4318	0.058
H(24)	0.6797	0.1308	0.4741	0.064
H(25)	0.5992	-0.0310	0.4405	0.055
H(26)	0.4549	0.0043	0.3675	0.044
H(32)	0.5151	0.5202	0.2466	0.042
H(33)	0.6560	0.6714	0.2224	0.053
H(34)	0.7133	0.7526	0.1195	0.063
H(35)	0.6157	0.7010	0.0398	0.062
H(36)	0.4681	0.5558	0.0630	0.051
H(42)	0.2535	0.2336	0.1197	0.044
H(43)	0.3350	0.0839	0.0605	0.057
H(44)	0.5508	0.0639	0.0247	0.065
H(45)	0.6851	0.1950	0.0491	0.062
H(46)	0.6073	0.3406	0.1116	0.047
H(51)	0.1223	0.6813	0.3897	0.044
H(52A)	0.2509	0.4494	0.4067	0.067
H(52B)	0.1303	0.4949	0.4511	0.067
H(53A)	0.2498	0.6253	0.4889	0.081
H(53B)	0.3211	0.4946	0.4974	0.081
H(54A)	0.4660	0.5459	0.4094	0.063
H(54B)	0.4630	0.6453	0.4547	0.063
H(55A)	0.3359	0.7789	0.3921	0.077
H(55B)	0.4567	0.7342	0.3474	0.077
H(56A)	0.2677	0.7305	0.3017	0.061

Table S8. Derived Parameters for Hydrogen Atoms for [Sm{C(Ph_2P=N$SiMe_3$)$_2$-κ^3*C,N,N'*}(NCy_2)(THF)]•0.5PhMe (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H(56B)	0.3395	0.6004	0.3117	0.061
H(61)	-0.0610	0.5892	0.2912	0.040
H(62A)	0.0296	0.8082	0.3101	0.052
H(62B)	0.0475	0.7571	0.2445	0.052
H(63A)	-0.1222	0.9077	0.2492	0.067
H(63B)	-0.1699	0.7834	0.2385	0.067
H(64A)	-0.2005	0.8756	0.3557	0.082
H(64B)	-0.3124	0.8615	0.3161	0.082
H(65A)	-0.2873	0.6568	0.3372	0.074
H(65B)	-0.3032	0.7095	0.4023	0.074
H(66A)	-0.0851	0.6768	0.4090	0.055
H(66B)	-0.1353	0.5538	0.3983	0.055
H(71A)	-0.2088	0.4543	0.2455	0.056
H(71B)	-0.2197	0.3742	0.3138	0.056
H(72A)	-0.3460	0.2745	0.2712	0.099
H(72B)	-0.2808	0.3158	0.2010	0.099
H(73A)[a]	-0.2103	0.1479	0.2088	0.104
H(73B)[a]	-0.2275	0.1313	0.2844	0.104
H(74A)[a]	-0.0194	0.1554	0.2767	0.068
H(74B)[a]	-0.0120	0.2036	0.2026	0.068
H(73C)[a]	-0.1899	0.1440	0.1983	0.067
H(73D)[a]	-0.1805	0.2716	0.1543	0.067
H(74C)[a]	0.0151	0.2613	0.1767	0.092
H(74D)[a]	-0.0128	0.1601	0.2366	0.092

[a]Included with an occupancy factor of 0.5.