Design, Isolation, and Spectroscopic Analysis of a Tetravalent Terbium Complex

Supporting Information

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Table of Contents

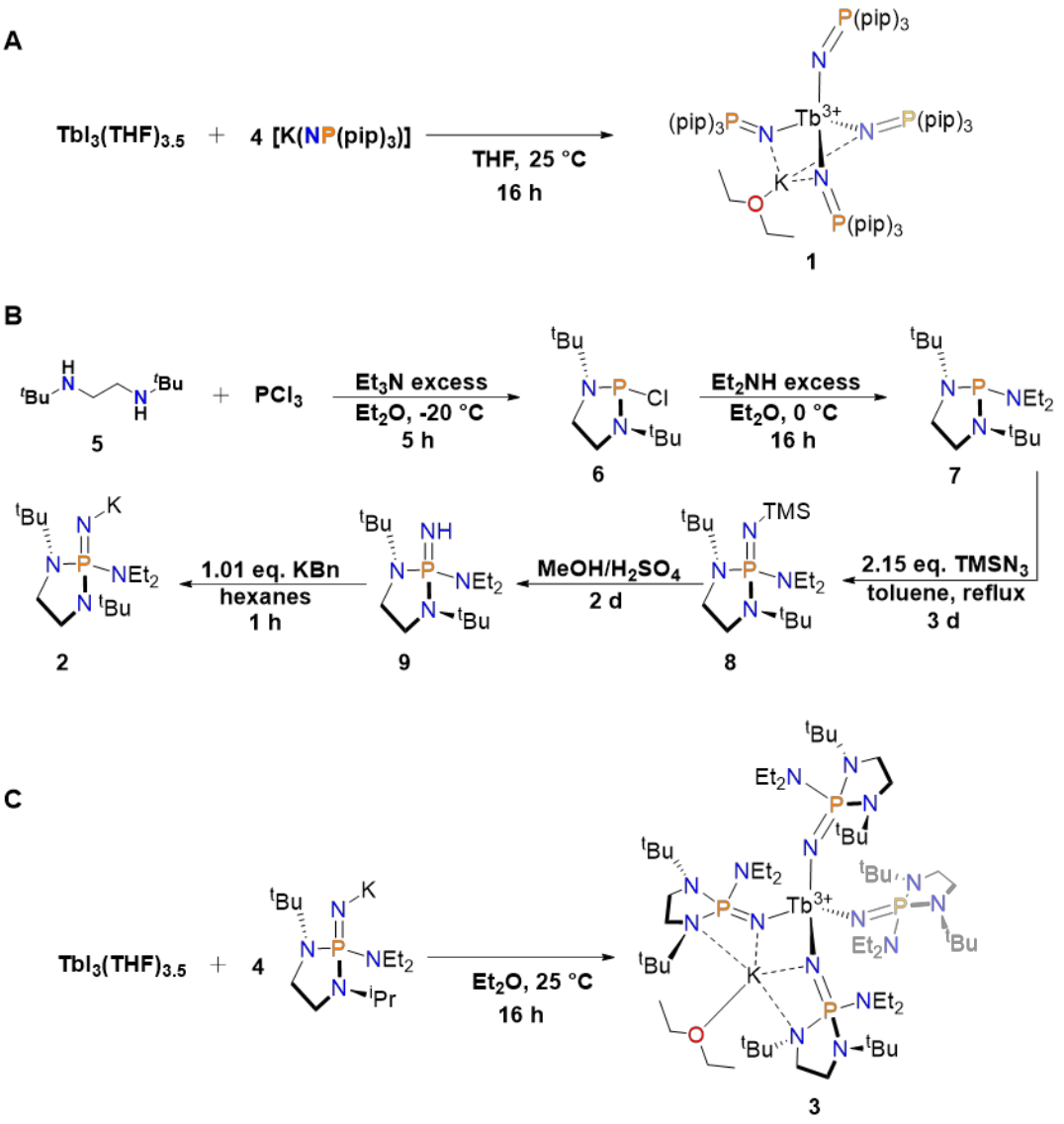

Figure S1. General synthetic route of the reported compounds.

NMR Spectra of Reported Compounds

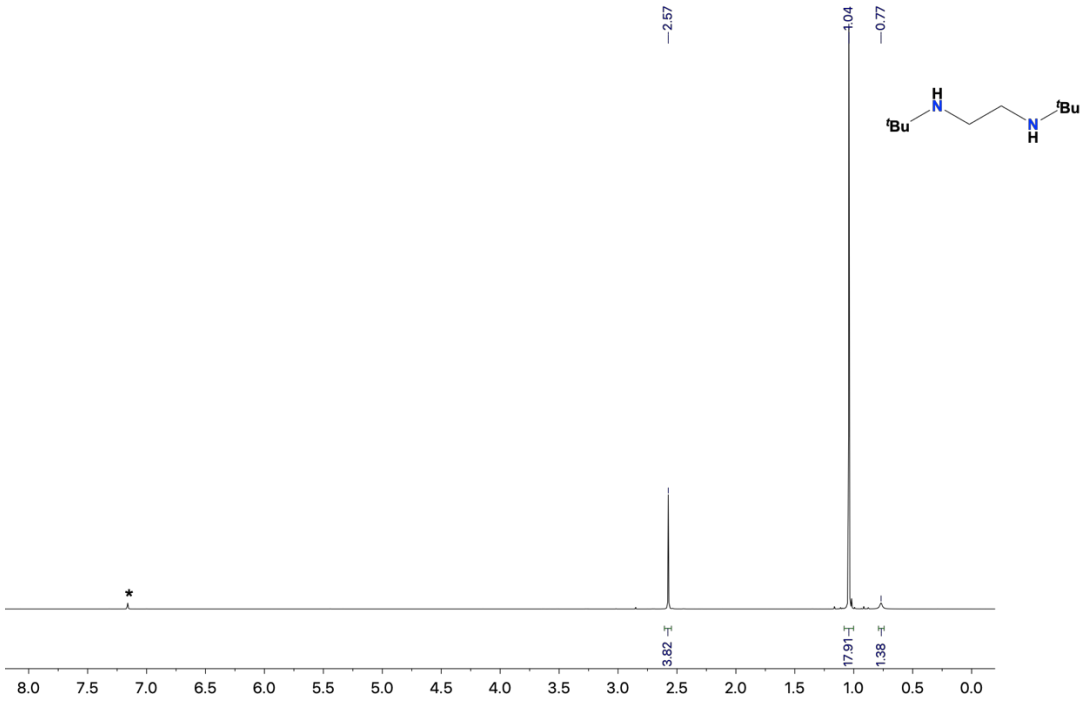

Figure S2. ^{1}H NMR of **5** in C_6D_6. Peak of C_6D_5H is noted as *.

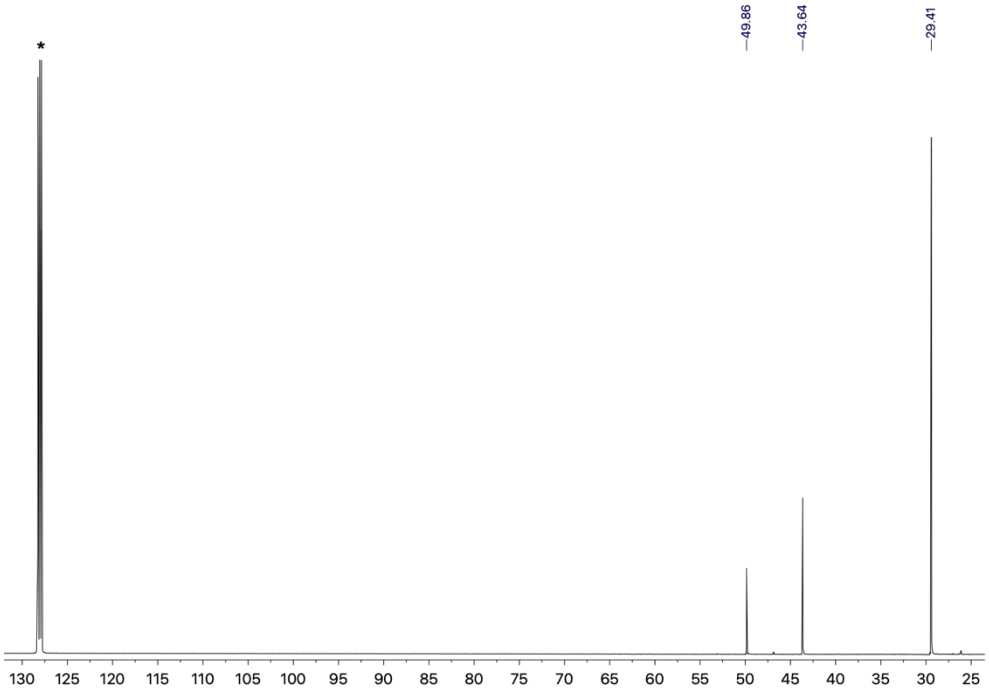

Figure S3. $^{13}C\{^{1}H\}$ NMR of **5** in C_6D_6. Peak of C_6D_5H is noted as *.

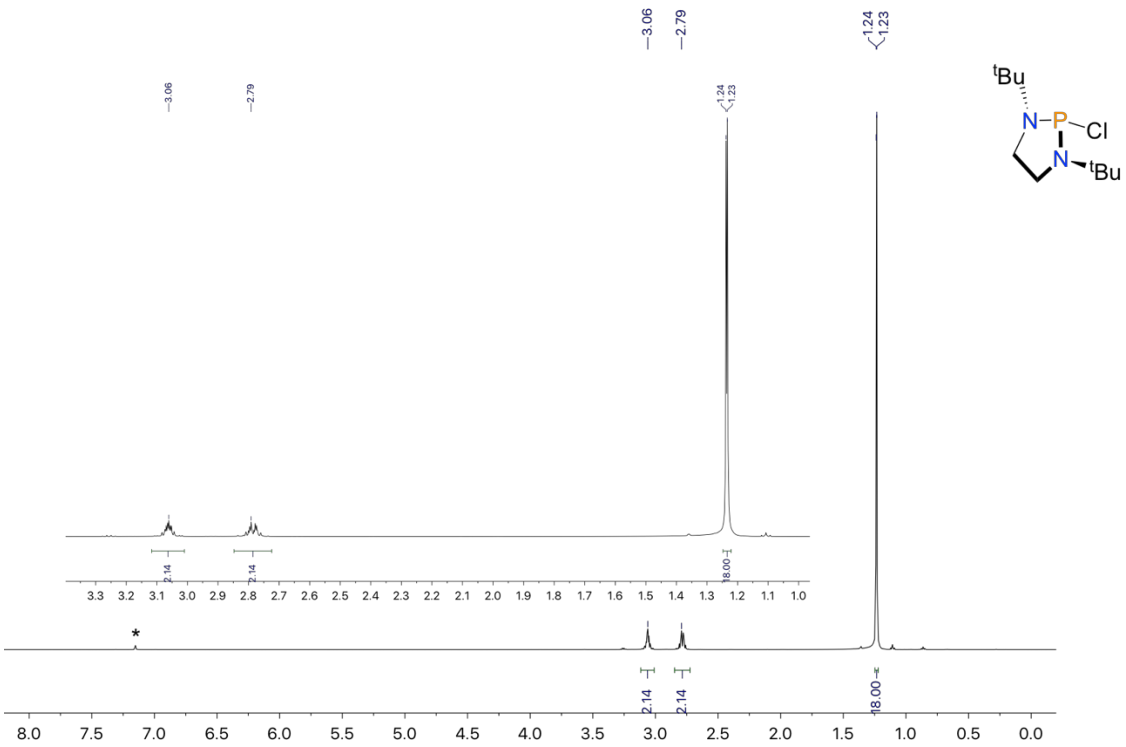

Figure S4. ^{1}H NMR of **6** in C_6D_6. Peak of C_6D_5H is noted as *.

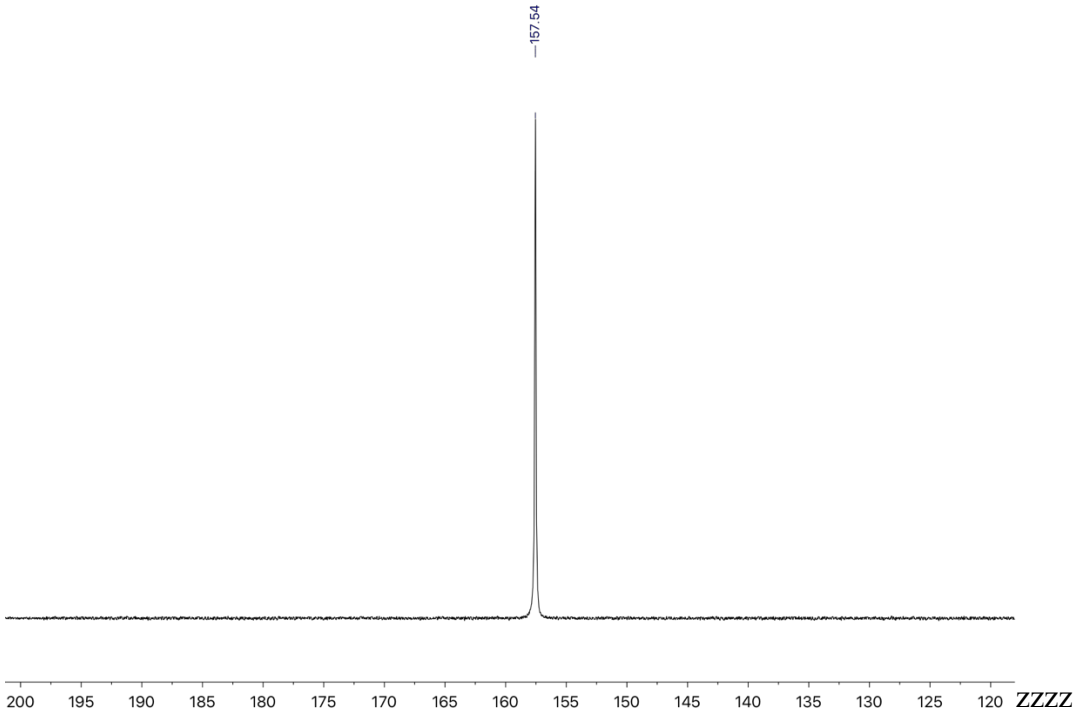

Figure S5. $^{31}P\{^{1}H\}$ NMR of **6** in C_6D_6.

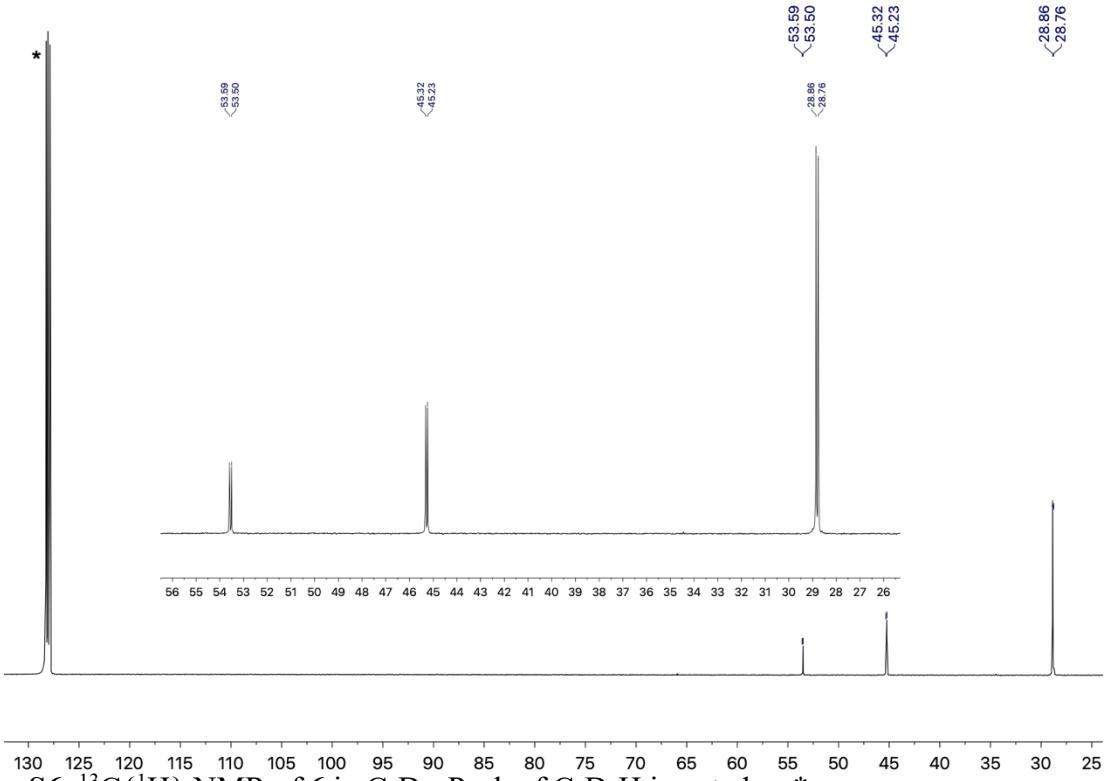

Figure S6. $^{13}C\{^{1}H\}$ NMR of **6** in C_6D_6. Peak of C_6D_5H is noted as *.

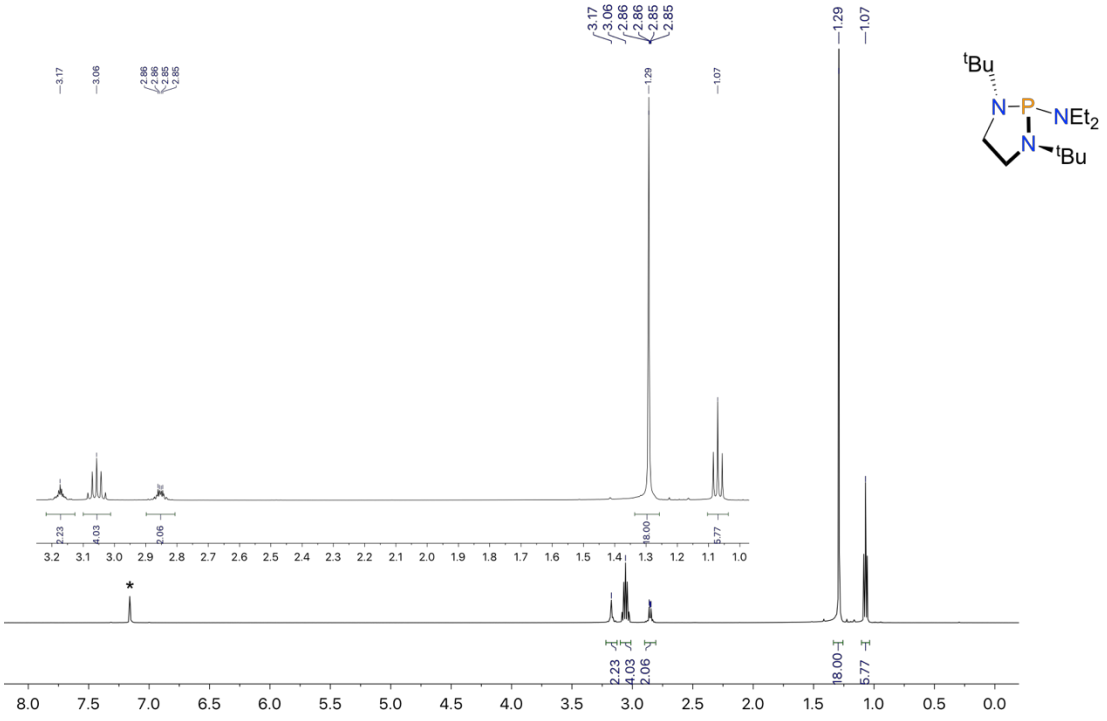

Figure S7. ^{1}H NMR of **7** in C_6D_6. Peak of C_6D_5H is noted as *.

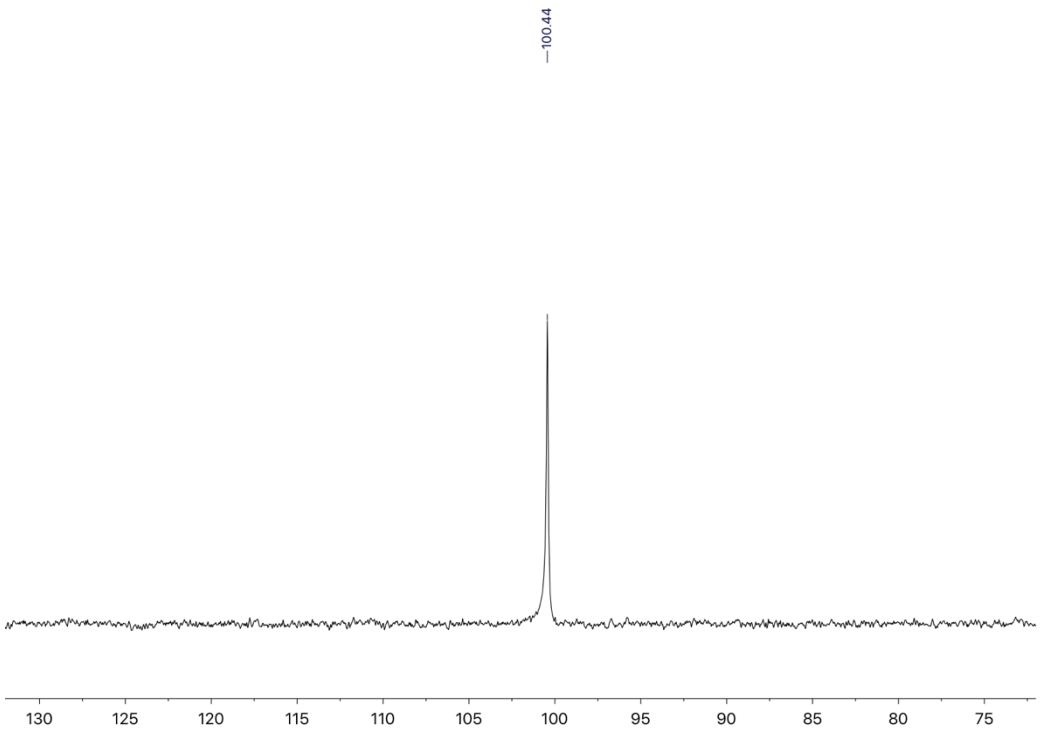

Figure S8. $^{31}P\{^{1}H\}$ NMR of **7** in C_6D_6.

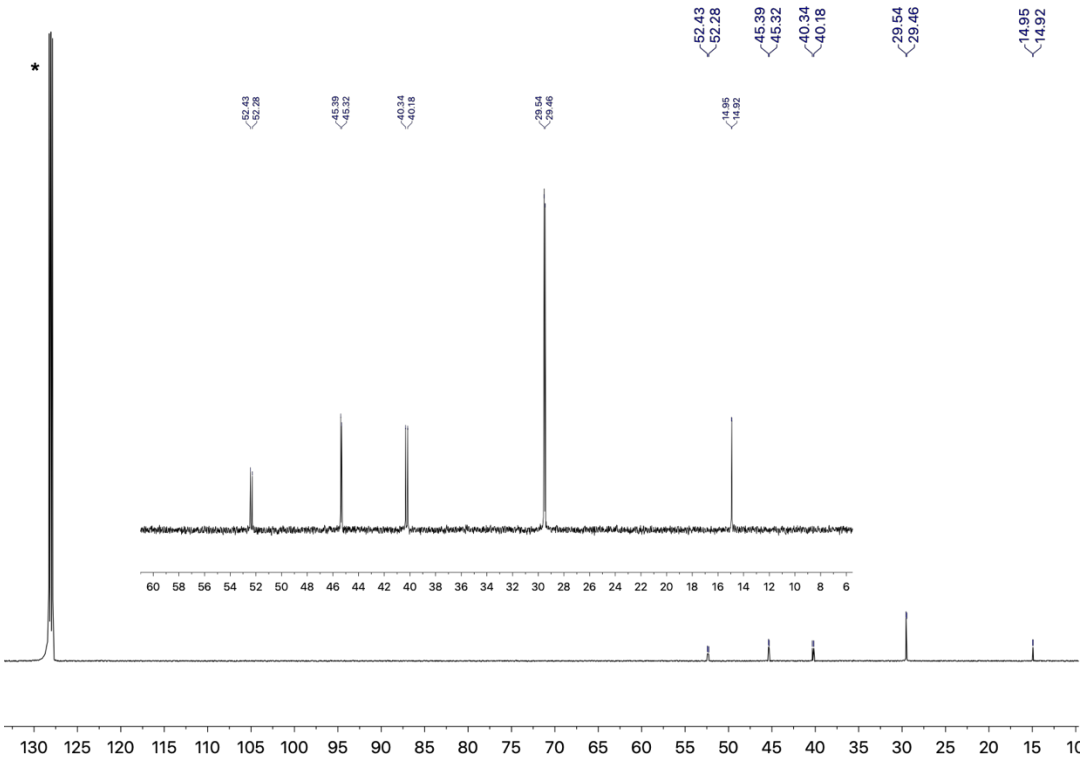

Figure S9. $^{13}C\{^{1}H\}$ NMR of **7** in C_6D_6. Peak of C_6D_5H is noted as *.

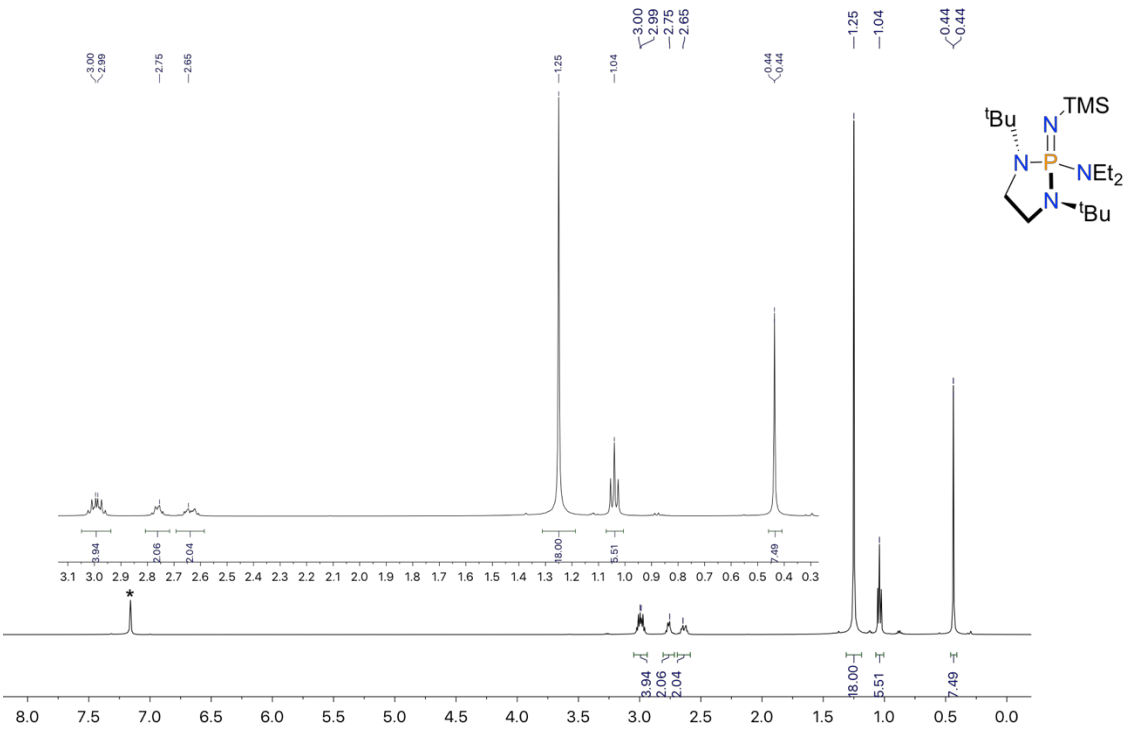

Figure S10. ^{1}H NMR of [TMSN=P(1,2-*bis*-^{t}Bu-diamidoethane)(NEt_2)] in C_6D_6. Peak of C_6D_5H is noted as *.

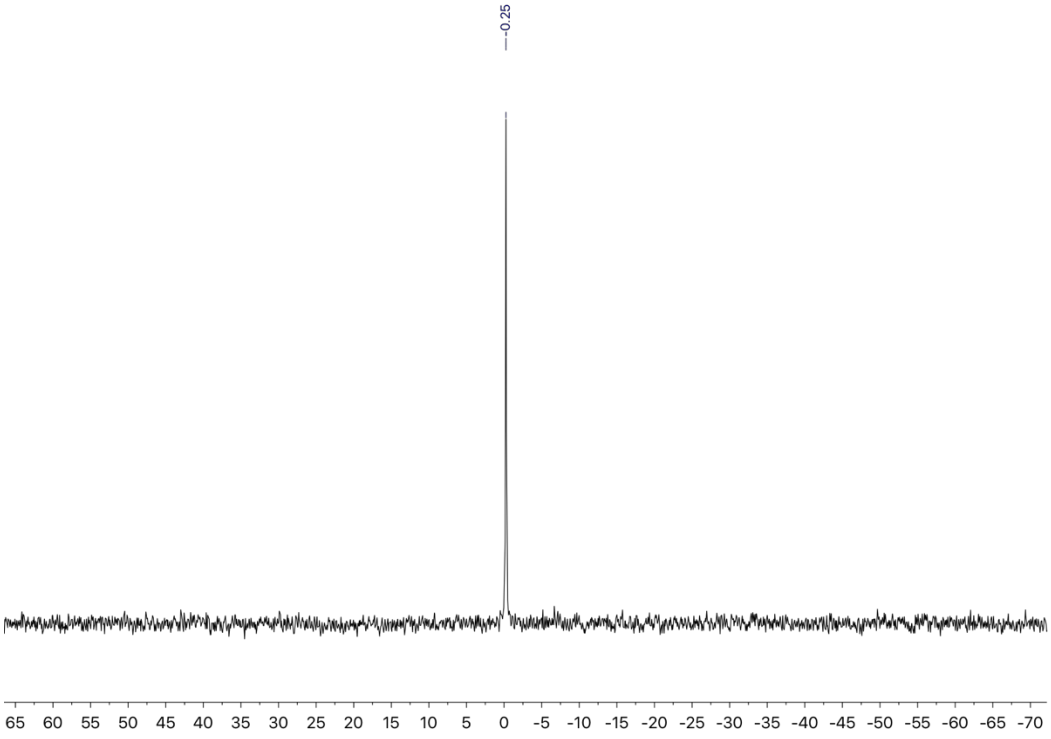

Figure S11. $^{31}P\{^{1}H\}$ NMR of [TMSN=P(1,2-*bis*-^{t}Bu-diamidoethane)(NEt_2)] in C_6D_6.

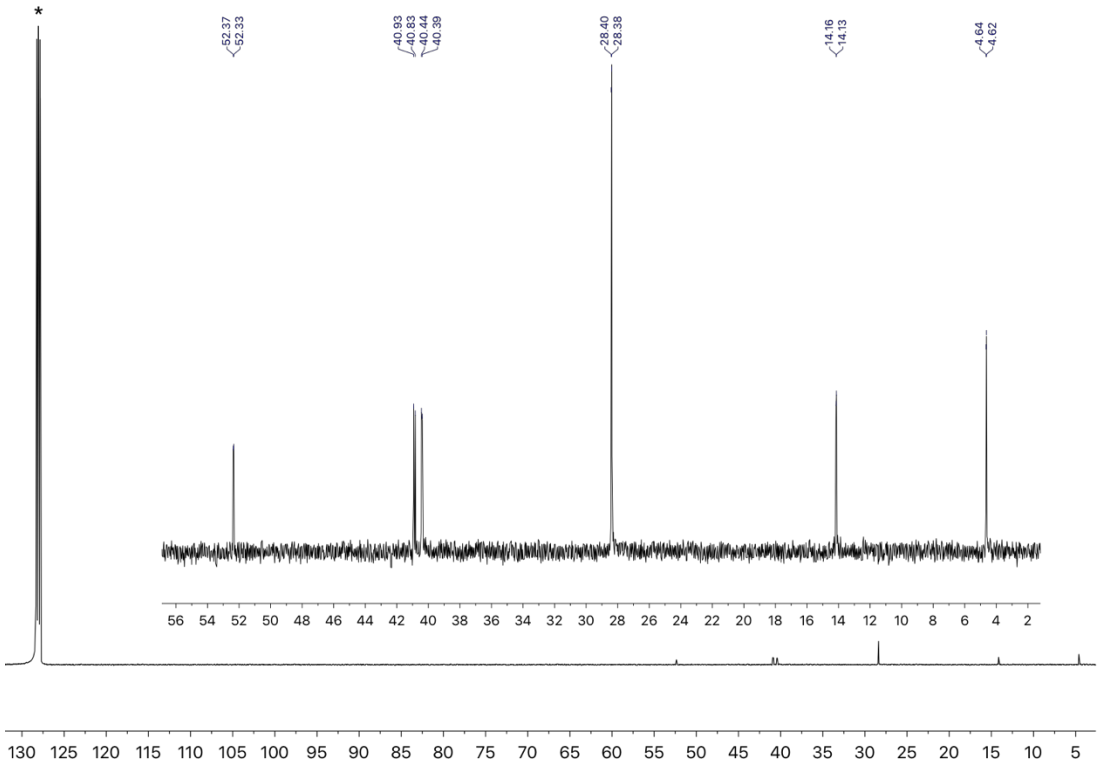

Figure S12. $^{13}C\{^{1}H\}$ NMR of [TMSN=P(1,2-*bis*-^{t}Bu-diamidoethane)(NEt_2)] in C_6D_6. Peak of C_6D_5H is noted as *.

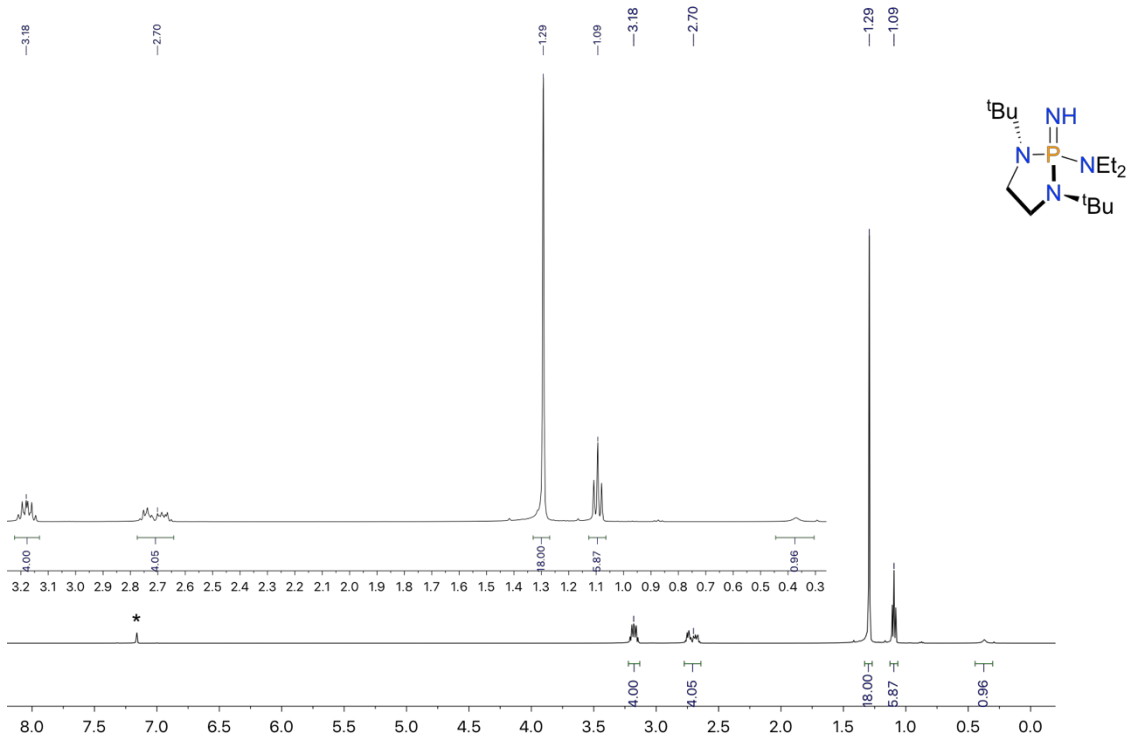

Figure S13. ^{1}H NMR of **8** in C_6D_6. Peak of C_6D_5H is noted as *.

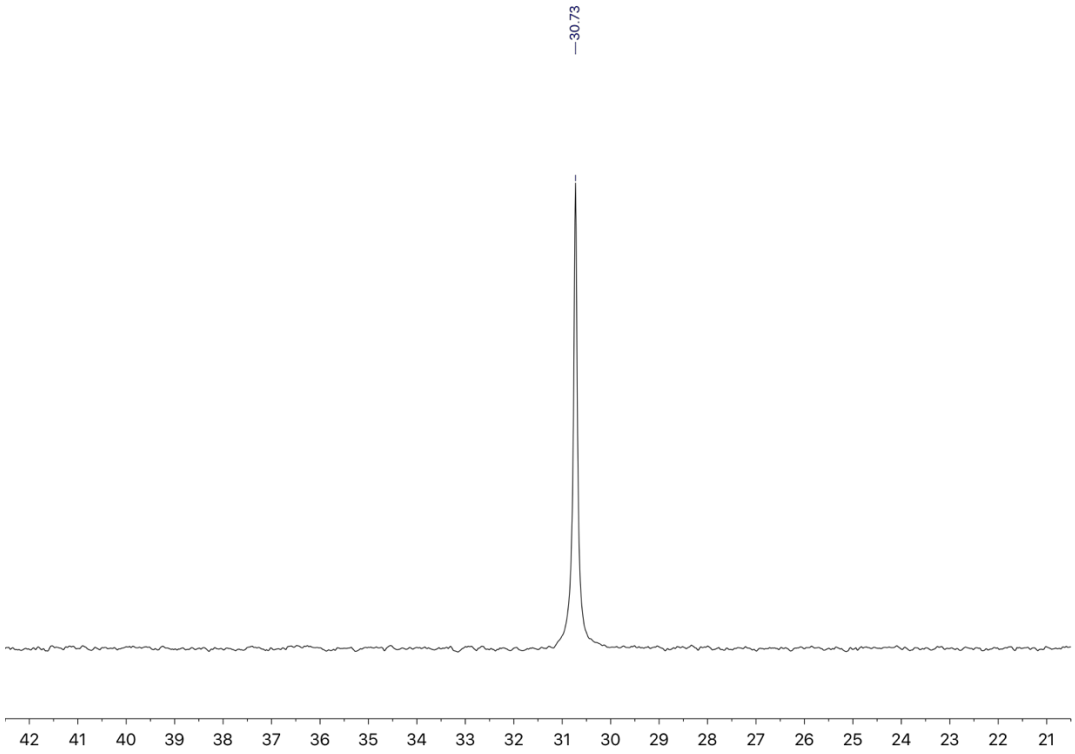

Figure S14. $^{31}P\{^{1}H\}$ NMR of **8** in C_6D_6.

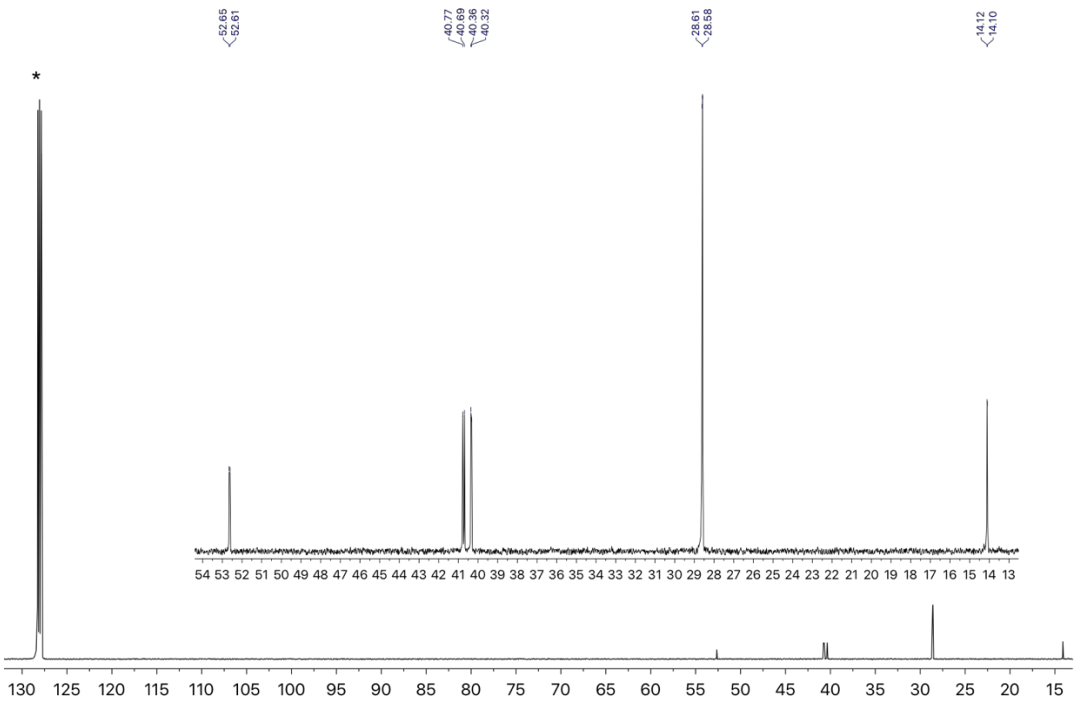

Figure S15. $^{13}C\{^{1}H\}$ NMR of **8** in C_6D_6. Peak of C_6D_5H is noted as *.

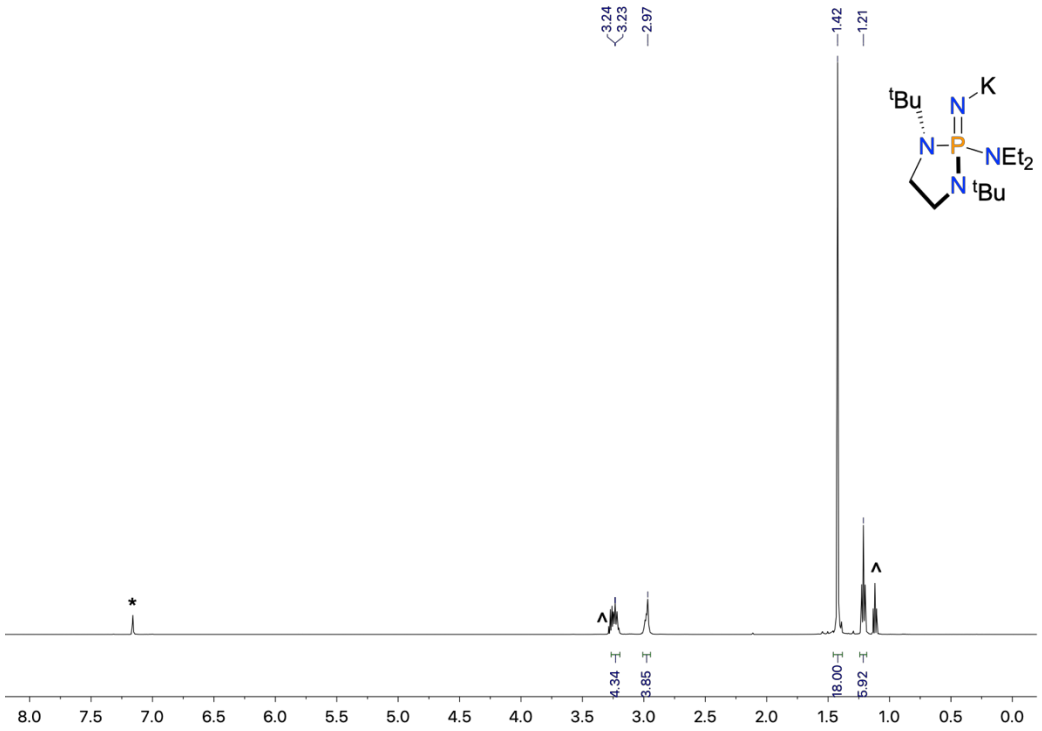

Figure S16. ^{1}H NMR of **2** in C_6D_6. Peak of C_6D_5H is noted as *. Residual diethyl ether is denoted as ^.

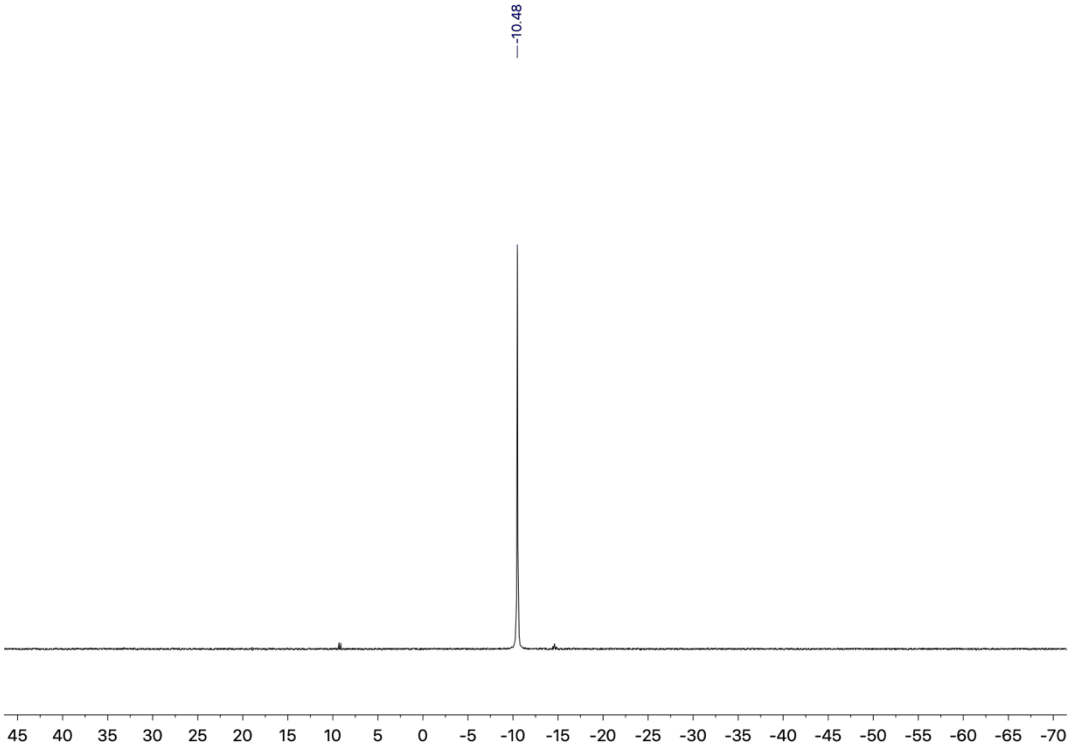

Figure S17. $^{31}P\{^{1}H\}$ NMR of **2** in C_6D_6.

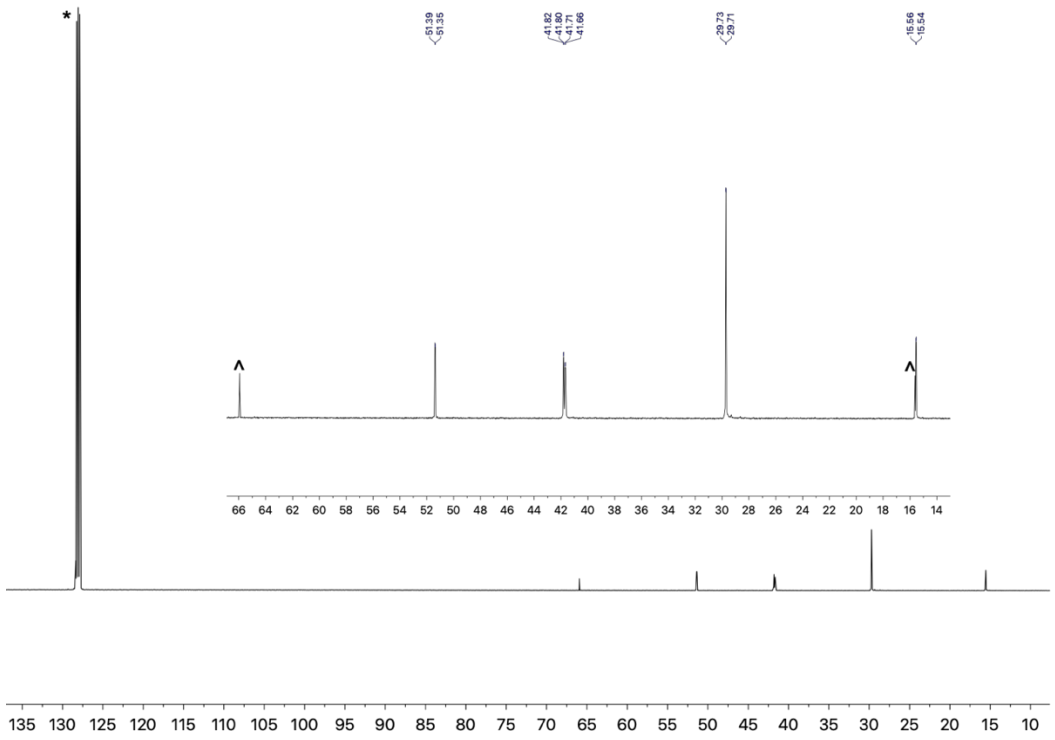

Figure S18. $^{13}C\{^{1}H\}$ NMR of **2** in C_6D_6. Peak of C_6D_5H is noted as *. Residual diethyl ether is denoted as ^.

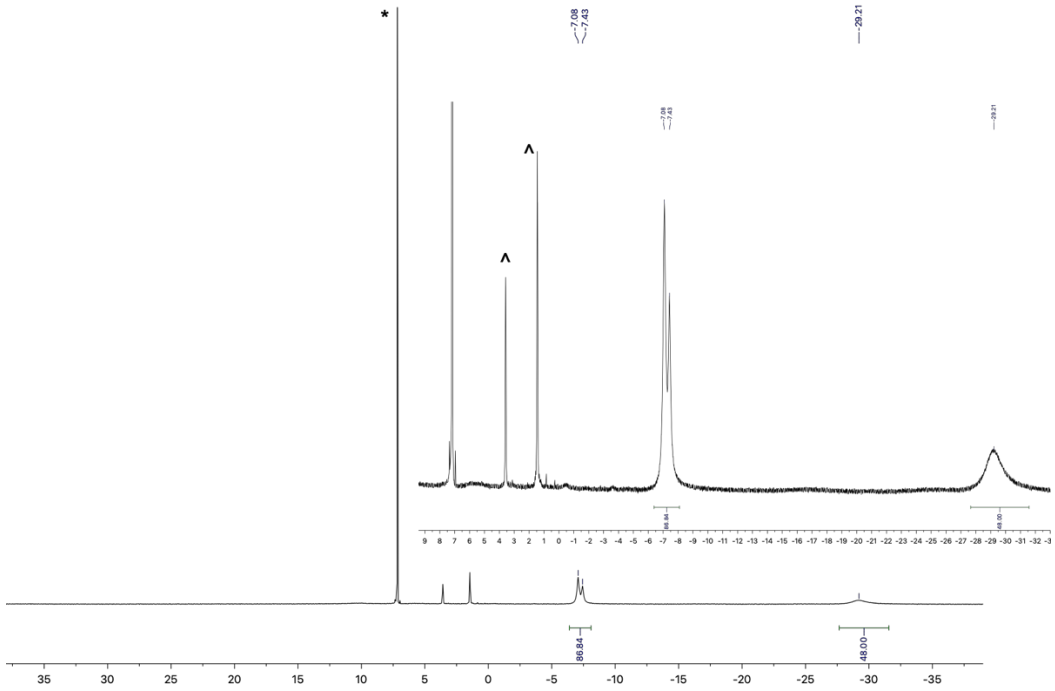

Figure S19. ^{1}H NMR of **1** in C_6D_6. Peak of C_6D_5H is noted as *. Residual THF is denoted as ^.

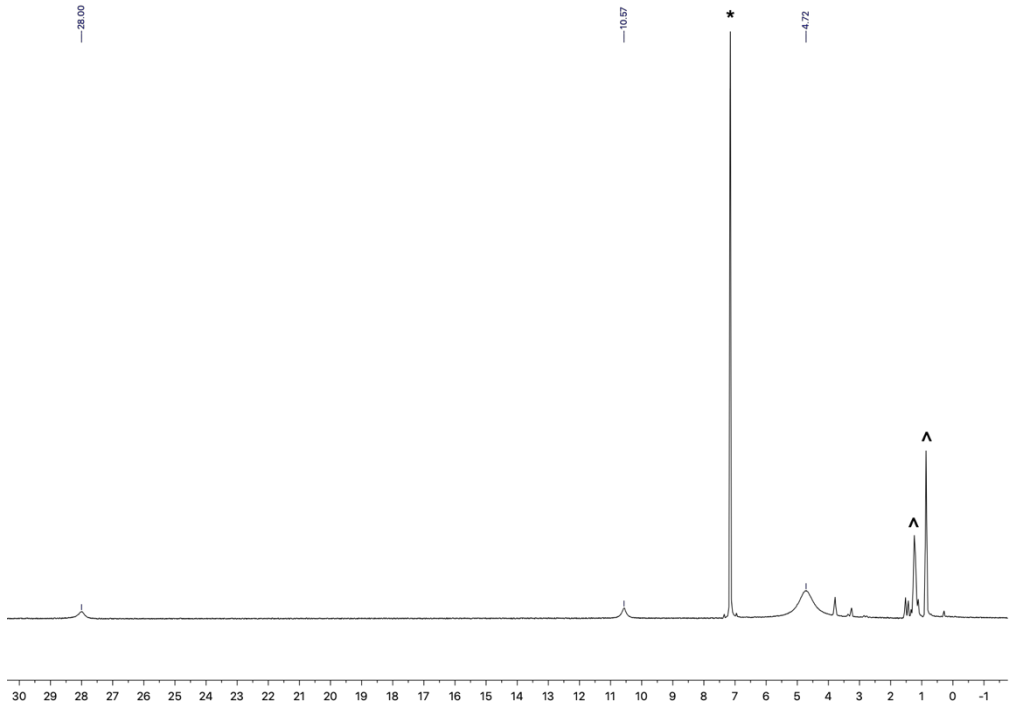

Figure S20. ^{1}H NMR of **3** in C_6D_6. Peak of C_6D_5H is noted as *. Residual *n*-pentane is denoted as ^.

Crystallographic Information

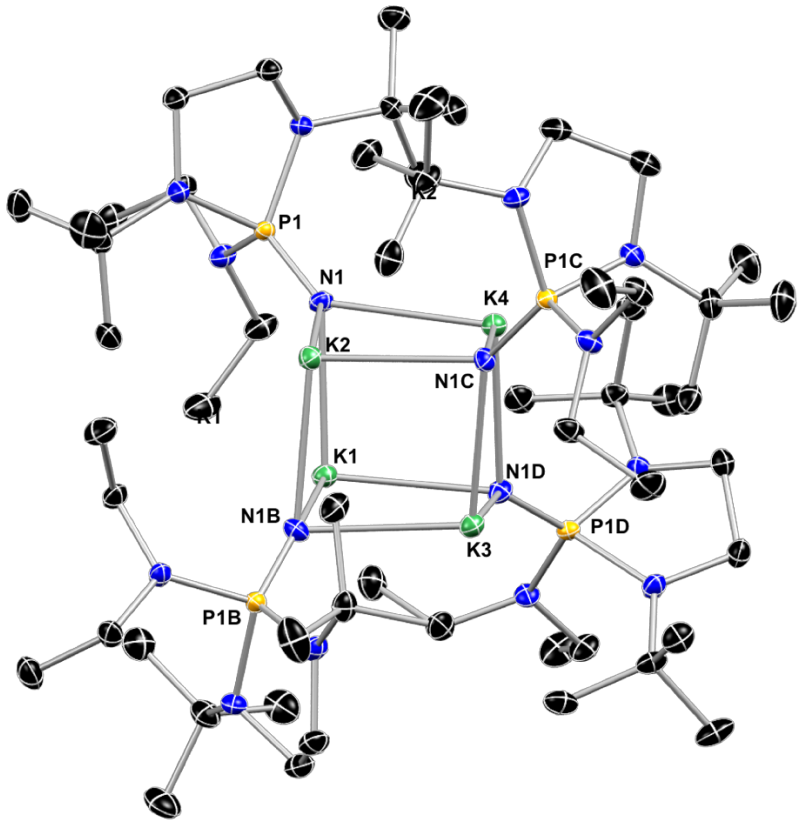

Figure S21. Molecular structure of **2** at with thermal ellipsoids shown at 50% probability. H atoms and co-crystallized diethyl ether molecule are omitted for clarity.

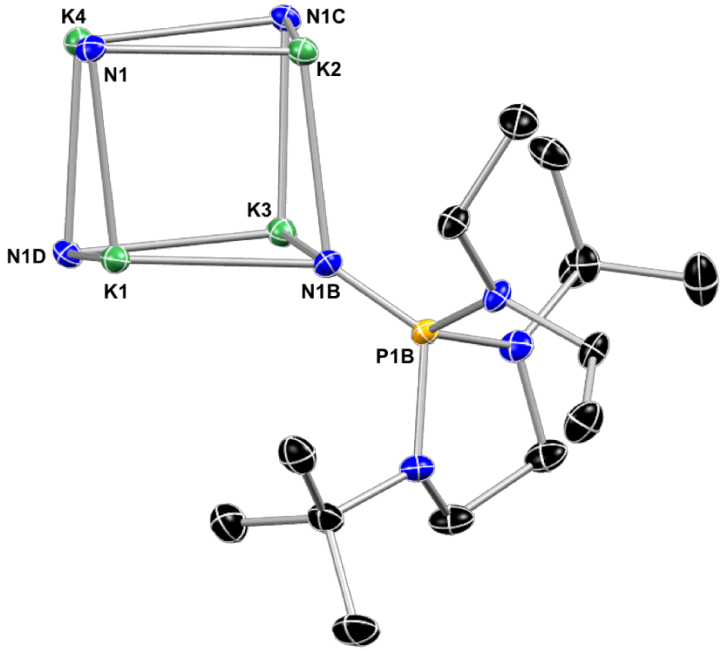

Figure S22. Molecular structure of **2** at with thermal ellipsoids shown at 50% probability. H atoms, co-crystallized diethyl ether molecule, and all but one ligand arm are omitted for clarity.

Table S1. Comparison of crystallographic metrics for **2** and $[PN(pip)_3]K$.

Metric Average	**$[PN(pip)_3]K$**	**2**
N_{imide}-P (Å)	1.519(4)	1.522(1)
P-N_{amido} (Å)	1.707(4)	1.703(1)
P-$N_{diamido}$ (Å)	-	1.722(1)
K-N_{imide} (Å)	2.728(4)	2.714(1)
N-P-N_{amido} (°)	116.8(2)	113.76(5)
N-P-$N_{diamido}$ (°)	-	121.00(4)

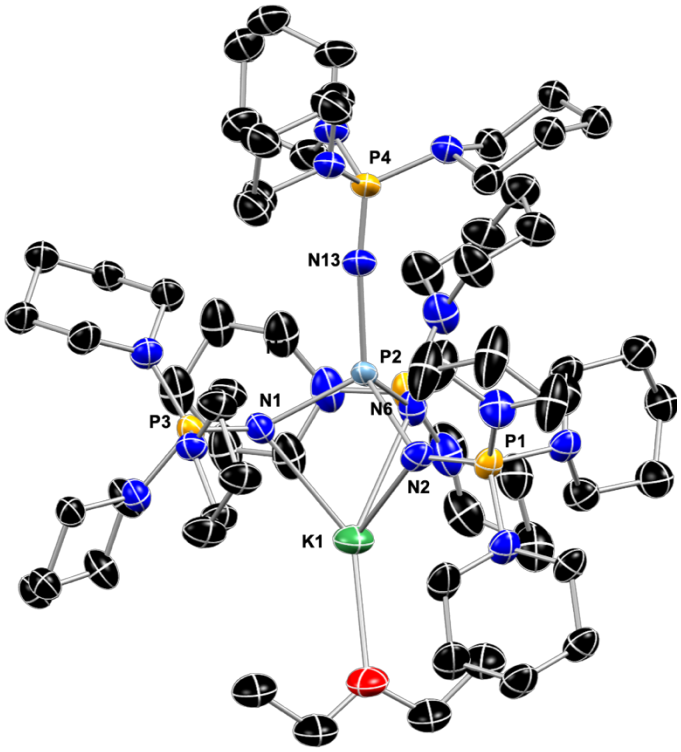

Figure S23. Molecular structure of **1** with thermal ellipsoids shown at 50% probability. H atoms are omitted for clarity.

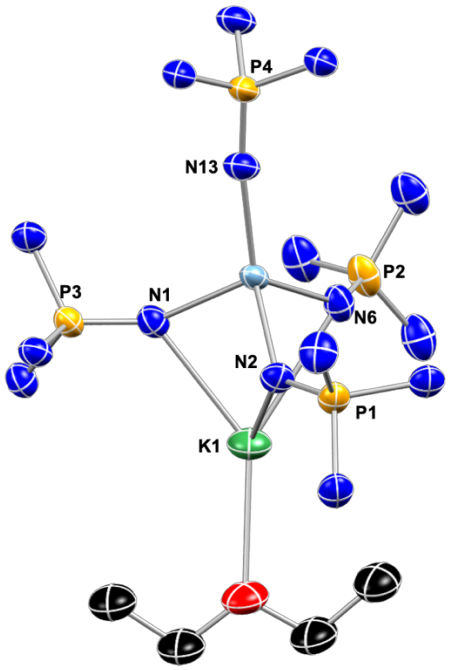

Figure S24. Molecular structure of **1** with thermal ellipsoids shown at 50% probability. H atoms and carbon atoms of the ligand are omitted for clarity.

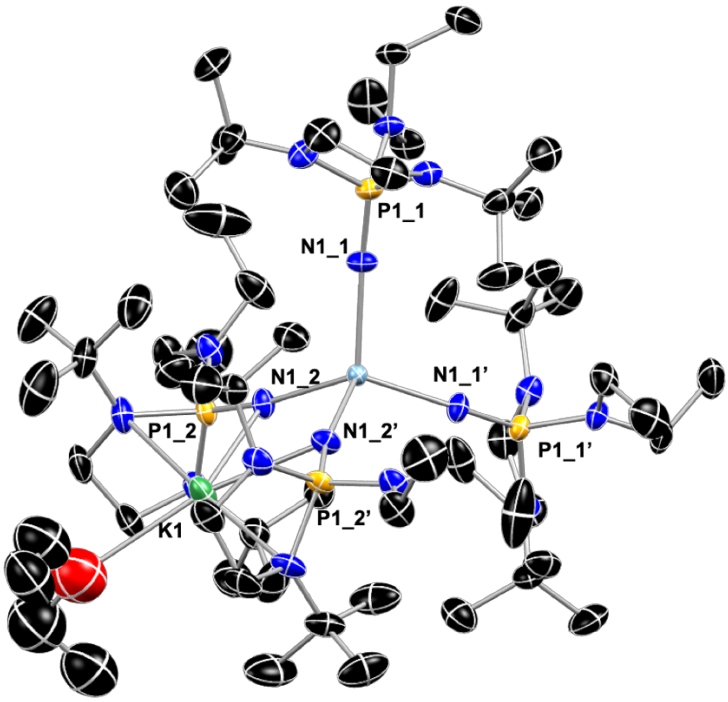

Figure S25. Molecular structure of **3** with thermal ellipsoids shown at 50% probability. H atoms are omitted for clarity.

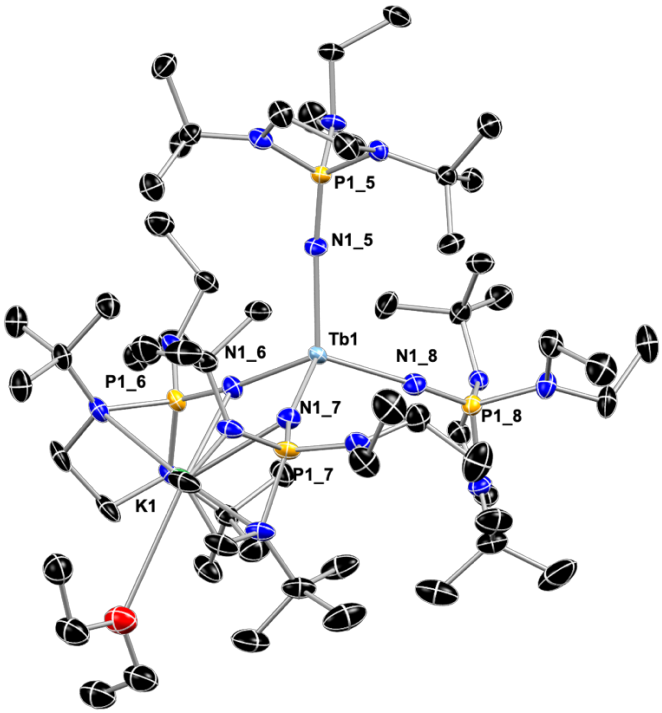

Figure S26. Molecular structure of **3-100K** with thermal ellipsoids shown at 50% probability. H atoms and one interstitial diethyl ether molecule as are omitted for clarity.

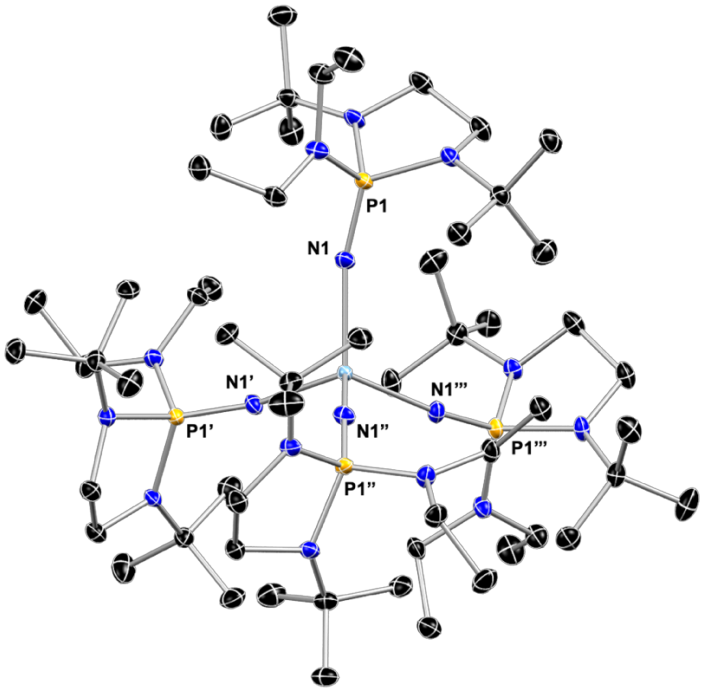

Figure S27. Molecular structure of **4** with thermal ellipsoids shown at 50% probability. H atoms are omitted for clarity.

Table S2. Crystallographic Data

	2	**1**	**3**	**3-100K**	**4**
Empirical Formula	$C_{116}H_{266}K_8N_{32}OP_8$	$C_{65}H_{129}KN_{15}OP_4Tb$	$C_{60}H_{138}KN_{16}OP_4Tb$	$C_{64}H_{148}N_{16}O_2P_4Tb$	$C_{66}H_{152}N_{16}P_4Tb$
Formula Weight	2686.15	1458.72	1421.76	1495.88	1452.83
Temperature (K)	100(2)	100(2)	180(2)	100(2)	107(2)
Crystal System	monoclinic	monoclinic	monoclinic	monoclinic	tetragonal
Space Group	$P2_1/c$	Cc	$C2/c$	$P2_1/n$	I-4
a/Å	22.6075(3)	24.279(5)	22.4833(11)	22.587(3)	13.2756(8)
b/Å	14.13495(15)	14.385(3)	15.9381(8)	15.454(2)	13.2756(8)
c/Å	24.5014(3)	23.002(5)	25.5112(16)	25.702(4)	21.077(3)
α/°	90	90	90	90	90
β/°	105.3668(12)	108.768(7)	114.512(2)	114.727(5)	90
γ/°	90	90	90	90	90
Volume/Å^3	7549.65(16)	7606(3)	8317.8(8)	3714.6(7)	3714.6(7)
Z	2	4	4	4	2
Z'	0.5	1	0.5	1	0.25
ρ(g/cm^3)	1.182	1.276	1.135	1.219	1.299
μ(mm^{-1})	0.367	1.118	1.020	1.045	1.088
F(000)	2932	3104	3048	3216	1570
Crystal Size/mm^3	0.47 x 0.43 x 0.33	0.47 x 0.39 x 0.20	0.41 x 0.33 x 0.32	0.38 x 0.37 x 0.28	0.29 x 0.18 x 0.13
Radiation	MoKα (λ=0.71073)	MoKα (λ=0.71073)	MoKα (λ=0.71073)	MoKα (λ=0.71073)	MoKα (λ=0.71073)
2θ range for data collection(°)	1.868 to 36.318	2.285 to 31.640	2.702 to 36.334	2.72 to 30.595	2.906 to 35.502
Index Ranges	*-36 ≤ h ≤ 37, -23 ≤ k ≤23, -40 ≤ l ≤ 40	*-35 ≤ h ≤ 24, -21 ≤ k ≤ 21, -33 ≤ l ≤ 33	*-34 ≤ h ≤ 37, -26 ≤ k ≤26, -40 ≤ l ≤ 42	*-32 ≤ h ≤ 32, -22 ≤ k ≤21, -36 ≤ l ≤ 36	*-21 ≤ h ≤ 20, -21 ≤ k ≤16, -33 ≤ l ≤ 34
Reflections Collected	207068	96071	79238	24862	27869
Independent Reflections	36590 [R_{int}=0.0812, R_{sigma}=0.0508]	20674 [R_{int}=0.0905, R_{sigma}=0.093]	20139 [R_{int}=0.0572, R_{sigma}=0.0449]	24826 [R_{int} = 0.0539, R_{sigma} =0.0406]	8221 [R_{int} = 0.0682, R_{sigma} =0.0713]
Data/Restraints/Parameters	207068/417/797	96071/607/788	79238/370/410	24826/152/855	27869/34/208
Goodness-of-Fit on F^2	1.048	1.017	1.042	1.219	1.052
Final R Indexes [I>=2σ (I)]	R_1 = 0.0362, wR_2= 0.721	R_1 = 0.0576, wR_2 = 0.1112	R_1=0.0.0392, wR_2=0.0996	R_1=00846, wR_2=0.1845	R_1=0.0327, wR_2=0.0863
Final R Indexes [all data]	R_1=0.0550, wR_2=0.0392	R_1 = 0.0977, wR_2 = 0.1303	R_1=0.0381, wR_2=0.0889	R_1 = 0.1015, wR_2= 0.1944	R_1 = 0.0375, wR_2= 0.0730
Largest Diff. Peak/Hole/ (e Å^3)	0.699/-0.599	1.054/-1.571	1.260/-1.283	4.30/-3.65	0.954/-0.784
Flack Parameter	-	0.018(11)	-	-	-
Completeness to 2θ	99.8	99.0	99.8	99.1	99.7

Table S3: Bond Lengths in Å for **2**.

Atom	Atom	Length/Å
C1	C2	1.5093(13)
C1	N2	1.4615(12)
C2	N3	1.4512(12)
C3	C4	1.5365(14)
C3	C5	1.5379(15)
C3	C6	1.5282(14)
C3	N2	1.4728(12)
C5	K4	3.4170(11)
C7	C8	1.5308(15)
C7	C9	1.5322(14)
C7	C10	1.5245(15)
C7	N3	1.4709(12)
C11	C12	1.5236(14)
C11	N4	1.4625(11)
C13	C14	1.5264(16)
C13	N4	1.4598(12)
C13	K1	3.4987(10)
C14	K1	3.3593(12)
N1	P1	1.5224(7)
N1	K1	2.7168(8)
N1	K2	2.7308(8)
N1	K4	2.7263(8)
N2	P1	1.7355(8)
N3	P1	1.7056(8)
N4	P1	1.7127(8)
P1	K2	3.7988(3)
C1D	C2D	1.5143(14)
C1D	N2D	1.4498(12)
C2D	N3D	1.4597(12)
C3D	C4D	1.5365(14)
C3D	C5D	1.5389(14)
C3D	C6D	1.5314(15)
C3D	N2D	1.4686(12)
C7D	C8D	1.5315(14)
C7D	C9D	1.5379(13)
C7D	C10D	1.5301(14)
C7D	N3D	1.4798(12)
C11D	C12D	1.5224(14)
C11D	N4D	1.4584(11)
C13D	C14D	1.5278(14)
C13D	N4D	1.4536(12)
C14D	K1	3.4174(11)
N1D	P1D	1.5221(7)
N1D	K1	2.7112(8)
N1D	K3	2.7299(8)
N1D	K4	2.7100(8)
N2D	P1D	1.7132(8)
N3D	P1D	1.7177(8)
N4D	P1D	1.7001(8)
P1D	K3	3.8658(3)
P1D	K4	3.8110(3)
C1C	C2C	1.5102(15)
C1C	N2C	1.4546(12)
C2C	N3C	1.4583(12)
C3C	C4C	1.5340(15)
C3C	C5C	1.5368(15)
C3C	C6C	1.5311(15)
C3C	N2C	1.4805(12)
C5C	K2	3.4106(12)
C6C	K2	3.5283(11)
C7C	C8C	1.5325(15)
C7C	C9C	1.5377(14)
C7C	C10C	1.5316(15)
C7C	N3C	1.4833(12)
C11C	C12C	1.5223(15)
C11C	N4C	1.4566(12)
C13C	C14C	1.5222(15)
C13C	N4C	1.4519(12)
N1C	P1C	1.5223(8)
N1C	K2	2.7313(7)
N1C	K3	2.7056(8)
N1C	K4	2.6826(8)
N2C	P1C	1.7244(8)
N3C	P1C	1.7319(8)
N3C	K4	3.4258(8)
N4C	P1C	1.7009(8)
P1C	K4	3.4789(3)
C1B	C2B	1.5101(16)
C1B	N2B	1.4562(13)
C2B	N3B	1.4596(12)
C3B	C4B	1.5362(14)
C3B	C5B	1.5336(13)
C3B	C6B	1.5304(14)
C3B	N2B	1.4778(13)
C7B	C8B	1.5322(15)
C7B	C9B	1.5334(15)
C7B	C10B	1.5295(15)
C7B	N3B	1.4812(13)
C11B	C12B	1.5206(14)
C11B	N4B	1.4595(11)
C13B	C14B	1.5206(14)
C13B	N4B	1.4526(11)
N1B	P1B	1.5234(8)
N1B	K1	2.7009(8)
N1B	K2	2.7126(8)
N1B	K3	2.7096(8)
N2B	P1B	1.7151(8)
N3B	P1B	1.7344(8)
N4B	P1B	1.6969(8)
P1B	K3	3.6065(3)
C1S	C2S	1.519(2)
C1S	O1S	1.352(2)
C3S	C4S	1.516(2)
C3S	O1S	1.443(2)

Table S4: Bond Angles in ° for **2**.

Atom	Atom	Atom	Angle/°
N2	C1	C2	104.02(7)
N3	C2	C1	104.96(7)
C4	C3	C5	109.41(9)
C6	C3	C4	107.58(9)
C6	C3	C5	110.04(8)
N2	C3	C4	108.89(8)
N2	C3	C5	111.03(8)
N2	C3	C6	109.82(8)
C3	C5	K4	104.69(6)
C8	C7	C9	108.75(9)
C10	C7	C8	108.80(9)
C10	C7	C9	107.95(9)
N3	C7	C8	109.35(9)
N3	C7	C9	110.60(8)
N3	C7	C10	111.34(8)
N4	C11	C12	114.47(8)
C14	C13	K1	72.08(6)
N4	C13	C14	113.57(9)
N4	C13	K1	103.90(5)
C13	C14	K1	82.30(6)
P1	N1	K1	131.40(4)
P1	N1	K2	124.05(4)
P1	N1	K4	135.82(4)
K1	N1	K2	81.08(2)
K1	N1	K4	82.81(2)
K4	N1	K2	82.41(2)
C1	N2	C3	115.96(7)
C1	N2	P1	109.54(6)
C3	N2	P1	121.44(6)
C2	N3	C7	117.39(7)
C2	N3	P1	114.18(6)
C7	N3	P1	127.46(7)
C11	N4	P1	119.46(6)
C13	N4	C11	115.06(7)
C13	N4	P1	119.11(6)
N1	P1	N2	122.78(4)
N1	P1	N3	120.11(4)
N1	P1	N4	113.65(4)
N1	P1	K2	36.55(3)
N2	P1	K2	122.66(3)
N3	P1	N2	90.17(4)
N3	P1	N4	104.16(4)
N3	P1	K2	84.02(3)
N4	P1	N2	102.05(4)
N4	P1	K2	134.72(3)
N2D	C1D	C2D	105.41(7)
N3D	C2D	C1D	104.85(8)
C4D	C3D	C5D	108.60(8)
C6D	C3D	C4D	107.61(9)
C6D	C3D	C5D	109.50(8)
N2D	C3D	C4D	110.22(8)
N2D	C3D	C5D	109.97(8)
N2D	C3D	C6D	110.89(8)
C8D	C7D	C9D	109.04(8)
C10D	C7D	C8D	108.27(8)
C10D	C7D	C9D	107.79(9)
N3D	C7D	C8D	111.75(8)
N3D	C7D	C9D	108.48(8)
N3D	C7D	C10D	111.41(7)
N4D	C11D	C12D	113.79(8)
N4D	C13D	C14D	114.66(8)
C13D	C14D	K1	82.09(5)
P1D	N1D	K1	136.53(4)
P1D	N1D	K3	128.51(4)
P1D	N1D	K4	126.12(4)
K1	N1D	K3	81.78(2)
K4	N1D	K1	83.22(2)
K4	N1D	K3	81.99(2)
C1D	N2D	C3D	117.57(7)
C1D	N2D	P1D	114.62(6)
C3D	N2D	P1D	127.81(6)
C2D	N3D	C7D	116.34(7)
C2D	N3D	P1D	109.73(6)
C7D	N3D	P1D	126.01(6)
C11D	N4D	P1D	120.32(6)
C13D	N4D	C11D	115.50(8)
C13D	N4D	P1D	119.25(6)
N1D	P1D	N2D	119.82(4)
N1D	P1D	N3D	123.66(4)
N1D	P1D	N4D	113.73(4)
N1D	P1D	K3	33.54(3)
N1D	P1D	K4	35.06(3)
N2D	P1D	N3D	90.01(4)
N2D	P1D	K3	87.13(3)
N2D	P1D	K4	117.79(3)
N3D	P1D	K3	137.49(3)
N3D	P1D	K4	89.61(3)
N4D	P1D	N2D	105.60(4)
N4D	P1D	N3D	99.99(4)
N4D	P1D	K3	121.60(3)
N4D	P1D	K4	135.55(3)
K4	P1D	K3	55.396(5)
N2C	C1C	C2C	105.32(8)
N3C	C2C	C1C	104.92(8)
C4C	C3C	C5C	108.91(9)
C6C	C3C	C4C	107.75(9)
C6C	C3C	C5C	109.62(9)
N2C	C3C	C4C	108.71(9)
N2C	C3C	C5C	111.34(8)
N2C	C3C	C6C	110.42(8)
C3C	C5C	K2	99.08(6)
C3C	C6C	K2	94.54(6)
C8C	C7C	C9C	108.52(9)
C10C	C7C	C8C	108.00(9)
C10C	C7C	C9C	108.11(9)
N3C	C7C	C8C	108.80(9)
N3C	C7C	C9C	112.48(8)
N3C	C7C	C10C	110.81(8)
N4C	C11C	C12C	114.78(8)
N4C	C13C	C14C	114.07(8)
P1C	N1C	K2	133.98(4)
P1C	N1C	K3	141.14(4)
P1C	N1C	K4	108.48(4)
K3	N1C	K2	83.21(2)
K4	N1C	K2	83.21(2)
K4	N1C	K3	82.95(2)
C1C	N2C	C3C	115.40(8)

Atom	Atom	Atom	Angle/°
C1C	N2C	P1C	111.32(6)
C3C	N2C	P1C	121.62(6)
C2C	N3C	C7C	115.86(8)
C2C	N3C	P1C	112.34(6)
C2C	N3C	K4	121.88(6)
C7C	N3C	P1C	124.88(6)
C7C	N3C	K4	98.13(5)
P1C	N3C	K4	77.18(3)
C11C	N4C	P1C	123.83(6)
C13C	N4C	C11C	116.14(7)
C13C	N4C	P1C	119.71(6)
N1C	P1C	N2C	122.40(4)
N1C	P1C	N3C	117.73(4)
N1C	P1C	N4C	114.00(4)
N1C	P1C	K4	47.00(3)
N2C	P1C	N3C	90.98(4)
N2C	P1C	K4	110.14(3)
N3C	P1C	K4	73.78(3)
N4C	P1C	N2C	101.24(4)
N4C	P1C	N3C	107.14(4)
N4C	P1C	K4	148.61(3)
N2B	C1B	C2B	104.76(8)
N3B	C2B	C1B	104.44(8)
C5B	C3B	C4B	108.53(8)
C6B	C3B	C4B	108.75(9)
C6B	C3B	C5B	107.67(8)
N2B	C3B	C4B	111.54(8)
N2B	C3B	C5B	109.02(8)
N2B	C3B	C6B	111.23(7)
C8B	C7B	C9B	109.02(9)
C10B	C7B	C8B	109.09(9)
C10B	C7B	C9B	108.18(9)
N3B	C7B	C8B	111.51(9)
N3B	C7B	C9B	109.09(9)
N3B	C7B	C10B	109.88(8)
N4B	C11B	C12B	115.47(8)
N4B	C13B	C14B	113.96(8)
P1B	N1B	K1	143.68(4)
P1B	N1B	K2	130.36(4)
P1B	N1B	K3	113.90(4)
K1	N1B	K2	81.70(2)
K1	N1B	K3	82.35(2)
K3	N1B	K2	83.48(2)
C1B	N2B	C3B	117.18(8)
C1B	N2B	P1B	113.27(7)
C3B	N2B	P1B	127.45(6)
C2B	N3B	C7B	115.71(8)
C2B	N3B	P1B	109.67(6)
C7B	N3B	P1B	121.02(6)
C11B	N4B	P1B	122.82(6)
C13B	N4B	C11B	115.79(7)
C13B	N4B	P1B	120.33(6)
N1B	P1B	N2B	119.53(4)
N1B	P1B	N3B	121.98(4)
N1B	P1B	N4B	113.66(4)
N1B	P1B	K3	43.38(3)
N2B	P1B	N3B	90.71(4)
N2B	P1B	K3	78.33(3)
N3B	P1B	K3	113.56(3)

Atom	Atom	Atom	Angle/°
N4B	P1B	N2B	104.73(4)
N4B	P1B	N3B	102.61(4)
N4B	P1B	K3	143.72(3)
O1S	C1S	C2S	106.7(2)
O1S	C3S	C4S	108.29(19)
C1S	O1S	C3S	115.33(14)
N1	K1	C14	78.32(3)
N1D	K1	C14	126.04(3)
N1D	K1	N1	96.28(2)
N1B	K1	C14	136.13(3)
N1B	K1	N1	98.62(2)
N1B	K1	N1D	97.83(2)
N1	K2	C5C	88.91(3)
N1	K2	N1C	96.12(2)
N1C	K2	C5C	72.78(2)
N1B	K2	N1	97.99(2)
N1B	K2	C5C	167.28(3)
N1B	K2	N1C	95.76(2)
N1D	K3	K1	48.882(16)
N1C	K3	N1D	96.69(2)
N1C	K3	N1B	96.44(2)
N1C	K3	K1	94.613(17)
N1B	K3	N1D	97.17(2)
N1B	K3	K1	48.723(17)
N1	K4	C5	70.85(2)
N1D	K4	C5	150.86(3)
N1D	K4	N1	96.08(2)
N1C	K4	C5	109.50(3)
N1C	K4	N1	97.38(2)
N1C	K4	N1D	97.72(2)

Table S5: Bond Lengths in Å for **1.**

Atom	Atom	Length/Å
Tb1	K1	3.2285(18)
Tb1	N6	2.235(8)
Tb1	N2	2.239(6)
Tb1	N1	2.241(6)
Tb1	N12	2.200(7)
K1	O1	2.771(7)
K1	N6	3.015(7)
K1	N2	2.780(7)
K1	N1	2.797(8)
P3	N9	1.677(7)
P3	N10	1.697(6)
P3	N1	1.534(8)
P3	N11	1.698(7)
P1	N3	1.701(8)
P1	N4	1.689(8)
P1	N2	1.532(7)
P1	N5	1.693(7)
P4	N13	1.667(9)
P4	N14	1.683(7)
P4	N15	1.703(7)
P4	N12	1.523(7)
P2	N6	1.516(7)
P2	N7	1.680(10)
P2	N8	1.705(8)
P2	C30	1.686(9)
O1	C1	1.444(14)
O1	C3	1.417(15)
N13	C51	1.480(12)
N13	C55	1.476(11)
N3	C5	1.483(10)
N3	C9	1.460(12)
N14	C56	1.434(12)
N14	C60	1.459(10)
N7	C20	1.444(13)
N7	C24	1.486(12)
N9	C36	1.438(14)
N9	C40	1.462(10)
N10	C41	1.459(11)
N10	C45	1.456(10)
N4	C10	1.456(12)
N4	C14	1.467(14)
N15	C61	1.481(10)
N15	C65	1.455(12)
C39	C38	1.520(13)
C39	C40	1.513(11)
N8	C25	1.485(15)
N8	C29	1.454(12)
N11	C46	1.462(10)
N11	C50	1.484(10)
N5	C15	1.459(10)
N5	C19	1.473(12)
C34	C33	1.517(12)
C34	C35	1.469(13)
C15	C16	1.523(11)
C19	C18	1.502(13)
C49	C50	1.508(12)
C49	C48	1.522(12)
C42	C43	1.513(12)
C42	C41	1.499(11)
C46	C47	1.509(12)
C64	C65	1.532(11)
C64	C63	1.506(11)
C43	C44	1.512(13)
C7	C8	1.534(13)
C7	C6	1.528(16)
C61	C62	1.501(11)
C38	C37	1.521(11)
C36	C37	1.533(13)
C31	C30	1.473(11)
C31	C32	1.468(14)
C33	C32	1.474(13)
C56	C57	1.475(14)
C45	C44	1.497(12)
C8	C9	1.513(14)
C60	C59	1.493(14)
C27	C26	1.514(14)
C27	C28	1.526(17)
C47	C48	1.506(12)
C6	C5	1.513(14)
C10	C11	1.459(15)
C25	C26	1.518(12)
C30	C35	1.503(13)
C16	C17	1.524(14)
C20	C21	1.528(15)
C51	C52	1.492(15)
C55	C54	1.524(14)
C59	C58	1.484(15)
C54	C53	1.532(15)
C28	C29	1.525(12)
C14	C13	1.407(17)
C57	C58	1.500(13)
C53	C52	1.529(14)
C13	C12	1.516(14)
C1	C2	1.468(18)
C11	C12	1.513(18)
C4	C3	1.496(16)
C23	C24	1.440(16)
C23	C22	1.502(17)
C63	C62	1.513(13)
C18	C17	1.516(13)
C21	C22	1.564(15)

Table S6: Bond Angles in ° **1.**

Atom	Atom	Atom	Angle/°
N6	Tb1	K1	64.01(17)
N6	Tb1	N2	95.8(3)
N6	Tb1	N1	98.5(3)
N2	Tb1	K1	57.78(17)
N2	Tb1	N1	97.1(2)
N1	Tb1	K1	58.21(19)
N12	Tb1	K1	172.1(2)
N12	Tb1	N6	123.3(3)
N12	Tb1	N2	121.2(2)
N12	Tb1	N1	115.5(3)

Atom	Atom	Atom	Angle/°
O1	K1	N6	149.2(2)
O1	K1	N2	111.38(19)
O1	K1	N1	139.5(2)
N2	K1	N6	69.76(18)
N2	K1	N1	74.0(2)
N1	K1	N6	71.2(2)
N9	P3	N10	108.5(4)
N9	P3	N11	100.8(4)
N10	P3	N11	99.7(3)
N1	P3	N9	113.8(4)
N1	P3	N10	112.5(4)
N1	P3	N11	120.0(3)
N4	P1	N3	100.7(4)
N4	P1	N5	108.1(4)
N2	P1	N3	121.1(3)
N2	P1	N4	113.0(4)
N2	P1	N5	112.1(3)
N5	P1	N3	100.4(4)
N13	P4	N14	107.3(4)
N13	P4	N15	98.9(4)
N14	P4	N15	101.6(3)
N12	P4	N13	114.4(4)
N12	P4	N14	113.0(4)
N12	P4	N15	119.8(4)
N6	P2	N7	112.6(4)
N6	P2	N8	120.6(4)
N6	P2	C30	113.4(4)
N7	P2	N8	99.2(4)
N7	P2	C30	108.1(5)
C30	P2	N8	101.3(4)
C1	O1	K1	128.6(7)
C3	O1	K1	116.4(6)
C3	O1	C1	113.9(8)
C51	N13	P4	117.9(6)
C55	N13	P4	125.5(6)
C55	N13	C51	109.9(8)
C5	N3	P1	111.5(6)
C9	N3	P1	115.2(6)
C9	N3	C5	109.3(7)
C56	N14	P4	122.5(6)
C56	N14	C60	112.6(7)
C60	N14	P4	123.6(6)
Tb1	N6	K1	74.23(19)
P2	N6	Tb1	140.2(4)
P2	N6	K1	122.7(3)
C20	N7	P2	114.4(6)
C20	N7	C24	110.2(9)
C24	N7	P2	119.3(7)
C36	N9	P3	125.6(5)
C36	N9	C40	112.4(7)
C40	N9	P3	122.0(7)
C41	N10	P3	122.1(6)
C45	N10	P3	114.1(5)
C45	N10	C41	111.0(6)
C10	N4	P1	126.1(7)
C10	N4	C14	112.7(8)
C14	N4	P1	120.9(6)
C61	N15	P4	115.4(5)
C65	N15	P4	114.8(5)

Atom	Atom	Atom	Angle/°
C65	N15	C61	110.2(7)
Tb1	N2	K1	79.27(18)
P1	N2	Tb1	135.2(4)
P1	N2	K1	130.7(4)
C40	C39	C38	110.9(7)
Tb1	N1	K1	78.9(2)
P3	N1	Tb1	135.8(4)
P3	N1	K1	128.0(3)
C25	N8	P2	111.7(6)
C29	N8	P2	115.9(6)
C29	N8	C25	109.2(8)
P4	N12	Tb1	172.5(5)
C46	N11	P3	114.2(5)
C46	N11	C50	109.6(6)
C50	N11	P3	114.4(6)
C15	N5	P1	121.1(5)
C15	N5	C19	110.8(6)
C19	N5	P1	114.3(6)
C35	C34	C33	113.4(8)
N5	C15	C16	111.0(7)
N5	C19	C18	111.8(9)
C50	C49	C48	111.7(8)
C41	C42	C43	111.8(7)
N11	C46	C47	111.5(7)
C63	C64	C65	110.6(7)
C44	C43	C42	110.3(7)
C6	C7	C8	108.2(9)
N15	C61	C62	110.4(6)
C39	C38	C37	109.4(7)
N9	C36	C37	112.0(9)
N10	C41	C42	110.7(8)
C32	C31	C30	112.7(8)
C38	C37	C36	110.7(7)
C32	C33	C34	112.4(7)
N14	C56	C57	113.7(10)
N10	C45	C44	111.8(7)
C9	C8	C7	112.5(9)
N14	C60	C59	111.5(8)
C26	C27	C28	110.1(9)
C48	C47	C46	112.5(9)
C5	C6	C7	111.2(8)
N4	C10	C11	111.0(10)
N8	C25	C26	110.3(9)
C31	C30	P2	125.3(7)
C31	C30	C35	110.9(8)
C35	C30	P2	120.7(6)
C31	C32	C33	113.1(9)
C15	C16	C17	110.3(8)
N3	C5	C6	111.3(8)
N7	C20	C21	110.5(8)
N13	C51	C52	111.2(8)
C27	C26	C25	110.9(9)
N13	C55	C54	110.3(7)
C58	C59	C60	112.3(10)
C55	C54	C53	111.5(9)
C29	C28	C27	110.2(9)
C13	C14	N4	113.4(10)
N9	C40	C39	110.8(7)
C56	C57	C58	110.8(8)

Atom	Atom	Atom	Angle/°
C52	C53	C54	107.7(10)
C14	C13	C12	111.1(12)
O1	C1	C2	109.6(9)
C34	C35	C30	110.5(9)
C10	C11	C12	110.6(10)
C45	C44	C43	111.5(9)
C3	C4	K1	86.8(7)
N3	C9	C8	110.4(8)
C51	C52	C53	112.3(8)
C24	C23	C22	114.1(9)
N8	C29	C28	110.2(8)
C23	C24	N7	109.1(9)
N11	C50	C49	109.4(8)
N15	C65	C64	109.8(7)
C64	C63	C62	110.7(7)
C19	C18	C17	109.9(8)
C20	C21	C22	108.5(9)
C59	C58	C57	111.5(8)
C47	C48	C49	108.2(7)
C61	C62	C63	111.3(7)
C11	C12	C13	111.2(10)
C23	C22	C21	108.9(11)
C18	C17	C16	108.8(7)
O1	C3	C4	110.0(9)

Atom	Atom	Length/Å
P1_2	N3_2	1.7034(12)
P1_2	N4_2	1.6771(12)
N2_2	C1_2	1.4498(18)
N2_2	C7_2	1.4814(19)
N3_2	C2_2	1.4495(18)
N3_2	C3_2	1.4815(19)
N4_2	C12_2	1.4601(17)
N4_2	C13_2	1.4569(18)
C1_2	C2_2	1.507(2)
C3_2	C4_2	1.536(2)
C3_2	C5_2	1.533(2)
C3_2	C6_2	1.524(2)
C7_2	C8_2	1.553(2)
C7_2	C9_2	1.524(2)
C7_2	C10_2	1.517(2)
C11_2	C12_2	1.509(2)
C13_2	C14_2	1.523(3)
O1_3	C1_3	1.430(3)
O1_3	C3_3	1.399(9)
C1_3	C2_3	1.483(5)
C3_3	C4_3	1.496(5)

[1]1-x,+y,3/2-

Table S7: Bond Lengths in Å for **3.**

Atom	Atom	Length/Å
Tb1	K1	3.7858(5)
Tb1	N1_1	2.2307(11)
Tb1	N1_1[1]	2.2307(11)
Tb1	N1_2	2.2637(11)
Tb1	N1_2[1]	2.2637(10)
K1	N1_2[1]	2.8057(14)
K1	N1_2	2.8058(14)
K1	N2_2[1]	3.1793(15)
K1	O1_3	2.939(5)
P1_1	N1_1	1.5283(11)
P1_1	N2_1	1.7165(12)
P1_1	N3_1	1.6955(12)
P1_1	N4_1	1.6826(11)
N2_1	C1_1	1.4537(18)
N2_1	C7_1	1.4817(18)
N3_1	C2_1	1.4463(18)
N3_1	C3_1	1.4718(19)
N4_1	C12_1	1.4568(17)
N4_1	C13_1	1.4519(17)
C1_1	C2_1	1.508(2)
C3_1	C4_1	1.536(2)
C3_1	C5_1	1.535(2)
C3_1	C6_1	1.522(2)
C7_1	C8_1	1.546(2)
C7_1	C9_1	1.527(2)
C7_1	C10_1	1.515(2)
C11_1	C12_1	1.510(2)
C13_1	C14_1	1.523(2)
P1_2	N1_2	1.5318(11)
P1_2	N2_2	1.7173(12)

Table S8: Bond Angles in ° for **3.**

Atom	Atom	Atom	Angle/°
N1_1[1]	Tb1	K1	125.39(3)
N1_1	Tb1	K1	125.39(3)
N1_1	Tb1	N1_1[1]	109.22(7)
N1_1	Tb1	N1_2	113.17(5)
N1_1[1]	Tb1	N1_2	112.91(5)
N1_1[1]	Tb1	N1_2[1]	113.18(5)
N1_1	Tb1	N1_2[1]	112.91(5)
N1_2	Tb1	K1	47.48(3)
N1_2[1]	Tb1	K1	47.48(3)
N1_2[1]	Tb1	N1_2	94.96(7)
N1_2[1]	K1	N1_2	72.97(4)
N1_2[1]	K1	N2_2[1]	54.41(3)
N1_2	K1	N2_2[1]	123.01(4)
N1_2	K1	O1_3	144.2(2)
N1_2[1]	K1	O1_3	142.3(2)
O1_3	K1	N2_2[1]	91.8(2)
N1_1	P1_1	N2_1	120.75(7)
N1_1	P1_1	N3_1	120.52(7)
N1_1	P1_1	N4_1	113.38(7)
N3_1	P1_1	N2_1	90.74(6)
N4_1	P1_1	N2_1	103.72(6)
N4_1	P1_1	N3_1	104.27(7)
P1_1	N1_1	Tb1	168.78(9)
C1_1	N2_1	P1_1	109.65(10)
C1_1	N2_1	C7_1	117.06(12)
C7_1	N2_1	P1_1	123.22(9)
C2_1	N3_1	P1_1	114.36(11)
C2_1	N3_1	C3_1	117.61(12)
C3_1	N3_1	P1_1	127.99(10)
C12_1	N4_1	P1_1	120.77(10)
C13_1	N4_1	P1_1	122.03(10)
C13_1	N4_1	C12_1	117.06(12)
N2_1	C1_1	C2_1	105.13(13)
N3_1	C2_1	C1_1	105.86(12)
N3_1	C3_1	C4_1	109.57(15)
N3_1	C3_1	C5_1	109.08(14)
N3_1	C3_1	C6_1	110.94(13)
C5_1	C3_1	C4_1	109.51(15)
C6_1	C3_1	C4_1	108.68(16)
C6_1	C3_1	C5_1	109.03(16)
N2_1	C7_1	C8_1	110.25(15)
N2_1	C7_1	C9_1	108.70(13)
N2_1	C7_1	C10_1	110.48(12)
C9_1	C7_1	C8_1	109.65(15)
C10_1	C7_1	C8_1	108.02(15)
C10_1	C7_1	C9_1	109.73(17)
N4_1	C12_1	C11_1	115.72(15)
N4_1	C13_1	C14_1	113.49(15)
N1_2	P1_2	K1	56.65(5)
N1_2	P1_2	N2_2	115.93(7)
N1_2	P1_2	N3_2	120.88(7)
N1_2	P1_2	N4_2	113.79(7)
N2_2	P1_2	K1	69.63(5)
N3_2	P1_2	K1	92.42(5)
N3_2	P1_2	N2_2	91.45(6)
N4_2	P1_2	K1	163.94(5)
N4_2	P1_2	N2_2	108.47(7)
N4_2	P1_2	N3_2	103.62(7)
Tb1	N1_2	K1	96.04(4)
P1_2	N1_2	Tb1	167.67(8)
P1_2	N1_2	K1	96.22(6)
P1_2	N2_2	K1	79.94(5)
C1_2	N2_2	K1	110.66(12)
C1_2	N2_2	P1_2	111.73(10)
C1_2	N2_2	C7_2	116.58(12)
C7_2	N2_2	K1	104.70(9)
C7_2	N2_2	P1_2	125.28(11)
C2_2	N3_2	P1_2	113.51(11)
C2_2	N3_2	C3_2	115.70(13)
C3_2	N3_2	P1_2	123.55(10)
C12_2	N4_2	P1_2	122.67(11)
C13_2	N4_2	P1_2	122.00(11)
C13_2	N4_2	C12_2	115.34(14)
N2_2	C1_2	C2_2	105.96(13)
N3_2	C2_2	C1_2	106.16(13)
N3_2	C3_2	C4_2	108.78(14)
N3_2	C3_2	C5_2	110.17(15)
N3_2	C3_2	C6_2	110.70(13)
C5_2	C3_2	C4_2	109.58(17)
C6_2	C3_2	C4_2	108.88(15)
C6_2	C3_2	C5_2	108.71(15)
N2_2	C7_2	C8_2	108.84(16)
N2_2	C7_2	C9_2	111.35(14)
N2_2	C7_2	C10_2	111.18(13)
C9_2	C7_2	C8_2	108.63(17)
C10_2	C7_2	C8_2	106.75(17)
C10_2	C7_2	C9_2	109.95(18)
N4_2	C12_2	C11_2	115.52(16)
N4_2	C13_2	C14_2	113.72(19)
C1_3	O1_3	K1	133.1(5)
C3_3	O1_3	K1	108.3(4)
C3_3	O1_3	C1_3	114.9(6)
O1_3	C1_3	C2_3	104.1(4)
O1_3	C3_3	C4_3	122.9(11)

[1]1-x,+y,3/2-

Table S9: Bond Lengths in Å for **3-100K.**

Atom	Atom	Length/Å
Tb1	N1_5	2.239(5)
Tb1	N1_6	2.256(5)
Tb1	N1_7	2.285(5)
Tb1	N1_8	2.235(5)
K1	O1S_1	3.146(6)
K1	O1S_2	3.148(6)
K1	N1_6	2.829(5)
K1	N6_6	3.098(6)
K1	N1_7	2.749(5)
K1	N6_7	3.208(6)
O1S_1	C2S_1	1.402(6)
O1S_1	C4S_1	1.402(6)
C2S_1	C3S_1	1.505(10)
C4S_1	C5S_1	1.484(11)
O1S_2	C2S_2	1.402(6)
O1S_2	C4S_2	1.403(6)
C2S_2	C3S_2	1.504(10)
C4S_2	C5S_2	1.484(11)
O1S_3	C2S_3	1.402(6)
O1S_3	C4S_3	1.402(6)
C2S_3	C3S_3	1.504(10)
C4S_3	C5S_3	1.484(11)
O1S_4	C2S_4	1.402(6)
O1S_4	C4S_4	1.402(6)
C2S_4	C3S_4	1.504(10)
C4S_4	C5S_4	1.484(11)
P1_5	N1_5	1.530(5)
P1_5	N5_5	1.680(5)
P1_5	N6_5	1.726(5)
P1_5	N7_5	1.687(5)
N5_5	C12_5	1.460(7)
N5_5	C13_5	1.455(8)
N6_5	C1_5	1.462(8)
N6_5	C7_5	1.483(8)
N7_5	C2_5	1.454(7)
N7_5	C3_5	1.483(8)
C1_5	C2_5	1.508(9)
C3_5	C4_5	1.530(9)
C3_5	C5_5	1.538(9)
C3_5	C6_5	1.527(9)
C7_5	C8_5	1.534(9)
C7_5	C9_5	1.544(9)
C7_5	C10_5	1.535(9)
C11_5	C12_5	1.540(9)
C13_5	C14_5	1.501(9)
P1_6	N1_6	1.530(5)
P1_6	N5_6	1.687(5)
P1_6	N6_6	1.743(5)
P1_6	N7_6	1.707(5)
N5_6	C12_6	1.460(8)
N5_6	C13_6	1.469(7)
N6_6	C1_6	1.469(8)
N6_6	C7_6	1.463(8)
N7_6	C2_6	1.464(7)
N7_6	C3_6	1.466(8)
C1_6	C2_6	1.500(10)
C3_6	C4_6	1.537(8)
C3_6	C5_6	1.543(9)
C3_6	C6_6	1.537(9)
C7_6	C8_6	1.536(9)
C7_6	C9_6	1.531(9)
C7_6	C10_6	1.528(8)
C11_6	C12_6	1.523(9)
C13_6	C14_6	1.532(9)
P1_7	N1_7	1.526(5)
P1_7	N5_7	1.678(6)
P1_7	N6_7	1.738(5)
P1_7	N7_7	1.701(5)
N5_7	C12_7	1.460(8)
N5_7	C13_7	1.464(9)
N6_7	C1_7	1.458(8)
N6_7	C7_7	1.482(8)
N7_7	C2_7	1.468(8)
N7_7	C3_7	1.474(8)
C1_7	C2_7	1.504(10)
C3_7	C4_7	1.523(9)
C3_7	C5_7	1.533(10)
C3_7	C6_7	1.535(8)
C7_7	C8_7	1.539(10)
C7_7	C9_7	1.526(10)
C7_7	C10_7	1.518(10)
C11_7	C12_7	1.524(11)
C13_7	C14_7	1.527(10)
P1_8	N1_8	1.526(5)
P1_8	N5_8	1.698(5)
P1_8	N6_8	1.710(5)
P1_8	N7_8	1.707(5)
N5_8	C12_8	1.452(8)
N5_8	C13_8	1.462(8)
N6_8	C1_8	1.461(7)
N6_8	C7_8	1.492(7)
N7_8	C2_8	1.442(8)
N7_8	C3_8	1.474(8)
C1_8	C2_8	1.513(9)
C3_8	C4_8	1.536(11)
C3_8	C5_8	1.535(11)
C3_8	C6_8	1.513(10)
C7_8	C8_8	1.535(9)
C7_8	C9_8	1.537(9)
C7_8	C10_8	1.535(9)
C11_8	C12_8	1.524(11)
C13_8	C14_8	1.531(10)

Table S10: Bond Angles in ° for **3-100K.**

Atom	Atom	Atom	Angle/°
N1_5	Tb1	N1_6	112.39(18)
N1_5	Tb1	N1_7	114.23(17)
N1_6	Tb1	N1_7	94.61(18)
N1_8	Tb1	N1_5	110.25(18)
N1_8	Tb1	N1_6	112.15(18)
N1_8	Tb1	N1_7	112.46(19)
O1S_1	K1	N6_7	89.4(2)
O1S_2	K1	N6_7	96.8(3)
N1_6	K1	O1S_1	132.70(19)
N1_6	K1	O1S_2	128.8(2)
N1_6	K1	N6_6	55.35(14)
N1_6	K1	N6_7	125.91(14)
N6_6	K1	O1S_1	96.7(2)
N6_6	K1	O1S_2	88.8(3)
N6_6	K1	N6_7	168.25(14)
N1_7	K1	O1S_1	141.1(2)
N1_7	K1	O1S_2	149.3(3)
N1_7	K1	N1_6	73.49(15)
N1_7	K1	N6_6	121.46(14)
N1_7	K1	N6_7	54.47(14)
C2S_1	O1S_1	K1	111.3(5)
C2S_1	O1S_1	C4S_1	112.7(6)
C4S_1	O1S_1	K1	133.6(5)
O1S_1	C2S_1	C3S_1	110.5(6)
C2S_1	C3S_1	K1	95.3(5)
O1S_1	C4S_1	C5S_1	111.8(6)
C2S_2	O1S_2	K1	108.7(6)
C2S_2	O1S_2	C4S_2	112.6(6)
C4S_2	O1S_2	K1	138.6(7)
O1S_2	C2S_2	C3S_2	110.5(6)
C2S_2	C3S_2	K1	97.7(5)
O1S_2	C4S_2	C5S_2	111.8(7)
C2S_3	O1S_3	C4S_3	112.7(6)
O1S_3	C2S_3	C3S_3	110.5(6)
O1S_3	C4S_3	C5S_3	111.8(7)
C2S_4	O1S_4	C4S_4	112.6(6)
O1S_4	C2S_4	C3S_4	110.5(6)
O1S_4	C4S_4	C5S_4	111.8(7)
N1_5	P1_5	N5_5	113.5(3)
N1_5	P1_5	N6_5	120.7(3)
N1_5	P1_5	N7_5	121.0(3)
N5_5	P1_5	N6_5	104.2(2)
N5_5	P1_5	N7_5	103.6(3)
N7_5	P1_5	N6_5	90.4(2)
P1_5	N1_5	Tb1	172.5(3)
C12_5	N5_5	P1_5	121.2(4)
C13_5	N5_5	P1_5	122.3(4)
C13_5	N5_5	C12_5	116.3(5)
C1_5	N6_5	P1_5	109.2(4)
C1_5	N6_5	C7_5	116.4(5)
C7_5	N6_5	P1_5	122.0(4)
C2_5	N7_5	P1_5	114.4(4)
C2_5	N7_5	C3_5	118.1(5)
C3_5	N7_5	P1_5	127.3(4)
N6_5	C1_5	C2_5	104.2(5)
N7_5	C2_5	C1_5	106.1(5)
N7_5	C3_5	C4_5	109.6(5)
N7_5	C3_5	C5_5	108.8(5)
N7_5	C3_5	C6_5	110.7(5)
C4_5	C3_5	C5_5	109.4(5)
C6_5	C3_5	C4_5	108.7(5)
C6_5	C3_5	C5_5	109.6(5)
N6_5	C7_5	C8_5	111.2(5)
N6_5	C7_5	C9_5	107.6(5)
N6_5	C7_5	C10_5	109.9(5)
C8_5	C7_5	C9_5	110.2(5)
C8_5	C7_5	C10_5	109.2(5)
C10_5	C7_5	C9_5	108.6(5)
N5_5	C12_5	C11_5	114.8(5)
N5_5	C13_5	C14_5	115.1(6)
N1_6	P1_6	N5_6	113.5(3)
N1_6	P1_6	N6_6	115.0(3)
N1_6	P1_6	N7_6	121.0(3)
N5_6	P1_6	N6_6	110.7(3)
N5_6	P1_6	N7_6	102.8(3)
N7_6	P1_6	N6_6	91.5(2)
Tb1	N1_6	K1	95.06(17)
P1_6	N1_6	Tb1	171.6(3)
P1_6	N1_6	K1	93.0(2)
C12_6	N5_6	P1_6	123.0(4)
C12_6	N5_6	C13_6	116.0(5)
C13_6	N5_6	P1_6	120.9(4)
P1_6	N6_6	K1	80.21(19)
C1_6	N6_6	K1	112.1(4)
C1_6	N6_6	P1_6	109.2(4)
C7_6	N6_6	K1	109.7(3)
C7_6	N6_6	P1_6	124.5(4)
C7_6	N6_6	C1_6	115.6(5)
C2_6	N7_6	P1_6	113.0(4)
C2_6	N7_6	C3_6	116.5(5)
C3_6	N7_6	P1_6	122.3(4)
N6_6	C1_6	C2_6	105.2(5)
N7_6	C2_6	C1_6	106.0(5)
N7_6	C3_6	C4_6	110.1(5)
N7_6	C3_6	C5_6	112.5(5)
N7_6	C3_6	C6_6	110.0(5)
C4_6	C3_6	C5_6	108.1(6)
C4_6	C3_6	C6_6	108.0(5)
C6_6	C3_6	C5_6	108.1(6)
C3_6	C5_6	K1	108.2(4)
N6_6	C7_6	C8_6	109.0(5)
N6_6	C7_6	C9_6	112.4(5)
N6_6	C7_6	C10_6	110.8(5)
C9_6	C7_6	C8_6	109.2(5)
C10_6	C7_6	C8_6	106.8(5)
C10_6	C7_6	C9_6	108.5(6)
N5_6	C12_6	C11_6	114.2(6)
N5_6	C13_6	C14_6	113.1(5)
N1_7	P1_7	N5_7	113.7(3)
N1_7	P1_7	N6_7	115.1(3)
N1_7	P1_7	N7_7	121.9(3)
N5_7	P1_7	N6_7	109.4(3)
N5_7	P1_7	N7_7	102.8(3)
N7_7	P1_7	N6_7	91.4(3)
Tb1	N1_7	K1	96.57(17)
P1_7	N1_7	Tb1	162.8(3)

Atom	Atom	Atom	Angle/°
P1_7	N1_7	K1	100.6(2)
C12_7	N5_7	P1_7	122.8(5)
C12_7	N5_7	C13_7	115.8(5)
C13_7	N5_7	P1_7	121.4(4)
P1_7	N6_7	K1	80.30(18)
C1_7	N6_7	K1	117.6(4)
C1_7	N6_7	P1_7	110.8(4)
C1_7	N6_7	C7_7	115.3(5)
C7_7	N6_7	K1	103.0(3)
C7_7	N6_7	P1_7	124.6(4)
C2_7	N7_7	P1_7	113.5(4)
C2_7	N7_7	C3_7	115.9(5)
C3_7	N7_7	P1_7	124.2(4)
N6_7	C1_7	C2_7	105.9(5)
N7_7	C2_7	C1_7	105.5(6)
N7_7	C3_7	C4_7	109.0(5)
N7_7	C3_7	C5_7	109.8(6)
N7_7	C3_7	C6_7	110.5(5)
C4_7	C3_7	C5_7	110.2(7)
C4_7	C3_7	C6_7	108.9(6)
C5_7	C3_7	C6_7	108.4(5)
N6_7	C7_7	C8_7	108.2(6)
N6_7	C7_7	C9_7	112.7(6)
N6_7	C7_7	C10_7	110.3(5)
C9_7	C7_7	C8_7	109.9(6)
C10_7	C7_7	C8_7	107.2(6)
C10_7	C7_7	C9_7	108.5(7)
N5_7	C12_7	C11_7	114.7(6)
N5_7	C13_7	C14_7	113.5(6)
N1_8	P1_8	N5_8	113.2(3)
N1_8	P1_8	N6_8	121.6(3)
N1_8	P1_8	N7_8	119.8(3)
N5_8	P1_8	N6_8	103.1(3)
N5_8	P1_8	N7_8	104.7(3)
N7_8	P1_8	N6_8	91.1(3)
P1_8	N1_8	Tb1	167.6(3)
C12_8	N5_8	P1_8	121.2(4)
C12_8	N5_8	C13_8	117.4(5)
C13_8	N5_8	P1_8	121.0(4)
C1_8	N6_8	P1_8	110.1(4)
C1_8	N6_8	C7_8	115.2(5)
C7_8	N6_8	P1_8	122.8(4)
C2_8	N7_8	P1_8	113.8(4)
C2_8	N7_8	C3_8	118.0(5)
C3_8	N7_8	P1_8	127.2(4)
N6_8	C1_8	C2_8	104.7(5)
N7_8	C2_8	C1_8	105.9(5)
N7_8	C3_8	C4_8	109.8(6)
N7_8	C3_8	C5_8	108.8(6)
N7_8	C3_8	C6_8	110.9(5)
C5_8	C3_8	C4_8	108.5(7)
C6_8	C3_8	C4_8	109.8(7)
C6_8	C3_8	C5_8	109.0(7)
N6_8	C7_8	C8_8	112.5(5)
N6_8	C7_8	C9_8	108.0(5)
N6_8	C7_8	C10_8	109.1(5)
C8_8	C7_8	C9_8	110.3(5)
C8_8	C7_8	C10_8	108.2(5)
C10_8	C7_8	C9_8	108.8(5)
N5_8	C12_8	C11_8	115.6(6)
N5_8	C13_8	C14_8	112.8(6)

Table S11: Bond Lengths in Å for **4**.

Atom	Atom	Length/Å
Tb1	N1	2.106(3)
Tb1	N1[1]	2.106(3)
Tb1	N1[2]	2.106(3)
Tb1	N1[3]	2.106(3)
P1	N3	1.680(3)
P1	N2	1.697(4)
P1	N4	1.667(4)
P1	N1	1.555(3)
N3	C7	1.482(5)
N3	C2	1.456(5)
N2	C3	1.493(6)
N2	C1	1.469(6)
N4	C11	1.462(7)
N4	C13	1.468(5)
C11	C12	1.529(6)
C3	C4	1.532(6)
C3	C5	1.538(6)
C3	C6	1.523(7)
C7	C8	1.548(9)
C7	C9	1.539(6)
C7	C10	1.530(6)
C1	C2	1.517(6)
C14	C13	1.525(6)
C1S_1	C2S_1	1.518(3)
C2S_1	C3S_1	1.519(3)
C3S_1	C4S_1	1.518(3)
C4S_1	C5S_1	1.518(3)

[1]+y,-1-x,-1-z; [2]-1-x,-1-y,+z; [3]-1-

Table S12: Bond Angles in ° for **4**.

Atom	Atom	Atom	Angle/°
N1	Tb1	N1[1]	108.26(7)
N1[2]	Tb1	N1[3]	108.26(7)
N1	Tb1	N1[3]	111.91(14)
N1	Tb1	N1[2]	108.26(7)
N1[1]	Tb1	N1[2]	111.91(14)
N1[1]	Tb1	N1[3]	108.26(7)
N3	P1	N2	91.58(19)
N4	P1	N3	105.60(19)
N4	P1	N2	106.0(2)
N1	P1	N3	119.1(3)
N1	P1	N2	120.0(2)
N1	P1	N4	112.04(18)
C7	N3	P1	127.9(2)
C2	N3	P1	113.9(3)
C2	N3	C7	118.2(3)
C3	N2	P1	124.5(4)
C1	N2	P1	109.1(3)
C1	N2	C3	116.1(4)
C11	N4	P1	122.6(3)
C11	N4	C13	116.9(3)
C13	N4	P1	120.4(3)
N4	C11	C12	113.3(3)
N2	C3	C4	110.3(4)
N2	C3	C5	111.7(4)
N2	C3	C6	108.1(4)
C4	C3	C5	108.4(4)
C6	C3	C4	108.3(4)
C6	C3	C5	109.9(4)
N3	C7	C8	108.8(3)
N3	C7	C9	109.7(3)
N3	C7	C10	111.5(3)
C9	C7	C8	110.8(4)
C10	C7	C8	108.1(3)
C10	C7	C9	108.0(4)
N2	C1	C2	104.1(4)
N4	C13	C14	114.9(4)
P1	N1	Tb1	164.7(4)
N3	C2	C1	105.8(3)
C1S_1	C2S_1	C3S_1	113.6(4)
C4S_1	C3S_1	C2S_1	113.9(4)
C5S_1	C4S_1	C3S_1	113.7(4)

[1]-1-y,+x,-1-z; [2]+y,-1-x,-1-z; [3]-1-x,-1-y

Electronic Absorption Spectra

General Considerations. Special measures were taken to obtain the UV-visible/NIR spectroscopy of **4** as the compound is very air and water sensitive. Spectra were taken immediately after solution preparation from dilution of stock solution with a 240 nm/min scan rate.

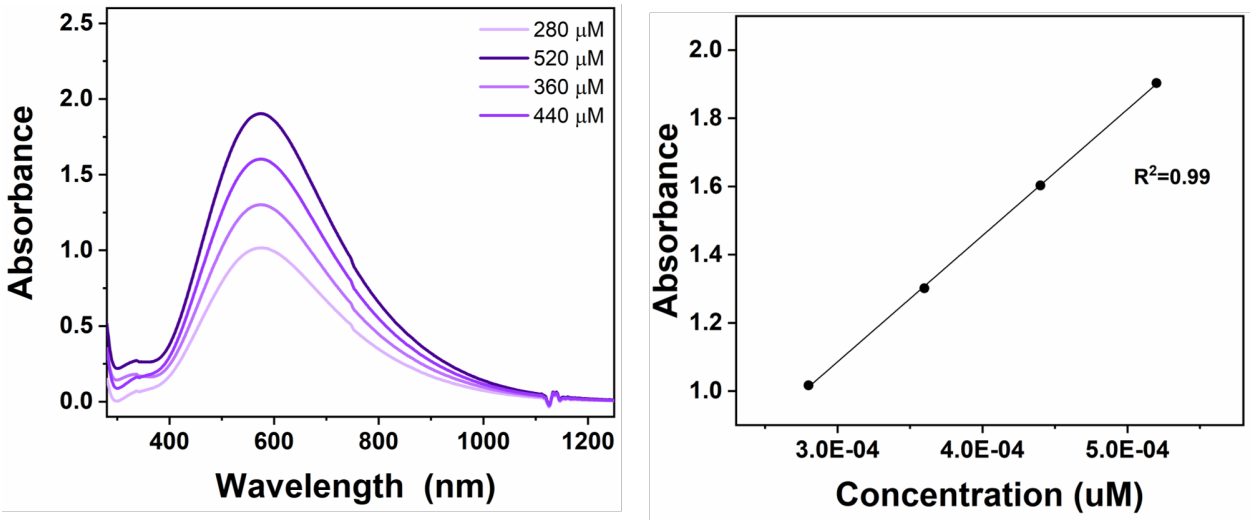

Figure S28. (left) UV-vis/NIR spectra of **4** in benzene. (right) Linear regression of absorbance at 575 nm maximum where ε= 3700 cm^{-1} M^{-1}.

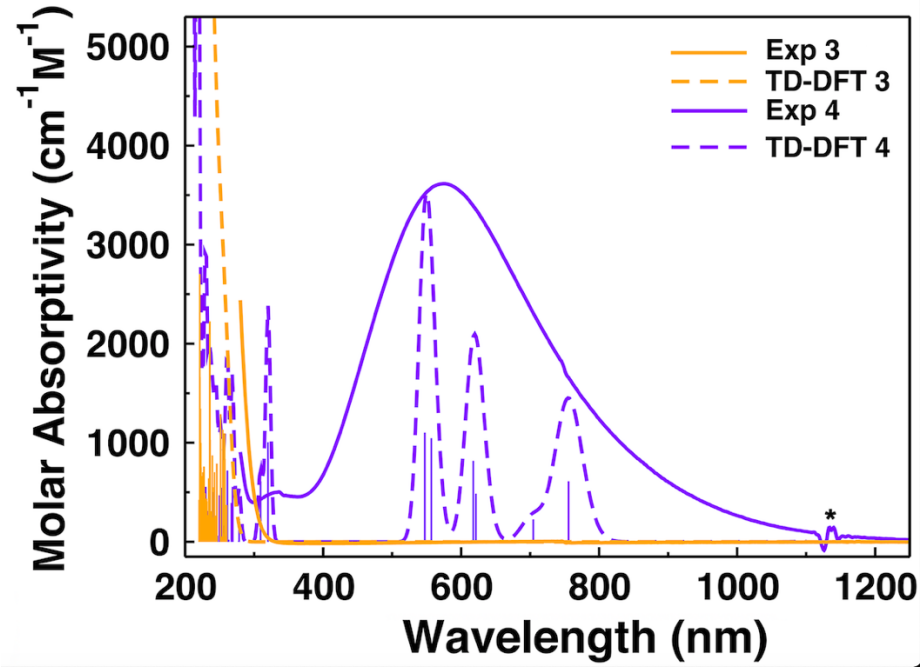

Figure S29. Experimental UV/vis/NIR spectra of **3** and **4** in benzene (solid lines) and their computed TD-DFT spectra in the UV/vis region (dashed lines). Vertical bars depict theoretical

oscillator strength of single-electron excitations. A * has been placed on the graphic to denote a grating change for the UV/vis/NIR instrument.

Magnetism

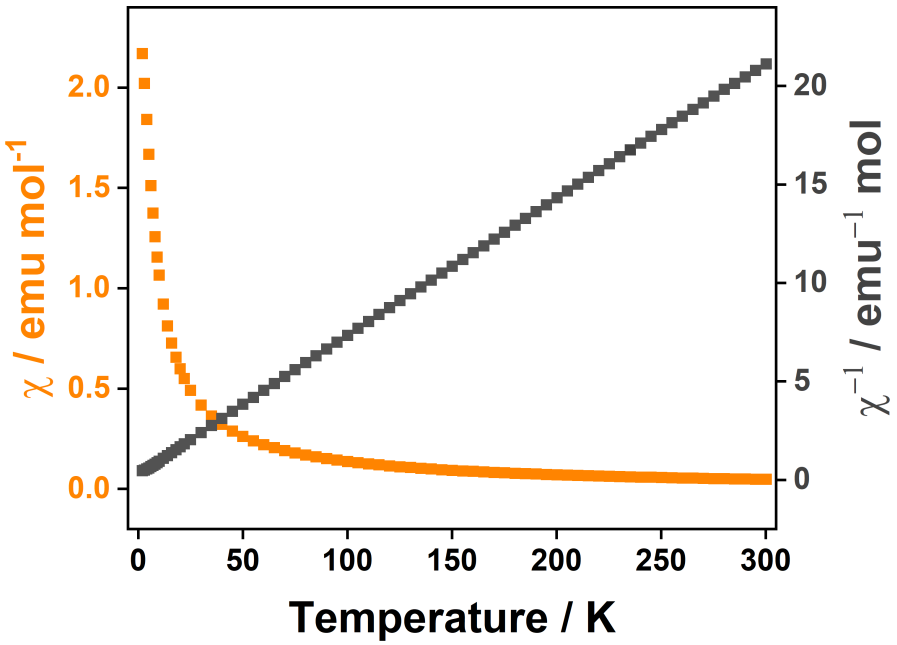

Figure S30. χT vs. T (orange, left axis) and $1/\chi$ vs. T (gray, right axis) for **3.**

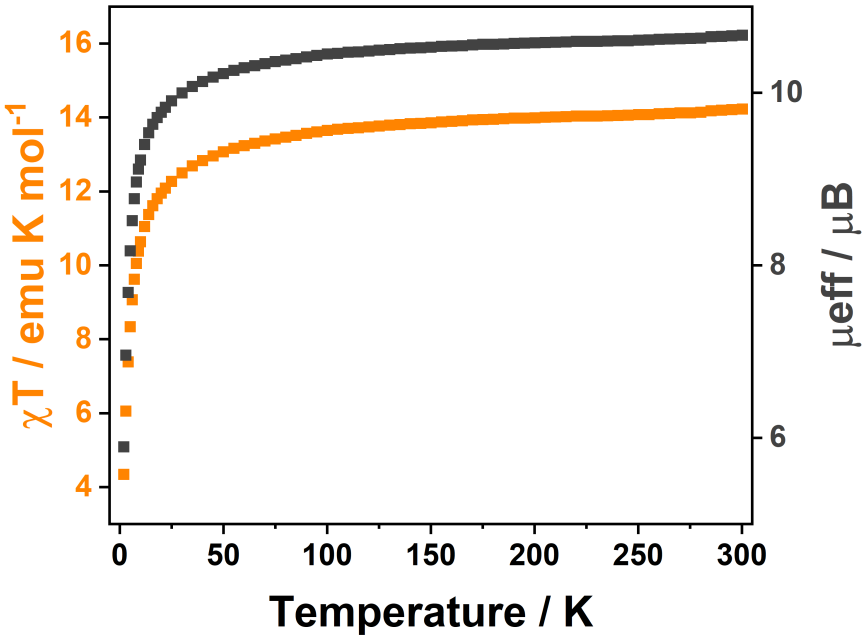

Figure S31. χT vs. T (orange, left axis) and μ_{eff} vs. T (gray, right axis) plot for **3.**

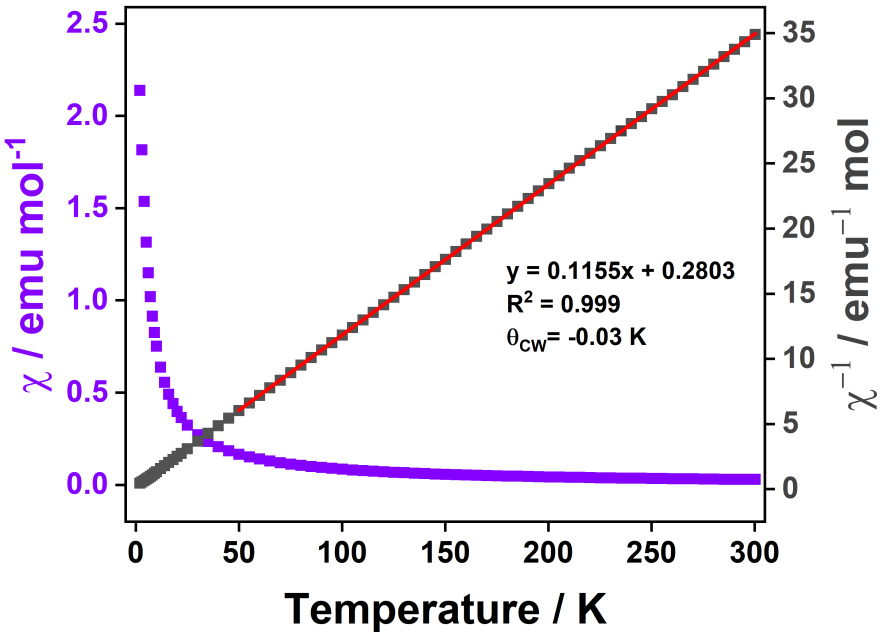

Figure S32. χT vs. T (purple, left axis) and $1/\chi$ vs. T (gray, right axis) for **4**.

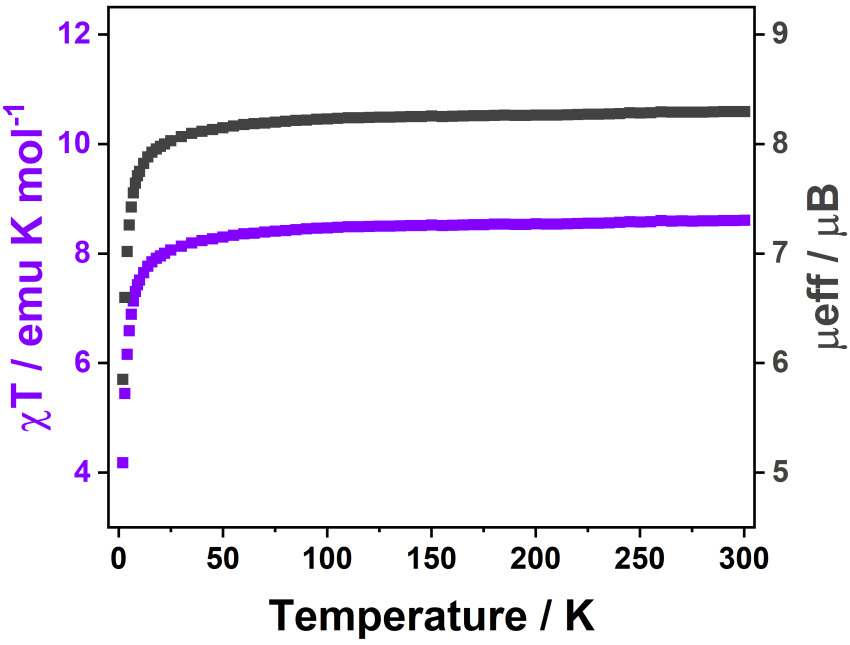

Figure S33. χT vs. T (purple, left axis) and μ_{eff} vs. T (gray, right axis) plot for **4**.

Fitting of Field-Dependent Magnetic Data for 4. A $S = 7/2$ spin Hamiltonian with only D and isotropic g was employed yielding a satisfactory fit using a previously described approach (the results are consistent with those obtained with PHI).[1,2] The fit uses all three field datasets, but because at the lower field the high T is less reliable (since χ is small), only the two higher field (1 T, 3 T) were employed for the final fit. The g value is determined from the high T data ($T \geq 100$

K), but even using the whole *T* range, the *g* value changes little, as does *D*. These different constraints are the basis for the error in *D* of ±0.5 cm^{-1}.

The Hamiltonian used is the sum of the electronic Zeeman (EZ), with only an isotropic *g* value, and zero-field splitting (ZFS) interactions, with only second order terms.

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\mathrm{EZ}} + \hat{\mathcal{H}}_{\mathrm{ZFS}}$$

$$= g\mu_{\mathrm{B}}\boldsymbol{B}\cdot\hat{\boldsymbol{S}} + \hat{\boldsymbol{S}}\cdot\boldsymbol{D}\cdot\hat{\boldsymbol{S}}$$

$$= g\mu_{\mathrm{B}}\boldsymbol{B}\cdot\hat{\boldsymbol{S}} + D\left\{\hat{S}_z^2 - \frac{1}{3}S(S+1)\hat{1}\right\} + E\left(\hat{S}_x^2 - \hat{S}_y^2\right)$$

μ_B is the Bohr magneton, $\hat{1}$ is the identity matrix, and *D* and *E* are the axial and rhombic zfs terms, respectively.

Goodness of fit calculated using established procedure.[3]

1 T, 3 T, D = 0, *g* varying, but *T* >= 100 K only
GINSBERG STANDARD ERROR OF ESTIMATE = 0.50274031E-01 (1e-02 is essentially perfect for any real system)

1 T, 3 T, D > 0, *g* varying, all *T*
GINSBERG STANDARD ERROR OF ESTIMATE = 0.13810961E+00

1 T, 3 T, D < 0, *g* varying, all *T*
GINSBERG STANDARD ERROR OF ESTIMATE = 0.15132256E+00

1 T, 3 T, D > 0, *g* fixed at high *T* value, all *T*
GINSBERG STANDARD ERROR OF ESTIMATE = 0.14273531E+00

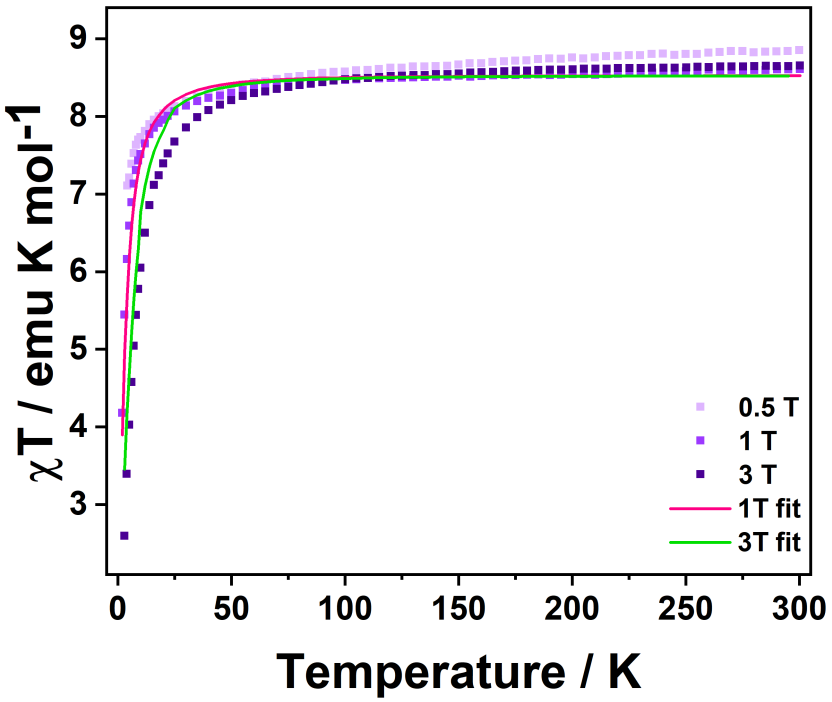

Figure S34. χT vs. T plot at 0.5, 1, and 3 T for **4** and fitting of the 1 and 3 T data with S = 7/2, D = ±5.5 cm^{-1}, g = 2.085.

Electron Paramagnetic Resonance

EPR simulations used the program SPIN (A. Ozarowski, NHMFL). Calculated resonant fields (±0.5 mT) for ν = 9.366 GHz, S = 7/2, D = ±5.5 cm^{-1}, E/D = 0.11, g = 2.085. The D and g values are based solely on magnetic susceptibility fits, shown in Figure S34.

	Orientation		
$\|S = 7/2, M_S\rangle$ multiplet	z	x	y
±1/2	542.5	245	52
±3/2	126.5	131.5	133
±5/2	65	---	---
±7/2	46	---	---

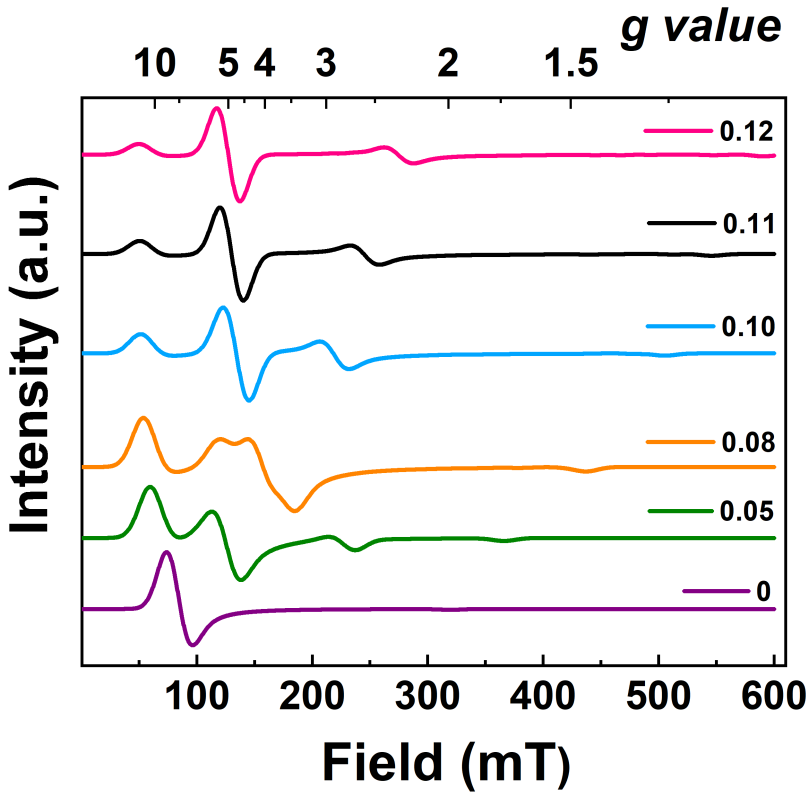

Figure S35. Simulation of EPR spectrum of **4** at 9.366 GHz and 12 K with changing $|E/D|$ value. The best match between the simulated and experimental features obtains for $|E/D|$ = 0.11, see main text for comparison with experimental spectrum.

Theoretical Details

Table S13. Experimental (exp) vs. optimized (opt) Tb–N and N–P bond lengths (Å) and Tb–N–P valence angles (º) of complexes **3** and **4**. See Figure 1 of the main text for atom labels.

	3 (exp)	**3** (opt)	**4** (exp)	**4** (opt)
Tb1–N1a	2.231	2.248	2.106	2.188
Tb1–N1b	2.264	2.249		
N1a–P1a	1.528	1.533	1.555	1.554
N1b–P1b	1.532	1.534		
Tb1–N1a–P1a	168.74	172.16	164.70	162.40
Tb1–N1b–P1b	167.64	173.03		

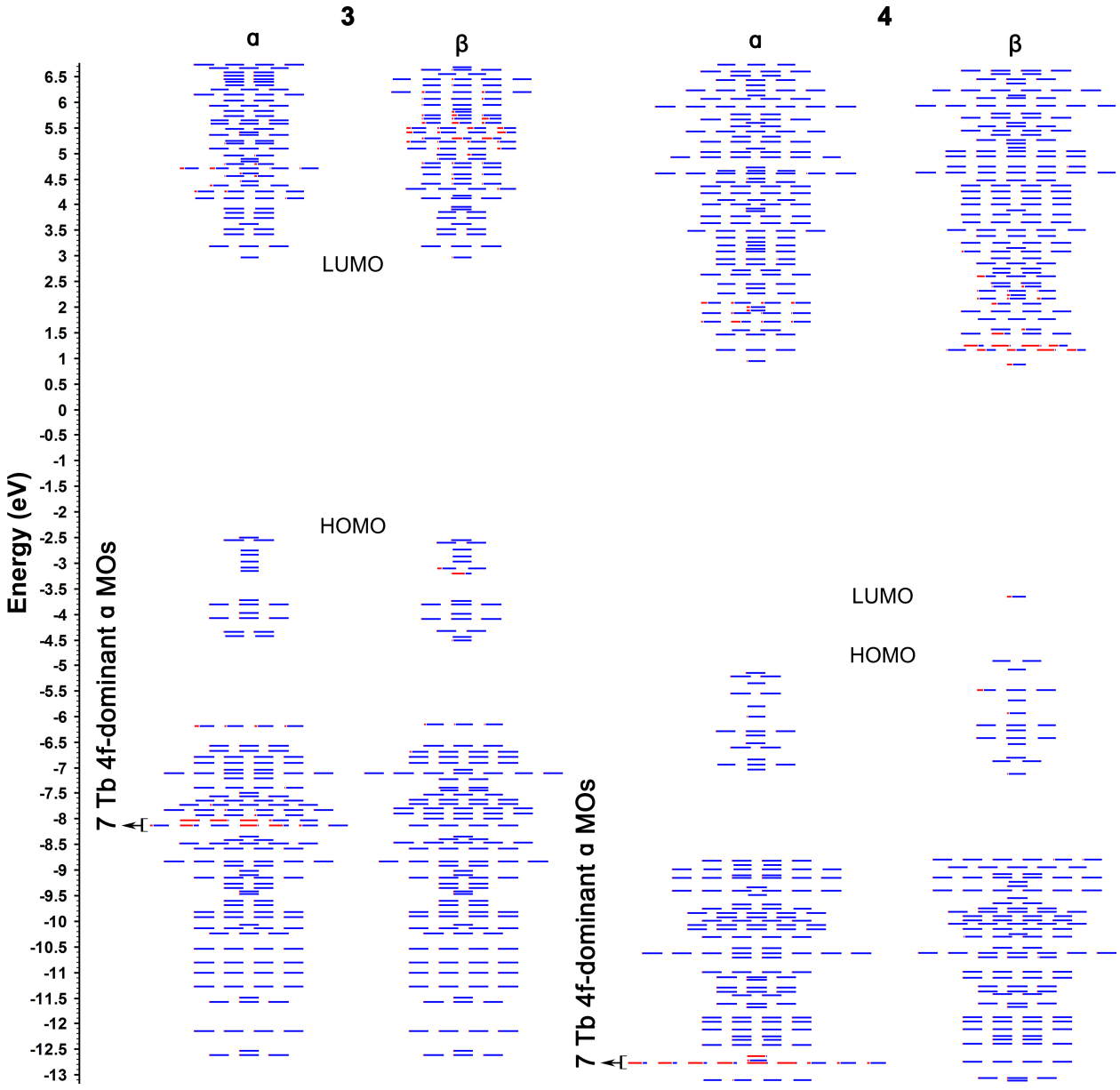

Figure S36. Combined (α+β) MO diagrams of **3** and **4**. The red fraction of the MO lines represents the percentage of Tb AOs in the MOs, and the blue lines are the ligand fraction. Degeneracy of the MO energy levels is set to 0.05eV.

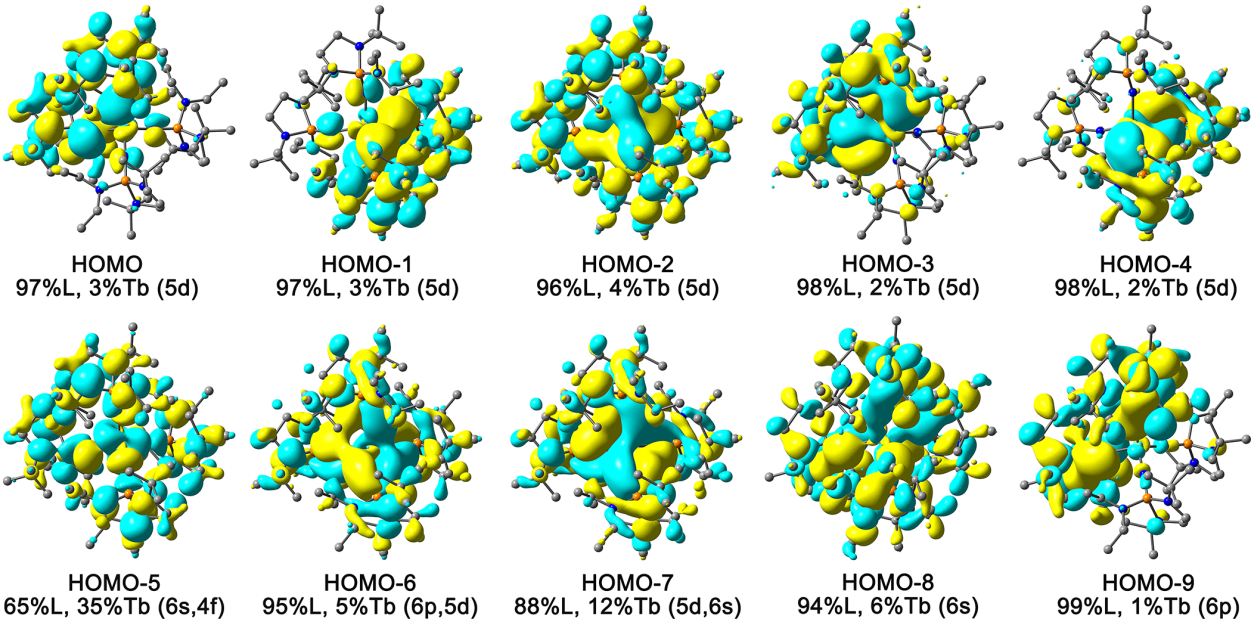

Figure S37. Ten highest occupied MOs of **4** (β electron density). Fragment composition (%) of the MOs is shown in colors in Figure 3 of the main text (Tb AOs, red vs. ligands AOs, blue). Dominant AOs of Tb are shown in parentheses.

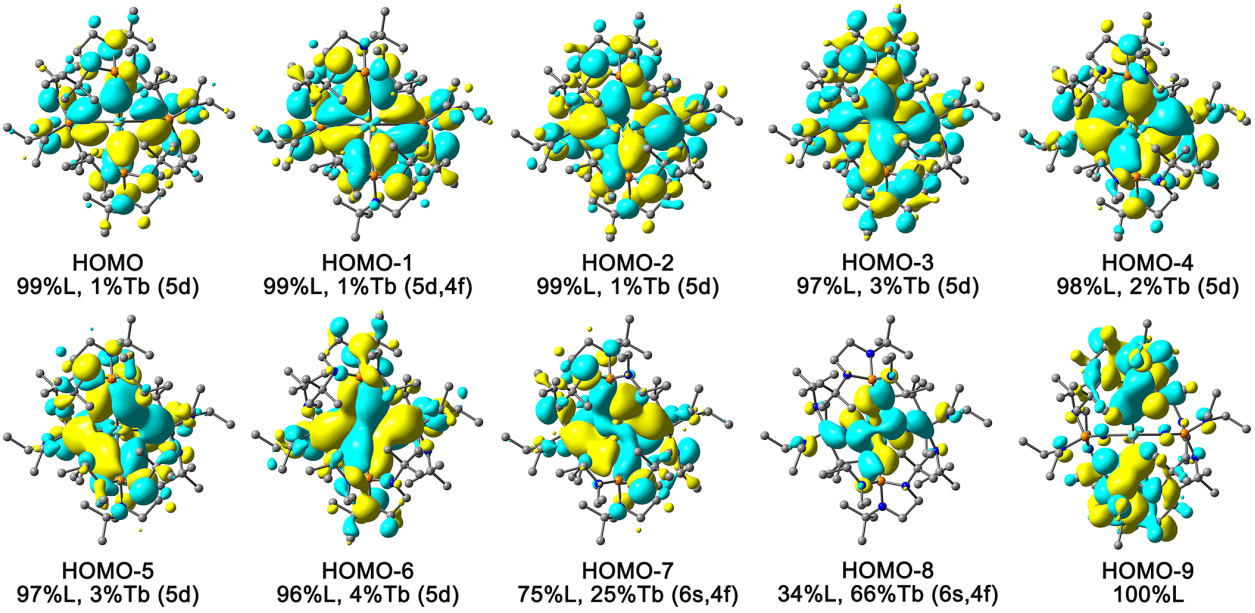

Figure S38. Ten highest occupied MOs of **3** (β electron density). Fragment composition (%) of the MOs is shown in colors in Figure 3 of the main text (Tb AOs, red vs. ligands AOs, blue). Dominant AOs of Tb are shown in parentheses.

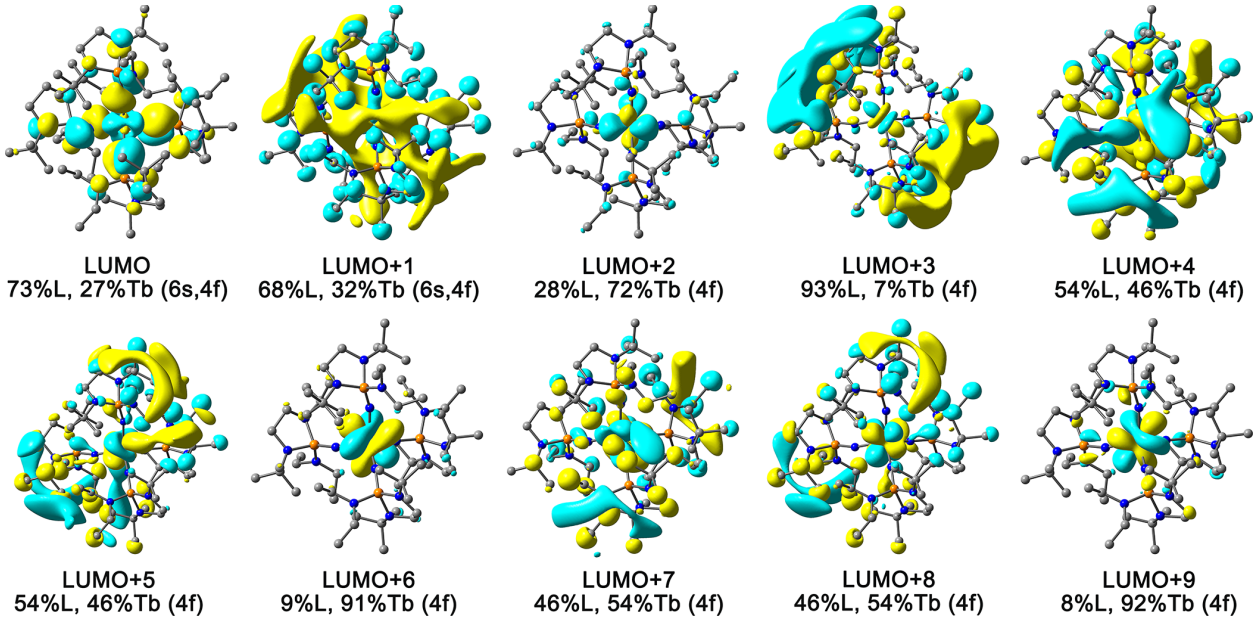

Figure S39. Ten lowest unoccupied MOs of **4** (β electron density). Fragment composition (%) of the MOs is shown in colors in Figure 3 of the main text (Tb AOs, red vs. ligands AOs, blue). Dominant AOs of Tb are shown in parentheses.

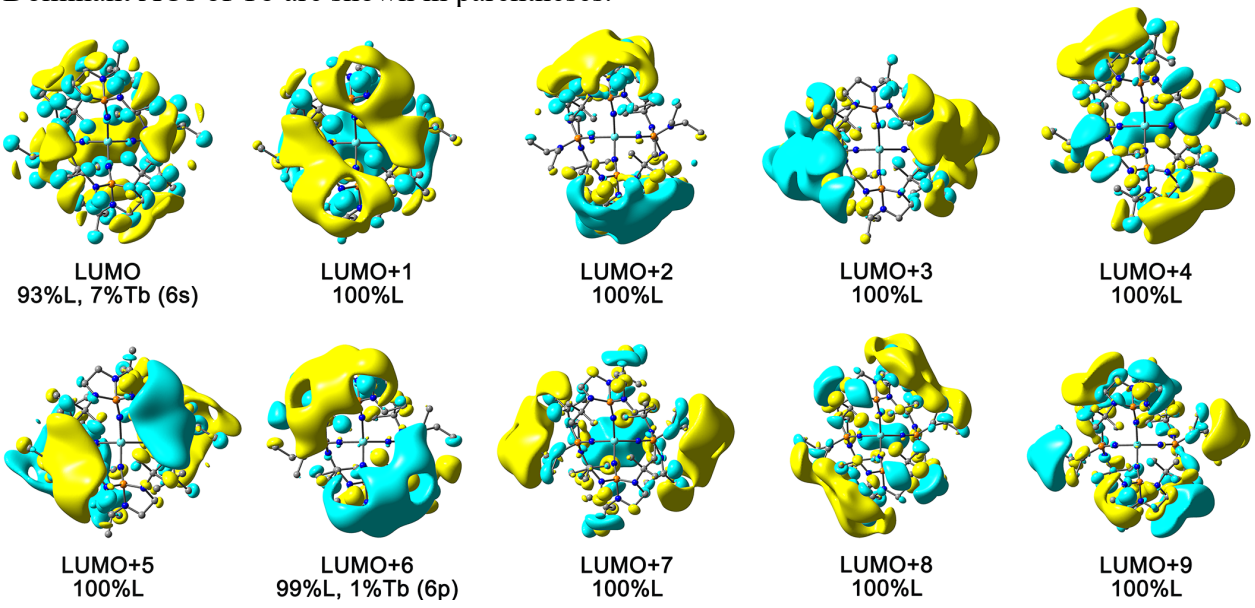

Figure S40. Ten lowest unoccupied MOs of **3** (β electron density). Fragment composition (%) of the MOs is shown in colors in Figure 3 of the main text (Tb AOs, red vs. ligands AOs, blue). Dominant AOs of Tb are shown in parentheses.

Table S14. Bond polarization (%) of the NBOs shown in Figure 4 of the main text.

Bonds	Tb–N σ bond		N–P σ bond		Tb–N–P π bonds		
	Tb	N	N	P	Tb	N	P
3	5.23	94.77	70.00	30.00	2.24	95.57	2.19
4	8.31	91.69	70.42	29.58	5.69	92.58	1.74

Table S15. Tb hybrids (%) of the Tb NBOs.

Bonds	3				4			
	s	p	d	f	s	p	d	f
Tb–N σ bond	15.27	0.40	73.49	10.62	18.13	0.34	75.19	6.10
Tb–N–P π bonds	2.83	0.99	72.12	32.23	9.71	2.11	62.11	25.44
1c-1e α NBO on Tb	0.00	0.01	0.01	99.98	0.00	0.01	0.01	99.98
1c-1e β NBO on Tb	57.59	0.00	0.01	42.40	N/A			

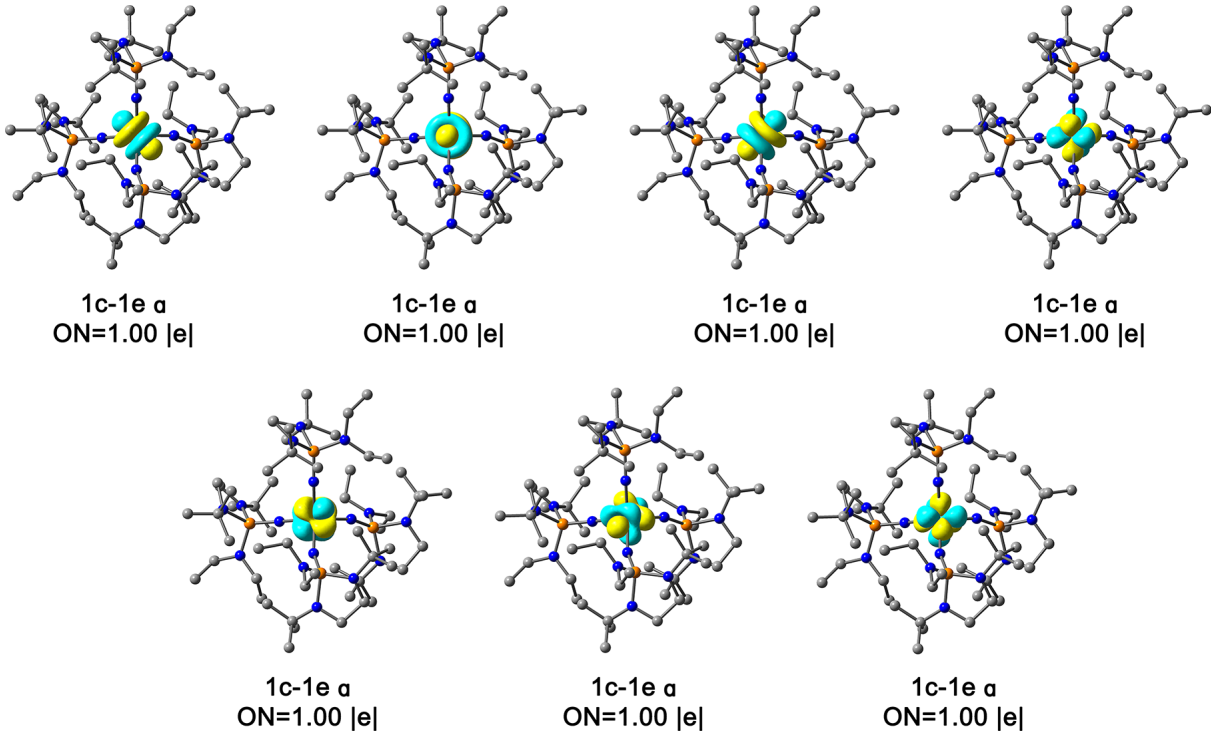

Figure S41. Seven unpaired electrons (1c-1e α NBOs) on Tb in **4**.

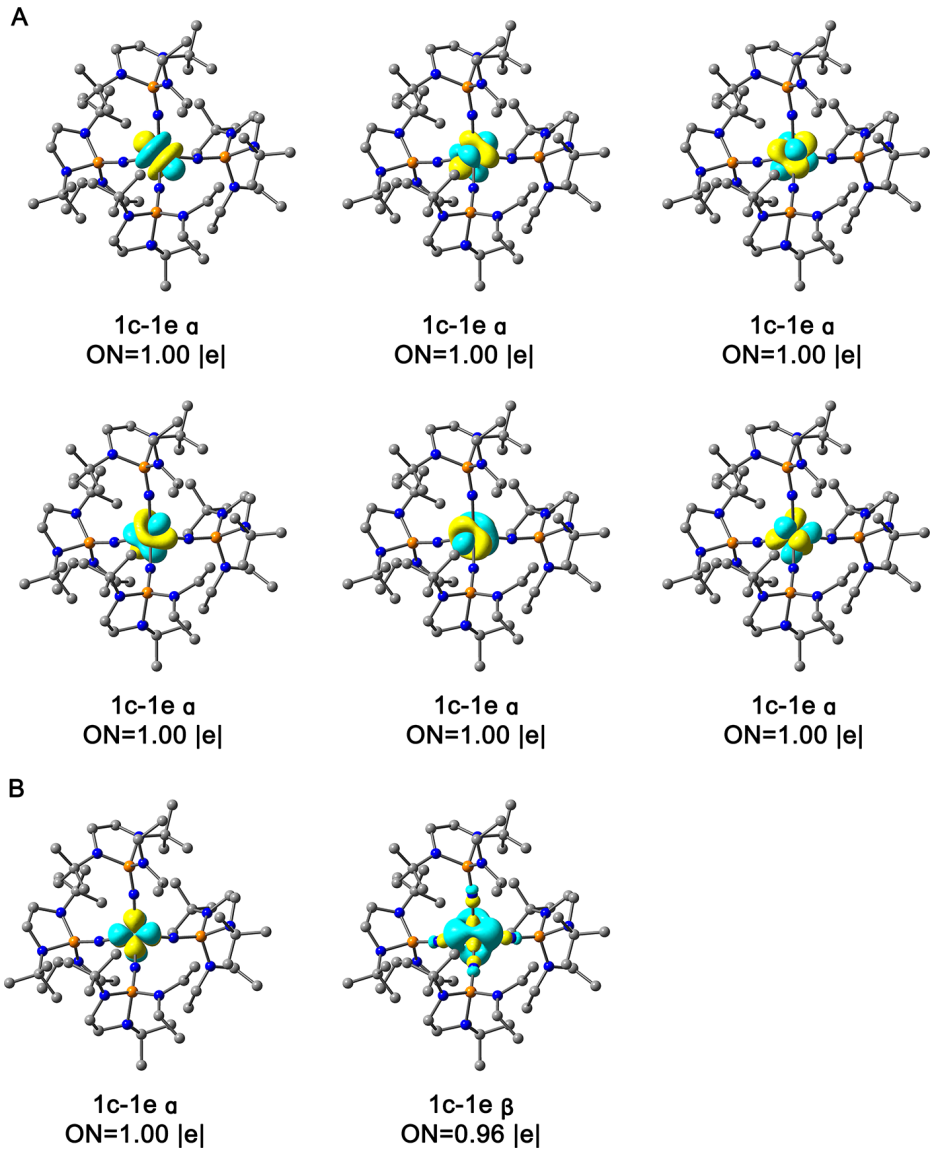

Figure S42. (A) Six unpaired electrons (1c-1e α NBOs) and (B) two electrons (α + β) composing a lone pair (1c-2e NBO) on Tb in **3**.

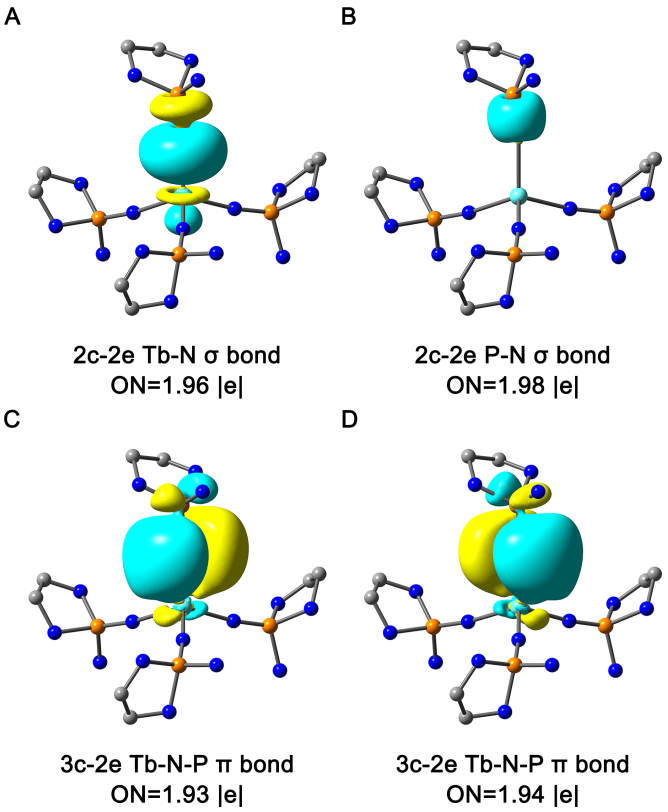

Figure S43. Bonding analysis of the Tb–N–P interactions in **3**. (A) Two-center two-electron Tb–N σ bond. (B) Two-center two-electron P–N σ bond. (C, D) Three-center two-electron Tb–N–P π bonds. ON denotes occupation number here and elsewhere. Side groups of the ligands (^{t}Bu, Et_2) are omitted for simplicity. An equivalent set of bonds is identified for other three ligands.

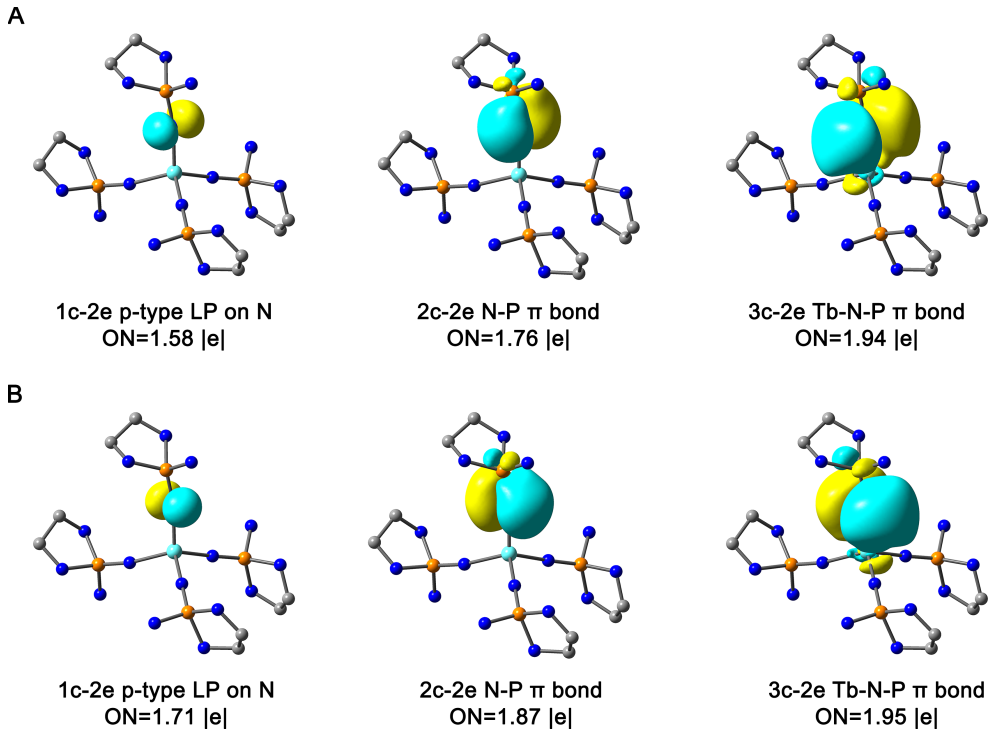

Figure S44. Representations of (A) two orthogonal p-type lone pairs of N as (B) two two-center two-electron N–P π bonds and (C) two three-center two-electron Tb–N–P π bonds in **4**. Side groups of the ligands (^{t}Bu, Et_2) are omitted for simplicity.

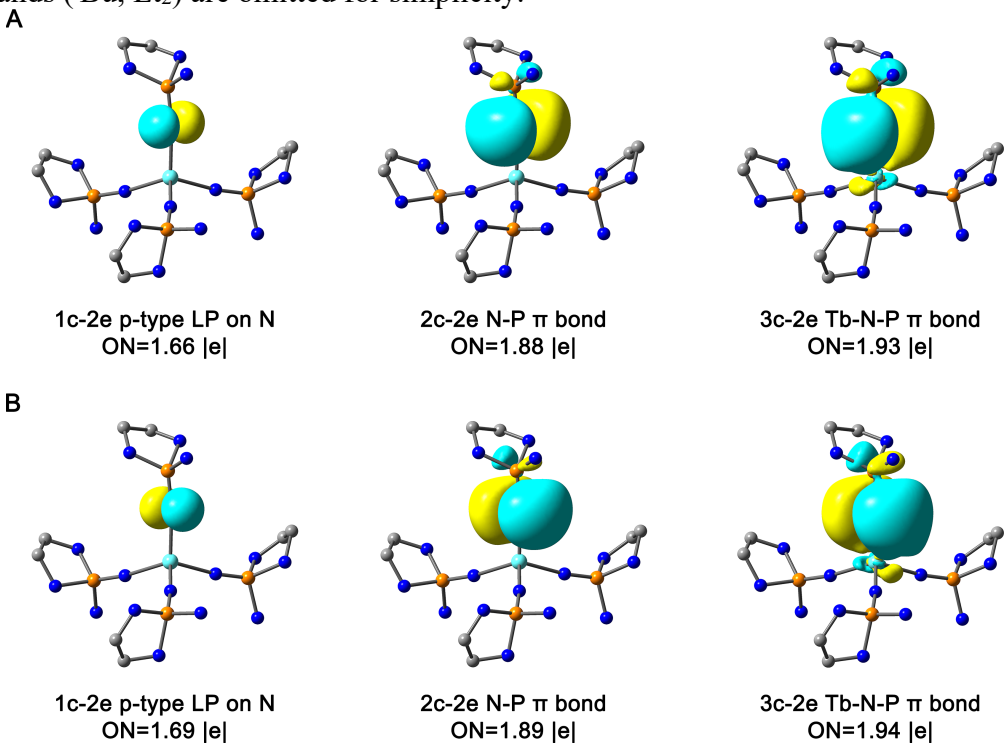

Figure S45. Representations of (A) two orthogonal p-type lone pairs of N as (B) two two-center two-electron N–P π bonds and (C) two three-center two-electron Tb–N–P π bonds in **3**. Side groups of the ligands (^{t}Bu, Et_2) are omitted for simplicity.

Table S16. Cartesian coordinates of optimized complexes **3** and **4**.

3				**4**			
Tb	0.00000000	0.00000000	0.02806200	Tb	0.00000000	0.00000000	0.00000000
P	-1.47314000	2.73846500	2.16523000	P	1.03065400	2.75097500	2.24771600
N	-0.76173300	1.66581600	1.33170000	N	2.40763300	2.76500100	3.25005800
N	-0.49328200	3.40085400	3.39519700	N	0.00000000	2.90592400	3.61553600
N	-2.97747000	2.40071700	2.98495600	N	0.99893200	4.26924000	1.51197900
N	-2.17947000	4.12667700	1.43765900	C	0.64529900	4.43793300	0.11542000
C	-4.06560200	2.91992900	2.17829300	H	-0.35067900	4.89717500	0.02722900
H	-4.98402900	3.01787000	2.76568700	H	0.55905400	3.43493300	-0.30652800
H	-4.28452400	2.28494800	1.30631400	C	-1.47276900	2.82596900	3.56252200
C	-3.58746000	4.27965900	1.70966000	C	-1.98858400	3.28881900	2.20287700
H	-4.14304200	4.59135000	0.81647300	H	-1.67486900	4.30946900	1.98055300
H	-3.77660900	5.03440000	2.49393900	H	-3.08101500	3.26384100	2.20788300
C	-1.51643600	5.12562200	0.59263600	H	-1.64354100	2.64157300	1.39351700
C	-1.87107900	6.53854900	1.07476300	C	3.81823800	2.71122000	2.83908000
H	-2.94121400	6.74863700	0.98322000	C	0.64943300	2.30109600	4.76401800
H	-1.33879500	7.28374200	0.47507600	H	0.58022700	1.20300200	4.75184600
H	-1.58405200	6.67703800	2.12093900	H	0.20446200	2.65557900	5.69785000
C	-1.96737800	4.96557800	-0.86305500	C	-1.96887800	1.40106800	3.82000400
H	-1.69209400	3.97815000	-1.23480500	H	-1.53486700	0.69084600	3.11053900
H	-1.49827500	5.72289500	-1.50056900	H	-3.05700500	1.36061500	3.72279700
H	-3.05089700	5.07658700	-0.96609000	H	-1.72536400	1.06583400	4.83315000
C	0.00000000	4.96708300	0.65396800	C	1.64331600	5.26093600	-0.68730600
H	0.38114100	5.21043900	1.64702200	H	1.72299200	6.29129000	-0.32753700
H	0.46268900	5.64437300	-0.06989200	H	1.32497400	5.31008600	-1.73243700
H	0.30204300	3.94439800	0.41806500	H	2.64080500	4.81772100	-0.66036100
C	-3.21074100	1.10464700	3.65047300	C	-2.04594100	3.76294800	4.63175100
C	-3.60798700	0.00670100	2.65818600	H	-1.75342000	3.46607800	5.64285200
H	-4.57331200	0.21502300	2.18789700	H	-3.13959000	3.75367500	4.59708900
H	-3.69601600	-0.95950100	3.16546200	H	-1.70485800	4.78828200	4.46826800
H	-2.85563000	-0.07987200	1.87126500	C	0.21001800	6.51956000	2.28975300
C	-4.32518700	1.28052400	4.68809200	H	-0.70645200	6.13726200	2.74455000
H	-4.07784800	2.08662700	5.38505800	H	-0.03452200	6.87303100	1.28414900
H	-4.45341100	0.35612000	5.26020500	H	0.53509800	7.38841100	2.87019900
H	-5.29058300	1.51049700	4.22803500	C	4.36521300	1.29631000	3.04279200
C	-1.94767300	0.66960100	4.38960900	H	4.28674600	0.97834000	4.08660000
H	-1.12810500	0.48870900	3.69215300	H	5.42167500	1.24110400	2.76057100
H	-2.14320400	-0.26039300	4.93068000	H	3.79939100	0.59418100	2.42960500
H	-1.62944800	1.42430300	5.11096600	C	4.63185600	3.70464400	3.67549100
C	-1.16475300	4.20343400	5.67860700	H	4.23000300	4.71704100	3.57667900
H	-1.45692400	5.11254600	6.21582500	H	5.67036500	3.71676900	3.33243600
H	-0.25931000	3.81709300	6.15672100	H	4.64274200	3.44270400	4.73711000
H	-1.95864700	3.46469300	5.80715000	C	1.30515100	5.46248600	2.28150300
C	-0.94924500	4.51129400	4.20160500	H	2.23775400	5.91374100	1.90950300
H	-1.88844200	4.86727800	3.77565500	H	1.50842700	5.15313800	3.30793400
H	-0.24105800	5.35127900	4.11184100	C	3.96743800	3.09073800	1.36976500
C	0.75963600	2.77447100	3.75510000	H	3.34130400	2.46399600	0.73184200
H	0.96187700	2.03340200	2.97921300	H	5.00946700	2.95792900	1.06494100
H	0.66488600	2.21874300	4.70226400	H	3.69591000	4.13441400	1.20447000
C	1.93126600	3.74058700	3.86554500	N	0.86796700	1.58295300	1.23556400
H	2.07711500	4.29037400	2.93268800	C	2.10074800	2.72877500	4.66423900
H	2.85182900	3.18685400	4.07604800	H	2.23758300	3.71893700	5.12702500
H	1.80191500	4.47058700	4.67183000	H	2.74461200	2.02215400	5.19939100
P	2.73749500	1.28132400	-2.23582600	P	-1.03065400	-2.75097500	2.24771600
N	1.69980700	0.75925900	-1.23380900	N	-2.40763300	-2.76500100	3.25005800
N	3.70249300	2.54857000	-1.62744400	N	0.00000000	-2.90592400	3.61553600
N	2.27041800	1.86821700	-3.77929000	N	-0.99893200	-4.26924000	1.51197900
N	3.90096600	0.22039300	-2.99069300	C	-0.64529900	-4.43793300	0.11542000
C	2.82389500	1.12928300	-4.88857700	H	0.35067900	-4.89717500	0.02722900

H	3.60825900	1.70779900	-5.40691900	H	-0.55905400	-3.43493300	-0.30652800
H	2.05908200	0.87858600	-5.63415300	C	1.47276900	-2.82596900	3.56252200
C	3.41043000	-0.14523100	-4.30591600	C	1.98858400	-3.28881900	2.20287700
H	2.63461300	-0.92362700	-4.26608600	H	1.67486900	-4.30946900	1.98055300
H	4.22202100	-0.51395300	-4.94116300	H	3.08101500	-3.26384100	2.20788300
C	4.57434100	-0.84349000	-2.22331600	H	1.64354100	-2.64157300	1.39351700
C	5.83266700	-1.27736700	-2.98312200	C	-3.81823800	-2.71122000	2.83908000
H	5.59733600	-1.78738700	-3.92175100	C	-0.64943300	-2.30109600	4.76401800
H	6.41465500	-1.97648700	-2.37432100	H	-0.58022700	-1.20300200	4.75184600
H	6.46205800	-0.41215500	-3.21211700	H	-0.20446200	-2.65557900	5.69785000
C	3.67148900	-2.05755500	-1.98935300	C	1.96887800	-1.40106800	3.82000400
H	2.78146400	-1.75945300	-1.43131600	H	1.53486700	-0.69084600	3.11053900
H	4.20129900	-2.82101000	-1.41083300	H	3.05700500	-1.36061500	3.72279700
H	3.35733500	-2.52245000	-2.92899500	H	1.72536400	-1.06583400	4.83315000
C	5.00473100	-0.30073600	-0.86295300	C	-1.64331600	-5.26093600	-0.68730600
H	5.65213900	0.57154900	-0.96451600	H	-1.72299200	-6.29129000	-0.32753700
H	5.55530700	-1.07523800	-0.32007900	H	-1.32497400	-5.31008600	-1.73243700
H	4.13457300	-0.02322000	-0.26576900	H	-2.64080500	-4.81772100	-0.66036100
C	1.17734600	2.81158000	-4.03285900	C	2.04594100	-3.76294800	4.63175100
C	-0.13345000	2.05619000	-4.27332700	H	1.75342000	-3.46607800	5.64285200
H	-0.05270100	1.38263900	-5.13322900	H	3.13959000	-3.75367500	4.59708900
H	-0.95637000	2.75161600	-4.47413600	H	1.70485800	-4.78828200	4.46826800
H	-0.38608000	1.45464800	-3.39687900	C	-0.21001800	-6.51956000	2.28975300
C	1.51796200	3.66621400	-5.25907000	H	0.70645200	-6.13726200	2.74455000
H	2.46697900	4.19117500	-5.11273800	H	0.03452200	-6.87303100	1.28414900
H	0.73583800	4.41460800	-5.42008500	H	-0.53509800	-7.38841100	2.87019900
H	1.59449300	3.07106500	-6.17374700	C	-4.36521300	-1.29631000	3.04279200
C	0.99851400	3.75184700	-2.84431600	H	-4.28674600	-0.97834000	4.08660000
H	0.77949700	3.19527600	-1.93143600	H	-5.42167500	-1.24110400	2.76057100
H	0.16476000	4.43168600	-3.04075400	H	-3.79939100	-0.59418100	2.42960500
H	1.89934400	4.34600400	-2.67507000	C	-4.63185600	-3.70464400	3.67549100
C	6.09808800	3.04970700	-2.20611700	H	-4.23000300	-4.71704100	3.57667900
H	6.35944200	3.28153000	-1.16865500	H	-5.67036500	-3.71676900	3.33243600
H	6.70585300	3.69554700	-2.84986900	H	-4.64274200	-3.44270400	4.73711000
H	6.37928800	2.01351800	-2.40478500	C	-1.30515100	-5.46248600	2.28150300
C	4.61622400	3.26929300	-2.48703900	H	-2.23775400	-5.91374100	1.90950300
H	4.39835100	4.34753200	-2.43081000	H	-1.50842700	-5.15313800	3.30793400
H	4.39911800	2.97825800	-3.51604100	C	-3.96743800	-3.09073800	1.36976500
C	3.73135100	2.84336700	-0.20996900	H	-3.34130400	-2.46399600	0.73184200
H	4.63401000	2.42381000	0.26628100	H	-5.00946700	-2.95792900	1.06494100
H	2.87820900	2.32180500	0.23006800	H	-3.69591000	-4.13441400	1.20447000
C	3.65378000	4.32858400	0.11327000	N	-0.86796700	-1.58295300	1.23556400
H	2.76361900	4.78284400	-0.32786700	C	-2.10074800	-2.72877500	4.66423900
H	4.52974200	4.88222700	-0.24124400	H	-2.23758300	-3.71893700	5.12702500
H	3.60163700	4.46803900	1.19675500	H	-2.74461200	-2.02215400	5.19939100
P	-2.73749500	-1.28132400	-2.23582600	P	-2.75097500	1.03065400	-2.24771600
N	-1.69980700	-0.75925900	-1.23380900	N	-2.76500100	2.40763300	-3.25005800
N	-3.70249300	-2.54857000	-1.62744400	N	-2.90592400	0.00000000	-3.61553600
N	-2.27041800	-1.86821700	-3.77929000	N	-4.26924000	0.99893200	-1.51197900
N	-3.90096600	-0.22039300	-2.99069300	C	-4.43793300	0.64529900	-0.11542000
C	-2.82389500	-1.12928300	-4.88857700	H	-4.89717500	-0.35067900	-0.02722900
H	-3.60825900	-1.70779900	-5.40691900	H	-3.43493300	0.55905400	0.30652800
H	-2.05908200	-0.87858600	-5.63415300	C	-2.82596900	-1.47276900	-3.56252200
C	-3.41043000	0.14523100	-4.30591600	C	-3.28881900	-1.98858400	-2.20287700
H	-2.63461300	0.92362700	-4.26608600	H	-4.30946900	-1.67486900	-1.98055300
H	-4.22202100	0.51395300	-4.94116300	H	-3.26384100	-3.08101500	-2.20788300
C	-4.57434100	0.84349000	-2.22331600	H	-2.64157300	-1.64354100	-1.39351700
C	-5.83266700	1.27736700	-2.98312200	C	-2.71122000	3.81823800	-2.83908000
H	-5.59733600	1.78738700	-3.92175100	C	-2.30109600	0.64943300	-4.76401800
H	-6.41465500	1.97648700	-2.37432100	H	-1.20300200	0.58022700	-4.75184600
H	-6.46205800	0.41215500	-3.21211700	H	-2.65557900	0.20446200	-5.69785000
C	-3.67148900	2.05755500	-1.98935300	C	-1.40106800	-1.96887800	-3.82000400

H	-2.78146400	1.75945300	-1.43131600	H	-0.69084600	-1.53486700	-3.11053900
H	-4.20129900	2.82101000	-1.41083300	H	-1.36061500	-3.05700500	-3.72279700
H	-3.35733500	2.52245000	-2.92899500	H	-1.06583400	-1.72536400	-4.83315000
C	-5.00473100	0.30073600	-0.86295300	C	-5.26093600	1.64331600	0.68730600
H	-5.65213900	-0.57154900	-0.96451600	H	-6.29129000	1.72299200	0.32753700
H	-5.55530700	1.07523800	-0.32007900	H	-5.31008600	1.32497400	1.73243700
H	-4.13457300	0.02322000	-0.26576900	H	-4.81772100	2.64080500	0.66036100
C	-1.17734600	-2.81158000	-4.03285900	C	-3.76294800	-2.04594100	-4.63175100
C	0.13345000	-2.05619000	-4.27332700	H	-3.46607800	-1.75342000	-5.64285200
H	0.05270100	-1.38263900	-5.13322900	H	-3.75367500	-3.13959000	-4.59708900
H	0.95637000	-2.75161600	-4.47413600	H	-4.78828200	-1.70485800	-4.46826800
H	0.38608000	-1.45464800	-3.39687900	C	-6.51956000	0.21001800	-2.28975300
C	-1.51796200	-3.66621400	-5.25907000	H	-6.13726200	-0.70645200	-2.74455000
H	-2.46697900	-4.19117500	-5.11273800	H	-6.87303100	-0.03452200	-1.28414900
H	-0.73583800	-4.41460800	-5.42008500	H	-7.38841100	0.53509800	-2.87019900
H	-1.59449300	-3.07106500	-6.17374700	C	-1.29631000	4.36521300	-3.04279200
C	-0.99851400	-3.75184700	-2.84431600	H	-0.97834000	4.28674600	-4.08660000
H	-0.77949700	-3.19527600	-1.93143600	H	-1.24110400	5.42167500	-2.76057100
H	-0.16476000	-4.43168600	-3.04075400	H	-0.59418100	3.79939100	-2.42960500
H	-1.89934400	-4.34600400	-2.67507000	C	-3.70464400	4.63185600	-3.67549100
C	-6.09808800	-3.04970700	-2.20611700	H	-4.71704100	4.23000300	-3.57667900
H	-6.37928800	-2.01351800	-2.40478500	H	-3.71676900	5.67036500	-3.33243600
H	-6.35944200	-3.28153000	-1.16865500	H	-3.44270400	4.64274200	-4.73711000
H	-6.70585300	-3.69554700	-2.84986900	C	-5.46248600	1.30515100	-2.28150300
C	-4.61622400	-3.26929300	-2.48703900	H	-5.91374100	2.23775400	-1.90950300
H	-4.39835100	-4.34753200	-2.43081000	H	-5.15313800	1.50842700	-3.30793400
H	-4.39911800	-2.97825800	-3.51604100	C	-3.09073800	3.96743800	-1.36976500
C	-3.73135100	-2.84336700	-0.20996900	H	-2.46399600	3.34130400	-0.73184200
H	-4.63401000	-2.42381000	0.26628100	H	-2.95792900	5.00946700	-1.06494100
H	-2.87820900	-2.32180500	0.23006800	H	-4.13441400	3.69591000	-1.20447000
C	-3.65378000	-4.32858400	0.11327000	N	-1.58295300	0.86796700	-1.23556400
H	-4.52974200	-4.88222700	-0.24124400	C	-2.72877500	2.10074800	-4.66423900
H	-3.60163700	-4.46803900	1.19675500	H	-3.71893700	2.23758300	-5.12702500
H	-2.76361900	-4.78284400	-0.32786700	H	-2.02215400	2.74461200	-5.19939100
P	1.47314000	-2.73846500	2.16523000	P	2.75097500	-1.03065400	-2.24771600
N	0.76173300	-1.66581600	1.33170000	N	2.76500100	-2.40763300	-3.25005800
N	0.49328200	-3.40085400	3.39519700	N	2.90592400	0.00000000	-3.61553600
N	2.97747000	-2.40071700	2.98495600	N	4.26924000	-0.99893200	-1.51197900
N	2.17947000	-4.12667700	1.43765900	C	4.43793300	-0.64529900	-0.11542000
C	4.06560200	-2.91992900	2.17829300	H	4.89717500	0.35067900	-0.02722900
H	4.98402900	-3.01787000	2.76568700	H	3.43493300	-0.55905400	0.30652800
H	4.28452400	-2.28494800	1.30631400	C	2.82596900	1.47276900	-3.56252200
C	3.58746000	-4.27965900	1.70966000	C	3.28881900	1.98858400	-2.20287700
H	4.14304200	-4.59135000	0.81647300	H	4.30946900	1.67486900	-1.98055300
H	3.77660900	-5.03440000	2.49393900	H	3.26384100	3.08101500	-2.20788300
C	1.51643600	-5.12562200	0.59263600	H	2.64157300	1.64354100	-1.39351700
C	1.87107900	-6.53854900	1.07476300	C	2.71122000	-3.81823800	-2.83908000
H	2.94121400	-6.74863700	0.98322000	C	2.30109600	-0.64943300	-4.76401800
H	1.33879500	-7.28374200	0.47507600	H	1.20300200	-0.58022700	-4.75184600
H	1.58405200	-6.67703800	2.12093900	H	2.65557900	-0.20446200	-5.69785000
C	1.96737800	-4.96557800	-0.86305500	C	1.40106800	1.96887800	-3.82000400
H	1.69209400	-3.97815000	-1.23480500	H	0.69084600	1.53486700	-3.11053900
H	1.49827500	-5.72289500	-1.50056900	H	1.36061500	3.05700500	-3.72279700
H	3.05089700	-5.07658700	-0.96609000	H	1.06583400	1.72536400	-4.83315000
C	0.00000000	-4.96708300	0.65396800	C	5.26093600	-1.64331600	0.68730600
H	-0.38114100	-5.21043900	1.64702200	H	6.29129000	-1.72299200	0.32753700
H	-0.46268900	-5.64437300	-0.06989200	H	5.31008600	-1.32497400	1.73243700
H	-0.30204300	-3.94439800	0.41806500	H	4.81772100	-2.64080500	0.66036100
C	3.21074100	-1.10464700	3.65047300	C	3.76294800	2.04594100	-4.63175100
C	3.60798700	-0.00670100	2.65818600	H	3.46607800	1.75342000	-5.64285200
H	4.57331200	-0.21502300	2.18789700	H	3.75367500	3.13959000	-4.59708900
H	3.69601600	0.95950100	3.16546200	H	4.78828200	1.70485800	-4.46826800

H	2.85563000	0.07987200	1.87126500	C	6.51956000	-0.21001800	-2.28975300
C	4.32518700	-1.28052400	4.68809200	H	6.13726200	0.70645200	-2.74455000
H	4.07784800	-2.08662700	5.38505800	H	6.87303100	0.03452200	-1.28414900
H	4.45341100	-0.35612000	5.26020500	H	7.38841100	-0.53509800	-2.87019900
H	5.29058300	-1.51049700	4.22803500	C	1.29631000	-4.36521300	-3.04279200
C	1.94767300	-0.66960100	4.38960900	H	0.97834000	-4.28674600	-4.08660000
H	1.12810500	-0.48870900	3.69215300	H	1.24110400	-5.42167500	-2.76057100
H	2.14320400	0.26039300	4.93068000	H	0.59418100	-3.79939100	-2.42960500
H	1.62944800	-1.42430300	5.11096600	C	3.70464400	-4.63185600	-3.67549100
C	1.16475300	-4.20343400	5.67860700	H	4.71704100	-4.23000300	-3.57667900
H	0.25931000	-3.81709300	6.15672100	H	3.71676900	-5.67036500	-3.33243600
H	1.95864700	-3.46469300	5.80715000	H	3.44270400	-4.64274200	-4.73711000
H	1.45692400	-5.11254600	6.21582500	C	5.46248600	-1.30515100	-2.28150300
C	0.94924500	-4.51129400	4.20160500	H	5.91374100	-2.23775400	-1.90950300
H	1.88844200	-4.86727800	3.77565500	H	5.15313800	-1.50842700	-3.30793400
H	0.24105800	-5.35127900	4.11184100	C	3.09073800	-3.96743800	-1.36976500
C	-0.75963600	-2.77447100	3.75510000	H	2.46399600	-3.34130400	-0.73184200
H	-0.96187700	-2.03340200	2.97921300	H	2.95792900	-5.00946700	-1.06494100
H	-0.66488600	-2.21874300	4.70226400	H	4.13441400	-3.69591000	-1.20447000
C	-1.93126600	-3.74058700	3.86554500	N	1.58295300	-0.86796700	-1.23556400
H	-2.85182900	-3.18685400	4.07604800	C	2.72877500	-2.10074800	-4.66423900
H	-1.80191500	-4.47058700	4.67183000	H	3.71893700	-2.23758300	-5.12702500
H	-2.07711500	-4.29037400	2.93268800	H	2.02215400	-2.74461200	-5.19939100

Tb L_3-edge XANES

Table S17. Summary of fit parameters for Tb L_3-edge XANES of **3** and **4**.

Complex	Peak 1		Peak 2		Peak 3	
	Intensity	Energy (eV)	Intensity	Energy (eV)	Intensity	Energy (eV)
3	4.34(4)	7519.20(4)	NA	NA	NA	NA
4	1.84(3)	7512.0(2)	3.48(3)	7520.30(3)	4.25(5)	7528.50(3)

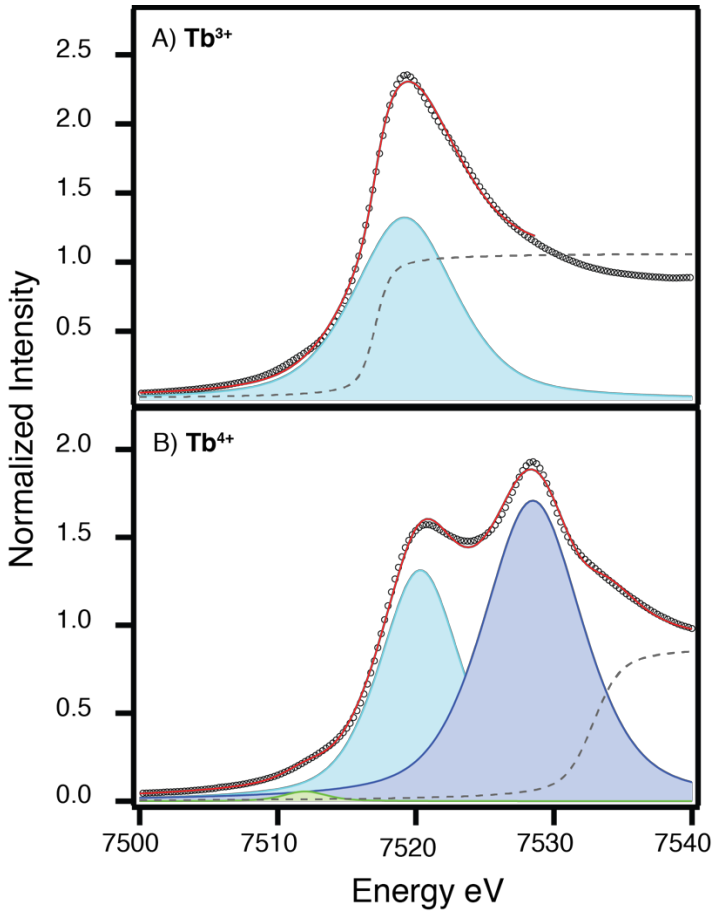

Figure S46. Tb L_3-edge XAS experimental data (black) obtained for **3**(A) and **4** (B) and the pseudo-Voigt [blue (p2) and purple (p3)] and steplike functions (gray dashed line), which sum to generate the curve fit (red). The shoulder feature observed near the edge onset has little intensity in **4** and is modeled with a single function [green (p1)] that is barely visible in the baseline of the spectrum.

Table S18. Normalized and Background Subtracted L_3-edge XAS of **3** and **4.**

3_TbL3_eV	3_TbL3_Int	4_TbL3_eV	3_TbL3_Int
6881.881	8.99E-03	6881.74	8.25E-03
6891.8785	8.03E-03	6891.7375	7.77E-03
6901.882	7.67E-03	6901.741	7.26E-03
6911.8815	7.37E-03	6911.7405	6.54E-03
6921.878	6.50E-03	6921.737	6.50E-03
6931.8795	6.22E-03	6931.7385	6.81E-03
6941.882	5.29E-03	6941.741	4.98E-03
6951.88	5.73E-03	6951.739	5.36E-03
6961.8785	6.23E-03	6961.7375	5.94E-03
6971.882	4.87E-03	6971.741	4.40E-03
6981.881	5.14E-03	6981.74	6.52E-03

6991.8795	5.39E-03	6991.7385	7.08E-03
7001.8824	5.10E-03	7001.7414	7.04E-03
7011.88	5.19E-03	7011.739	7.38E-03
7021.8815	4.40E-03	7021.7405	8.10E-03
7031.8776	4.12E-03	7031.7366	8.05E-03
7041.8776	3.92E-03	7041.7366	7.82E-03
7051.881	3.99E-03	7051.74	7.45E-03
7061.8785	4.14E-03	7061.7375	7.43E-03
7071.879	4.54E-03	7071.738	7.54E-03
7081.878	3.69E-03	7081.737	7.04E-03
7091.88	3.56E-03	7091.739	7.41E-03
7092.132	3.99E-03	7091.991	7.64E-03
7092.3785	4.44E-03	7092.2375	8.15E-03
7092.6305	4.07E-03	7092.4895	7.81E-03
7092.8776	4.24E-03	7092.7366	7.75E-03
7093.1295	4.39E-03	7092.9885	7.68E-03
7093.3815	4.35E-03	7093.2405	7.80E-03
7093.6285	4.31E-03	7093.4875	7.91E-03
7093.8805	4.32E-03	7093.7395	7.90E-03
7094.1324	4.08E-03	7093.9914	8.11E-03
7094.3795	4.21E-03	7094.2385	8.00E-03
7094.6315	4.20E-03	7094.4905	8.00E-03
7094.8785	4.21E-03	7094.7375	7.93E-03
7095.1305	4.24E-03	7094.9895	7.87E-03
7095.378	4.40E-03	7095.237	8.32E-03
7095.63	4.32E-03	7095.489	8.06E-03
7095.882	4.53E-03	7095.741	8.01E-03
7096.129	4.18E-03	7095.988	8.18E-03
7096.3815	4.30E-03	7096.2405	8.07E-03
7096.6285	4.55E-03	7096.4875	8.08E-03
7096.881	4.41E-03	7096.74	7.80E-03
7097.128	4.32E-03	7096.987	8.09E-03
7097.3805	4.77E-03	7097.2395	7.38E-03
7097.6276	4.59E-03	7097.4866	7.22E-03
7097.88	4.10E-03	7097.739	6.93E-03
7098.1324	3.86E-03	7097.9914	7.14E-03
7098.3795	3.94E-03	7098.2385	7.42E-03
7098.632	3.96E-03	7098.491	7.33E-03
7098.8795	4.09E-03	7098.7385	7.40E-03
7099.132	4.30E-03	7098.991	6.90E-03

7099.3795	4.08E-03	7099.2385	6.33E-03
7099.632	4.11E-03	7099.491	6.32E-03
7099.8795	4.27E-03	7099.7385	6.21E-03
7100.132	4.55E-03	7099.991	6.50E-03
7100.3795	3.67E-03	7100.2385	6.57E-03
7100.632	3.18E-03	7100.491	6.69E-03
7100.8795	3.75E-03	7100.7385	6.37E-03
7101.132	3.83E-03	7100.991	6.87E-03
7101.3795	3.69E-03	7101.2385	7.53E-03
7101.6324	3.74E-03	7101.4914	7.77E-03
7101.88	3.81E-03	7101.739	8.16E-03
7102.1276	5.05E-03	7101.9866	7.90E-03
7102.3805	5.13E-03	7102.2395	7.50E-03
7102.628	5.01E-03	7102.487	6.77E-03
7102.8805	5.07E-03	7102.7395	6.75E-03
7103.1285	5.07E-03	7102.9875	6.50E-03
7103.381	5.02E-03	7103.24	6.60E-03
7103.629	4.76E-03	7103.488	6.61E-03
7103.882	4.05E-03	7103.741	6.53E-03
7104.1295	4.44E-03	7103.9885	6.36E-03
7104.3776	4.55E-03	7104.2366	6.45E-03
7104.6305	4.83E-03	7104.4895	5.68E-03
7104.8785	4.82E-03	7104.7375	5.64E-03
7105.131	4.77E-03	7104.99	5.79E-03
7105.379	4.79E-03	7105.238	5.62E-03
7105.632	4.67E-03	7105.491	5.24E-03
7105.88	4.58E-03	7105.739	5.57E-03
7106.128	4.75E-03	7105.987	5.65E-03
7106.381	4.62E-03	7106.24	4.86E-03
7106.629	4.62E-03	7106.488	4.37E-03
7106.882	4.67E-03	7106.741	4.38E-03
7107.1305	4.40E-03	7106.9895	4.94E-03
7107.3785	3.89E-03	7107.2375	4.60E-03
7107.6315	3.90E-03	7107.4905	4.31E-03
7107.8795	3.95E-03	7107.7385	4.62E-03
7108.128	3.85E-03	7107.987	4.52E-03
7108.381	3.81E-03	7108.24	4.96E-03
7108.629	3.85E-03	7108.488	4.36E-03
7108.8824	4.39E-03	7108.7414	4.44E-03
7109.1305	5.44E-03	7108.9895	3.99E-03

7109.379	5.88E-03	7109.238	4.08E-03
7109.632	5.74E-03	7109.491	4.23E-03
7109.8805	5.73E-03	7109.7395	4.06E-03
7110.129	5.76E-03	7109.988	4.11E-03
7110.382	5.76E-03	7110.241	4.61E-03
7110.6305	5.40E-03	7110.4895	4.35E-03
7110.879	5.18E-03	7110.738	4.56E-03
7111.1324	5.31E-03	7110.9914	4.02E-03
7111.3805	5.31E-03	7111.2395	3.84E-03
7111.629	6.20E-03	7111.488	4.13E-03
7111.8776	6.47E-03	7111.7366	4.52E-03
7112.131	6.50E-03	7111.99	4.79E-03
7112.3795	6.47E-03	7112.2385	4.97E-03
7112.628	5.67E-03	7112.487	5.42E-03
7112.8815	5.73E-03	7112.7405	5.35E-03
7113.1305	5.84E-03	7112.9895	5.73E-03
7113.379	6.15E-03	7113.238	5.58E-03
7113.6324	6.15E-03	7113.4914	4.67E-03
7113.881	6.79E-03	7113.74	5.22E-03
7114.1295	6.96E-03	7113.9885	4.30E-03
7114.3785	6.98E-03	7114.2375	4.39E-03
7114.632	6.76E-03	7114.491	5.44E-03
7114.881	5.92E-03	7114.74	5.01E-03
7115.1295	6.08E-03	7114.9885	4.76E-03
7115.3785	5.86E-03	7115.2375	6.18E-03
7115.632	6.20E-03	7115.491	6.38E-03
7115.881	6.09E-03	7115.74	6.52E-03
7116.1295	6.22E-03	7115.9885	7.55E-03
7116.3785	6.43E-03	7116.2375	8.14E-03
7116.6324	6.13E-03	7116.4914	8.47E-03
7116.881	5.36E-03	7116.74	8.77E-03
7117.13	5.54E-03	7116.989	8.74E-03
7117.379	6.23E-03	7117.238	7.78E-03
7117.628	6.30E-03	7117.487	7.97E-03
7117.882	6.33E-03	7117.741	7.84E-03
7118.131	6.29E-03	7117.99	8.19E-03
7118.38	6.43E-03	7118.239	8.19E-03
7118.629	6.60E-03	7118.488	7.93E-03
7118.878	6.60E-03	7118.737	7.45E-03
7119.132	6.45E-03	7118.991	7.25E-03

7119.381	6.45E-03	7119.24	7.75E-03
7119.63	6.53E-03	7119.489	6.59E-03
7119.8795	6.74E-03	7119.7385	6.44E-03
7120.1285	6.88E-03	7119.9875	7.33E-03
7120.3776	7.00E-03	7120.2366	7.75E-03
7120.632	6.67E-03	7120.491	8.26E-03
7120.881	6.28E-03	7120.74	8.52E-03
7121.13	6.88E-03	7120.989	8.23E-03
7121.3795	6.58E-03	7121.2385	8.15E-03
7121.6285	6.53E-03	7121.4875	8.10E-03
7121.878	6.54E-03	7121.737	8.13E-03
7122.132	6.63E-03	7121.991	8.16E-03
7122.3815	6.48E-03	7122.2405	8.39E-03
7122.631	6.20E-03	7122.49	8.66E-03
7122.8805	6.37E-03	7122.7395	8.69E-03
7123.1295	6.50E-03	7122.9885	8.74E-03
7123.379	6.78E-03	7123.238	8.69E-03
7123.6285	6.78E-03	7123.4875	8.72E-03
7123.878	6.95E-03	7123.737	9.89E-03
7124.1324	7.05E-03	7123.9914	9.88E-03
7124.382	7.07E-03	7124.241	1.01E-02
7124.6315	7.11E-03	7124.4905	1.03E-02
7124.881	7.80E-03	7124.74	9.90E-03
7125.1305	7.71E-03	7124.9895	9.72E-03
7125.38	8.25E-03	7125.239	9.71E-03
7125.6295	8.84E-03	7125.4885	9.82E-03
7125.879	8.82E-03	7125.738	9.90E-03
7126.129	8.99E-03	7125.988	1.01E-02
7126.3785	8.84E-03	7126.2375	1.12E-02
7126.628	8.87E-03	7126.487	1.17E-02
7126.878	8.99E-03	7126.737	1.14E-02
7127.1324	9.25E-03	7126.9914	1.16E-02
7127.382	9.22E-03	7127.241	1.22E-02
7127.632	9.36E-03	7127.491	1.14E-02
7127.8815	9.35E-03	7127.7405	1.23E-02
7128.1315	9.29E-03	7127.9905	1.23E-02
7128.3815	9.46E-03	7128.2405	1.26E-02
7128.631	9.72E-03	7128.49	1.27E-02
7128.881	9.77E-03	7128.74	1.26E-02
7129.131	1.03E-02	7128.99	1.25E-02

7129.3805	1.04E-02	7129.2395	1.27E-02
7129.6305	1.05E-02	7129.4895	1.26E-02
7129.8805	1.12E-02	7129.7395	1.29E-02
7130.1305	1.10E-02	7129.9895	1.41E-02
7130.3805	1.11E-02	7130.2395	1.38E-02
7130.6305	1.11E-02	7130.4895	1.39E-02
7130.8805	1.10E-02	7130.7395	1.37E-02
7131.1305	1.06E-02	7130.9895	1.36E-02
7131.3805	1.12E-02	7131.2395	1.35E-02
7131.6305	1.11E-02	7131.4895	1.38E-02
7131.8805	1.12E-02	7131.7395	1.42E-02
7132.131	1.08E-02	7131.99	1.37E-02
7132.381	1.08E-02	7132.24	1.37E-02
7132.631	1.10E-02	7132.49	1.40E-02
7132.8815	1.07E-02	7132.7405	1.39E-02
7133.1315	1.08E-02	7132.9905	1.40E-02
7133.3815	1.07E-02	7133.2405	1.39E-02
7133.632	1.04E-02	7133.491	1.41E-02
7133.882	1.01E-02	7133.741	1.42E-02
7134.1324	9.93E-03	7133.9914	1.39E-02
7134.3776	9.99E-03	7134.2366	1.42E-02
7134.628	9.73E-03	7134.487	1.42E-02
7134.8785	9.65E-03	7134.7375	1.59E-02
7135.1285	9.66E-03	7134.9875	1.63E-02
7135.379	1.06E-02	7135.238	1.64E-02
7135.6295	1.10E-02	7135.4885	1.60E-02
7135.88	1.07E-02	7135.739	1.53E-02
7136.1305	1.01E-02	7135.9895	1.46E-02
7136.3805	9.68E-03	7136.2395	1.50E-02
7136.631	9.63E-03	7136.49	1.53E-02
7136.8815	9.87E-03	7136.7405	1.52E-02
7137.132	9.71E-03	7136.991	1.57E-02
7137.3776	9.64E-03	7137.2366	1.55E-02
7137.6285	9.71E-03	7137.4875	1.57E-02
7137.879	9.65E-03	7137.738	1.69E-02
7138.1295	9.59E-03	7137.9885	1.73E-02
7138.38	9.72E-03	7138.239	1.70E-02
7138.6305	1.03E-02	7138.4895	1.55E-02
7138.8815	1.03E-02	7138.7405	1.55E-02
7139.132	1.04E-02	7138.991	1.53E-02

7139.3776	1.07E-02	7139.2366	1.56E-02
7139.6285	1.07E-02	7139.4875	1.53E-02
7139.879	1.07E-02	7139.738	1.54E-02
7140.13	1.06E-02	7139.989	1.54E-02
7140.3805	1.07E-02	7140.2395	1.52E-02
7140.6315	1.06E-02	7140.4905	1.52E-02
7140.8824	1.05E-02	7140.7414	1.52E-02
7141.128	9.60E-03	7140.987	1.47E-02
7141.379	9.13E-03	7141.238	1.51E-02
7141.63	8.86E-03	7141.489	1.46E-02
7141.8805	8.75E-03	7141.7395	1.52E-02
7144.878	8.71E-03	7144.737	1.43E-02
7147.878	8.43E-03	7147.737	1.39E-02
7150.881	7.85E-03	7150.74	1.37E-02
7153.882	7.47E-03	7153.741	1.33E-02
7156.881	8.01E-03	7156.74	1.40E-02
7159.8776	7.81E-03	7159.7366	1.36E-02
7162.882	7.51E-03	7162.741	1.37E-02
7165.8795	7.63E-03	7165.7385	1.36E-02
7168.8795	7.27E-03	7168.7385	1.36E-02
7171.878	7.13E-03	7171.737	1.34E-02
7174.879	7.06E-03	7174.738	1.34E-02
7177.8776	7.37E-03	7177.7366	1.32E-02
7180.879	6.88E-03	7180.738	1.24E-02
7183.8785	6.97E-03	7183.7375	1.26E-02
7186.881	6.91E-03	7186.74	1.14E-02
7189.881	6.62E-03	7189.74	1.20E-02
7192.879	6.72E-03	7192.738	1.19E-02
7195.88	6.50E-03	7195.739	1.18E-02
7198.8785	6.14E-03	7198.7375	1.15E-02
7201.88	5.96E-03	7201.739	1.07E-02
7204.879	5.57E-03	7204.738	1.01E-02
7207.881	5.50E-03	7207.74	1.08E-02
7210.881	5.22E-03	7210.74	1.04E-02
7213.8785	5.16E-03	7213.7375	1.06E-02
7216.8785	5.15E-03	7216.7375	1.12E-02
7219.882	5.67E-03	7219.741	1.13E-02
7222.878	5.35E-03	7222.737	1.04E-02
7225.8815	4.91E-03	7225.7405	1.18E-02
7228.878	4.78E-03	7228.737	1.19E-02

7231.8824	4.35E-03	7231.7414	1.10E-02
7234.8795	3.94E-03	7234.7385	1.09E-02
7237.879	4.04E-03	7237.738	1.10E-02
7240.882	3.82E-03	7240.741	1.04E-02
7243.882	3.16E-03	7243.741	1.04E-02
7246.88	2.60E-03	7246.739	1.02E-02
7249.881	2.35E-03	7249.74	1.04E-02
7252.8795	2.27E-03	7252.7385	9.07E-03
7255.881	2.13E-03	7255.74	9.81E-03
7258.8795	1.28E-03	7258.7385	9.52E-03
7261.8815	1.59E-03	7261.7405	9.83E-03
7264.881	6.64E-04	7264.74	9.62E-03
7267.878	1.23E-05	7267.737	9.58E-03
7270.878	-4.08E-04	7270.737	9.02E-03
7273.8805	-6.83E-04	7273.7395	8.89E-03
7276.881	-2.38E-04	7276.74	9.69E-03
7279.879	-6.92E-04	7279.738	1.00E-02
7282.88	-1.44E-04	7282.739	1.01E-02
7285.878	-1.46E-04	7285.737	9.78E-03
7288.8795	-5.94E-04	7288.7385	9.62E-03
7291.878	-1.76E-03	7291.737	9.38E-03
7294.8795	-2.14E-03	7294.7385	8.45E-03
7297.879	-3.42E-03	7297.738	8.97E-03
7300.881	-4.39E-03	7300.74	8.63E-03
7303.8805	-4.33E-03	7303.7395	8.42E-03
7306.8824	-4.40E-03	7306.7414	7.99E-03
7309.8824	-4.48E-03	7309.7414	7.73E-03
7312.88	-3.93E-03	7312.739	8.00E-03
7315.88	-4.10E-03	7315.739	7.75E-03
7318.878	-4.66E-03	7318.737	7.01E-03
7321.8785	-4.68E-03	7321.7375	6.28E-03
7324.8815	-3.69E-03	7324.7405	6.07E-03
7327.8824	-3.70E-03	7327.7414	6.13E-03
7330.881	-3.65E-03	7330.74	4.50E-03
7333.882	-3.04E-03	7333.741	4.52E-03
7336.8805	-3.14E-03	7336.7395	4.21E-03
7339.882	-3.39E-03	7339.741	4.03E-03
7342.881	-3.61E-03	7342.74	4.18E-03
7345.8776	-3.53E-03	7345.7366	3.46E-03
7348.882	-2.88E-03	7348.741	3.68E-03

7351.8785	-3.20E-03	7351.7375	3.77E-03
7354.878	-3.30E-03	7354.737	3.40E-03
7357.88	-3.48E-03	7357.739	3.15E-03
7360.8795	-3.59E-03	7360.7385	3.26E-03
7363.882	-3.42E-03	7363.741	3.16E-03
7366.882	-3.68E-03	7366.741	1.77E-03
7369.879	-4.13E-03	7369.738	1.45E-03
7372.879	-4.48E-03	7372.738	1.27E-03
7375.882	-3.94E-03	7375.741	1.14E-03
7378.882	-4.52E-03	7378.741	9.10E-04
7381.8795	-4.70E-03	7381.7385	5.43E-04
7384.88	-5.08E-03	7384.739	5.77E-04
7387.8776	-5.12E-03	7387.7366	3.57E-04
7390.878	-5.42E-03	7390.737	-3.49E-04
7393.8815	-5.39E-03	7393.7405	-6.08E-04
7396.882	-5.35E-03	7396.741	-5.80E-04
7399.88	-5.10E-03	7399.739	3.14E-04
7402.8805	-5.23E-03	7402.7395	3.17E-04
7405.879	-5.18E-03	7405.738	9.56E-04
7408.8795	-5.40E-03	7408.7385	3.75E-04
7411.878	-5.56E-03	7411.737	-7.32E-04
7414.8785	-5.67E-03	7414.7375	-6.42E-04
7417.8824	-5.58E-03	7417.7414	-4.53E-04
7420.878	-5.33E-03	7420.737	-6.09E-04
7423.8815	-4.91E-03	7423.7405	3.41E-04
7426.8776	-4.81E-03	7426.7366	6.76E-04
7429.881	-5.03E-03	7429.74	3.73E-05
7432.882	-5.20E-03	7432.741	-1.10E-04
7435.8805	-5.39E-03	7435.7395	1.12E-03
7438.8815	-5.20E-03	7438.7405	1.17E-03
7441.88	-4.66E-03	7441.739	1.43E-03
7444.881	-4.21E-03	7444.74	1.69E-03
7447.8795	-3.53E-03	7447.7385	2.00E-03
7450.8805	-3.33E-03	7450.7395	2.25E-03
7453.879	-3.22E-03	7453.738	2.83E-03
7456.88	-3.14E-03	7456.739	3.78E-03
7459.8785	-2.34E-03	7459.7375	4.12E-03
7462.8795	-1.78E-03	7462.7385	4.92E-03
7465.878	-7.61E-04	7465.737	5.61E-03
7468.879	4.07E-05	7468.738	6.37E-03

7471.8824	1.16E-03	7471.7414	7.19E-03
7474.878	2.64E-03	7474.737	8.43E-03
7477.8815	4.03E-03	7477.7405	1.06E-02
7480.8824	6.23E-03	7480.7414	1.25E-02
7483.8805	8.81E-03	7483.7395	1.46E-02
7484.132	8.24E-03	7483.991	1.47E-02
7484.3776	7.91E-03	7484.2366	1.50E-02
7484.629	8.25E-03	7484.488	1.48E-02
7484.8805	8.67E-03	7484.7395	1.51E-02
7485.132	9.01E-03	7484.991	1.58E-02
7485.3776	9.18E-03	7485.2366	1.59E-02
7485.629	9.64E-03	7485.488	1.62E-02
7485.8805	9.75E-03	7485.7395	1.65E-02
7486.132	1.03E-02	7485.991	1.65E-02
7486.378	1.05E-02	7486.237	1.69E-02
7486.6295	1.06E-02	7486.4885	1.68E-02
7486.881	1.07E-02	7486.74	1.76E-02
7487.1271	1.14E-02	7486.9861	1.78E-02
7487.379	1.16E-02	7487.238	1.80E-02
7487.6305	1.20E-02	7487.4895	1.85E-02
7487.882	1.23E-02	7487.741	1.87E-02
7488.128	1.27E-02	7487.987	1.87E-02
7488.38	1.32E-02	7488.239	1.89E-02
7488.6315	1.37E-02	7488.4905	1.91E-02
7488.8776	1.40E-02	7488.7366	1.93E-02
7489.1295	1.41E-02	7488.9885	1.94E-02
7489.381	1.48E-02	7489.24	2.02E-02
7489.6276	1.49E-02	7489.4866	2.05E-02
7489.879	1.53E-02	7489.738	2.07E-02
7490.131	1.53E-02	7489.99	2.06E-02
7490.3829	1.55E-02	7490.2419	2.14E-02
7490.629	1.62E-02	7490.488	2.16E-02
7490.881	1.55E-02	7490.74	2.21E-02
7491.1271	1.61E-02	7490.9861	2.25E-02
7491.379	1.66E-02	7491.238	2.29E-02
7491.631	1.70E-02	7491.49	2.32E-02
7491.8776	1.78E-02	7491.7366	2.41E-02
7492.1295	1.82E-02	7491.9885	2.44E-02
7492.3815	1.87E-02	7492.2405	2.48E-02
7492.628	1.91E-02	7492.487	2.52E-02

7492.88	1.95E-02	7492.739	2.56E-02
7493.132	2.05E-02	7492.991	2.65E-02
7493.3785	2.12E-02	7493.2375	2.68E-02
7493.6305	2.18E-02	7493.4895	2.68E-02
7493.8824	2.27E-02	7493.7414	2.67E-02
7494.129	2.32E-02	7493.988	2.77E-02
7494.381	2.35E-02	7494.24	2.99E-02
7494.6276	2.42E-02	7494.4866	2.95E-02
7494.88	2.50E-02	7494.739	2.96E-02
7495.132	2.57E-02	7494.991	3.03E-02
7495.3785	2.66E-02	7495.2375	3.13E-02
7495.631	2.71E-02	7495.49	3.22E-02
7495.8776	2.76E-02	7495.7366	3.23E-02
7496.13	2.94E-02	7495.989	3.25E-02
7496.382	3.02E-02	7496.241	3.20E-02
7496.629	3.10E-02	7496.488	3.31E-02
7496.881	3.20E-02	7496.74	3.52E-02
7497.128	3.39E-02	7496.987	3.56E-02
7497.3805	3.55E-02	7497.2395	3.62E-02
7497.6324	3.70E-02	7497.4914	3.70E-02
7497.8795	3.80E-02	7497.7385	3.77E-02
7498.132	3.91E-02	7497.991	3.85E-02
7498.3785	4.10E-02	7498.2375	3.90E-02
7498.631	4.19E-02	7498.49	3.96E-02
7498.878	4.32E-02	7498.737	4.04E-02
7499.1305	4.46E-02	7498.9895	4.07E-02
7499.3776	4.61E-02	7499.2366	4.15E-02
7499.63	4.73E-02	7499.489	4.24E-02
7499.8824	4.87E-02	7499.7414	4.33E-02
7500.1295	5.03E-02	7499.9885	4.41E-02
7500.382	5.18E-02	7500.241	4.50E-02
7500.629	5.33E-02	7500.488	4.60E-02
7500.882	5.46E-02	7500.741	4.67E-02
7501.129	5.64E-02	7500.988	4.74E-02
7501.3815	5.78E-02	7501.2405	4.86E-02
7501.6285	5.95E-02	7501.4875	4.93E-02
7501.8815	6.15E-02	7501.7405	5.07E-02
7502.1285	6.34E-02	7501.9875	5.22E-02
7502.381	6.55E-02	7502.24	5.22E-02
7502.6285	6.74E-02	7502.4875	5.32E-02

7502.881	6.95E-02	7502.74	5.44E-02
7503.1285	7.15E-02	7502.9875	5.57E-02
7503.381	7.40E-02	7503.24	5.71E-02
7503.6285	7.61E-02	7503.4875	5.79E-02
7503.881	7.87E-02	7503.74	5.97E-02
7504.1285	8.15E-02	7503.9875	6.16E-02
7504.3815	8.42E-02	7504.2405	6.33E-02
7504.6285	8.70E-02	7504.4875	6.47E-02
7504.8815	8.99E-02	7504.7405	6.71E-02
7505.129	9.31E-02	7504.988	6.92E-02
7505.382	9.66E-02	7505.241	7.10E-02
7505.6295	0.10016511	7505.4885	7.32E-02
7505.8824	0.10385003	7505.7414	7.76E-02
7506.13	0.10792794	7505.989	8.00E-02
7506.3771	0.1120441	7506.2361	8.22E-02
7506.6305	0.11677193	7506.4895	8.45E-02
7506.878	0.12188348	7506.737	8.71E-02
7507.131	0.12690383	7506.99	9.03E-02
7507.3785	0.13172564	7507.2375	9.30E-02
7507.6315	0.13778136	7507.4905	9.66E-02
7507.879	0.14389869	7507.738	9.98E-02
7508.1324	0.1504027	7507.9914	0.1041356
7508.38	0.15725092	7508.239	0.10854797
7508.6276	0.16464096	7508.4866	0.11280535
7508.881	0.17373648	7508.74	0.11741849
7509.1285	0.18329261	7508.9875	0.12260055
7509.3815	0.19372481	7509.2405	0.1282532
7509.6295	0.20477011	7509.4885	0.13399226
7509.8824	0.2169477	7509.7414	0.14061587
7510.1305	0.2301936	7509.9895	0.14732811
7510.378	0.24398367	7510.237	0.1547655
7510.6315	0.25899366	7510.4905	0.16363626
7510.8795	0.27442305	7510.7385	0.17249556
7511.1329	0.29049903	7510.9919	0.18154182
7511.3805	0.30648521	7511.2395	0.19170033
7511.6285	0.32242349	7511.4875	0.2024197
7511.882	0.3391277	7511.741	0.21347595
7512.13	0.35602978	7511.989	0.22522294
7512.3776	0.37301515	7512.2366	0.23593695
7512.631	0.39217906	7512.49	0.24762862

7512.879	0.4127516	7512.738	0.25972517
7513.1324	0.43703399	7512.9914	0.27276108
7513.3805	0.46298442	7513.2395	0.2869753
7513.6285	0.49264853	7513.4875	0.30055441
7513.8824	0.52837159	7513.7414	0.31526914
7514.1305	0.567739	7513.9895	0.330348
7514.3785	0.61150436	7514.2375	0.3480076
7514.632	0.66443964	7514.491	0.36791968
7514.88	0.72236581	7514.739	0.38947341
7515.128	0.78851523	7514.987	0.41484755
7515.382	0.8657957	7515.241	0.44303948
7515.63	0.95016461	7515.489	0.47589151
7515.878	1.0442672	7515.737	0.51447021
7516.132	1.152439	7515.991	0.55850932
7516.38	1.2672395	7516.239	0.6091655
7516.6285	1.3898238	7516.4875	0.66585983
7516.8824	1.5217756	7516.7414	0.72947445
7517.1305	1.6538792	7516.9895	0.79785008
7517.379	1.78632	7517.238	0.87223466
7517.6324	1.9154792	7517.4914	0.95163801
7517.881	2.0308221	7517.74	1.0314846
7518.1295	2.1341045	7517.9885	1.111066
7518.3776	2.2184694	7518.2366	1.1887743
7518.6315	2.285376	7518.4905	1.2629806
7518.88	2.3288549	7518.739	1.329522
7519.1285	2.3501961	7518.9875	1.3890638
7519.3824	2.3549279	7519.2414	1.4412091
7519.631	2.3393706	7519.49	1.48258
7519.8795	2.3123253	7519.7385	1.5147959
7520.128	2.2758619	7519.987	1.5382799
7520.382	2.2333428	7520.241	1.5562866
7520.6305	2.1887194	7520.4895	1.5673747
7520.879	2.1435499	7520.738	1.5720363
7521.1276	2.1006304	7520.9866	1.5710504
7521.382	2.0582416	7521.241	1.5643735
7521.6305	2.017911	7521.4895	1.5547881
7521.879	1.97905	7521.738	1.5428819
7522.1276	1.940704	7521.9866	1.5310066
7522.382	1.9015424	7522.241	1.5182631
7522.6305	1.8620236	7522.4895	1.5081118

7522.879	1.8220044	7522.738	1.4981079
7523.128	1.7836277	7522.987	1.4906687
7523.3824	1.744184	7523.2414	1.4837692
7523.631	1.7032747	7523.49	1.4793667
7523.88	1.6629709	7523.739	1.478018
7524.1285	1.6233613	7523.9875	1.478475
7524.3776	1.5845661	7524.2366	1.4831657
7524.632	1.5460828	7524.491	1.4902322
7524.8805	1.510463	7524.7395	1.4986708
7525.1295	1.4750324	7524.9885	1.5088418
7525.3785	1.4436111	7525.2375	1.5264337
7525.6271	1.4119165	7525.4861	1.5442117
7525.882	1.3816971	7525.741	1.5689516
7526.1305	1.3543147	7525.9895	1.5975397
7526.3795	1.3283151	7526.2385	1.6314046
7526.6285	1.3037113	7526.4875	1.6702004
7526.8776	1.2790105	7526.7366	1.7119291
7527.132	1.2570327	7526.991	1.7559676
7527.381	1.236728	7527.24	1.7996295
7527.6305	1.2169782	7527.4895	1.8424082
7527.8795	1.197893	7527.7385	1.8792241
7528.1285	1.179987	7527.9875	1.9067655
7528.3776	1.1629217	7528.2366	1.9247427
7528.6324	1.1468984	7528.4914	1.929716
7528.8815	1.1304773	7528.7405	1.918385
7529.1305	1.1150176	7528.9895	1.8930509
7529.3795	1.1003308	7529.2385	1.8536428
7529.629	1.0863778	7529.488	1.8052595
7529.878	1.0736138	7529.737	1.7498789
7530.1276	1.0612633	7529.9866	1.694442
7530.382	1.0484457	7530.241	1.6376631
7530.6315	1.0371055	7530.4905	1.5870466
7530.881	1.026414	7530.74	1.5441202
7531.13	1.016016	7530.989	1.5033825
7531.3795	1.0060919	7531.2385	1.4706738
7531.6285	0.99647741	7531.4875	1.4432249
7531.878	0.98679443	7531.737	1.4169097
7532.1276	0.9787525	7531.9866	1.3954856
7532.3824	0.97014072	7532.2414	1.3749317
7532.632	0.96308831	7532.491	1.3568296

7532.8815	0.95616081	7532.7405	1.3396902
7533.131	0.95048532	7532.99	1.3232153
7533.38	0.94445787	7533.239	1.3054698
7533.6295	0.9388672	7533.4885	1.2886098
7533.879	0.93386543	7533.738	1.2719593
7534.129	0.92905178	7533.988	1.2558838
7534.3785	0.92487674	7534.2375	1.2410842
7534.628	0.92168483	7534.487	1.2252947
7534.8776	0.91817525	7534.7366	1.2098889
7535.1324	0.91463408	7534.9914	1.1934409
7535.3824	0.91176194	7535.2414	1.1788221
7535.632	0.90872727	7535.491	1.1643961
7535.8815	0.90573249	7535.7405	1.1508937
7536.1315	0.90299991	7535.9905	1.138393
7536.381	0.9006713	7536.24	1.1241691
7536.6305	0.89855916	7536.4895	1.1110538
7536.8805	0.89643309	7536.7395	1.0990948
7537.13	0.89401955	7536.989	1.0858838
7537.38	0.89198966	7537.239	1.0743854
7537.6295	0.89062247	7537.4885	1.0636911
7537.8795	0.888784	7537.7385	1.0527602
7538.1295	0.88735158	7537.9885	1.0429445
7538.379	0.88647644	7538.238	1.0342546
7538.629	0.88520419	7538.488	1.0240654
7538.879	0.88534879	7538.738	1.0156745
7539.129	0.88645951	7538.988	1.0073917
7539.379	0.88680986	7539.238	0.99987066
7539.6285	0.88765218	7539.4875	0.994004
7539.8785	0.88803133	7539.7375	0.98845479
7540.1285	0.88801937	7539.9875	0.98164605
7540.3785	0.8892012	7540.2375	0.9768121
7540.6285	0.89082246	7540.4875	0.97262984
7540.8785	0.89303067	7540.7375	0.96838803
7541.1285	0.89541996	7540.9875	0.963341
7541.379	0.89815992	7541.238	0.96057032
7541.629	0.90134226	7541.488	0.95558558
7541.879	0.90450358	7541.738	0.95139536
7542.129	0.9081021	7541.988	0.94784121
7542.3795	0.91124096	7542.2385	0.9455671
7542.6295	0.91444369	7542.4885	0.94311949

7542.8795	0.9181262	7542.7385	0.94032311
7543.13	0.92194317	7542.989	0.93786816
7543.38	0.92642126	7543.239	0.93535338
7543.6305	0.92978001	7543.4895	0.93253843
7543.8805	0.93237197	7543.7395	0.93099297
7544.1808	0.93705057	7544.0398	0.92990824
7544.4811	0.94107415	7544.3401	0.92905139
7544.7814	0.9461022	7544.6404	0.92722155
7545.0821	0.95024127	7544.9411	0.92608236
7545.3824	0.9542154	7545.2414	0.92521713
7545.6774	0.95764427	7545.5364	0.92486139
7545.9777	0.96165504	7545.8367	0.92305798
7546.2784	0.96475819	7546.1374	0.922885
7546.5787	0.96699856	7546.4377	0.92402598
7546.8795	0.96892111	7546.7385	0.92384781
7547.1798	0.97115613	7547.0388	0.92493173
7547.4806	0.9722775	7547.3396	0.92461435
7547.7814	0.97388368	7547.6404	0.92484193
7548.0821	0.97488081	7547.9411	0.92623044
7548.3829	0.97647871	7548.2419	0.92599016
7548.6779	0.97685065	7548.5369	0.92708795
7548.9786	0.97633292	7548.8376	0.9300079
7549.2794	0.97712991	7549.1384	0.93111433
7549.5802	0.97789728	7549.4392	0.93359755
7549.881	0.97881399	7549.74	0.93488061
7550.1818	0.97964777	7550.0408	0.9371038
7550.4825	0.98002694	7550.3415	0.93817548
7550.7779	0.98159517	7550.6369	0.9405312
7551.0792	0.9822663	7550.9382	0.9421978
7551.38	0.98331319	7551.239	0.94348397
7551.6808	0.98507751	7551.5398	0.94512611
7551.9821	0.9861175	7551.8411	0.94618292
7552.2775	0.98698039	7552.1365	0.94917082
7552.5787	0.9893145	7552.4377	0.9508087
7552.8795	0.99146103	7552.7385	0.95142794
7553.1808	0.9933864	7553.0398	0.95452356
7553.4821	0.99476999	7553.3411	0.95572988
7553.7775	0.99699573	7553.6365	0.95761809
7554.0787	0.99875058	7553.9377	0.95941306
7554.38	1.0009464	7554.239	0.96148904

7554.6813	1.0026158	7554.5403	0.9624912
7554.9825	1.0048647	7554.8415	0.96354208
7555.2784	1.0066089	7555.1374	0.96534373
7555.5797	1.0084886	7555.4387	0.96693469
7555.881	1.0096849	7555.74	0.9693086
7556.1822	1.0113803	7556.0412	0.97113661
7556.4781	1.0134336	7556.3371	0.97243784
7556.7794	1.0153083	7556.6384	0.97528296
7557.0812	1.0175404	7556.9402	0.97663227
7557.3824	1.019635	7557.2414	0.9792617
7557.6783	1.0215356	7557.5373	0.98084955
7557.9801	1.0239416	7557.8391	0.9827834
7558.2819	1.0257927	7558.1409	0.98414326
7558.5778	1.0270363	7558.4368	0.98512331
7558.8795	1.0281078	7558.7385	0.98608063
7559.1808	1.0300295	7559.0398	0.98769313
7559.4825	1.0314756	7559.3415	0.98808973
7559.7789	1.032576	7559.6379	0.9888516
7560.0807	1.0340248	7559.9397	0.99033828
7560.3824	1.0346707	7560.2414	0.98998085
7560.6783	1.0358041	7560.5373	0.98938985
7560.9801	1.0369476	7560.8391	0.99095351
7561.2823	1.0381016	7561.1413	0.99110088
7561.5782	1.0394429	7561.4372	0.99035398
7561.8805	1.0397018	7561.7395	0.9906272
7562.1822	1.0397269	7562.0412	0.99114572
7562.4786	1.040295	7562.3376	0.99052546
7562.7804	1.0406457	7562.6394	0.99042713
7563.0826	1.0420767	7562.9416	0.99022591
7563.379	1.0428919	7563.238	0.98957441
7563.6813	1.0431153	7563.5403	0.9895484
7563.9777	1.0434652	7563.8367	0.98902359
7564.2799	1.0434708	7564.1389	0.98744892
7564.5817	1.0437476	7564.4407	0.98812896
7564.8785	1.0432396	7564.7375	0.98713276
7565.1808	1.044787	7565.0398	0.98753723
7565.483	1.0440526	7565.342	0.98672312
7565.7794	1.0439785	7565.6384	0.98646077
7566.0817	1.0436282	7565.9407	0.98711098
7566.3785	1.0442149	7566.2375	0.98704066

7566.6808	1.044107	7566.5398	0.98745184
7566.9777	1.0442861	7566.8367	0.98771624
7567.2799	1.0440211	7567.1389	0.98893119
7567.5821	1.0439036	7567.4411	0.99031754
7567.879	1.0436274	7567.738	0.99087724
7568.1818	1.0438998	7568.0408	0.99108927
7568.4786	1.0439253	7568.3376	0.99195244
7568.7809	1.0429651	7568.6399	0.99184489
7569.0778	1.0435849	7568.9368	0.9923616
7569.3805	1.0439428	7569.2395	0.99435712
7569.6774	1.0420764	7569.5364	0.99517398
7569.9801	1.0418393	7569.8391	0.99598201
7570.2828	1.0411768	7570.1418	0.99584712
7570.5797	1.0403084	7570.4387	0.99783279
7570.8824	1.0394068	7570.7414	0.99826545
7571.1798	1.0381429	7571.0388	0.9992906
7571.4825	1.0366734	7571.3415	1.0000697
7571.7794	1.0358043	7571.6384	1.0011861
7572.0821	1.0344424	7571.9411	1.0013443
7572.3795	1.0333023	7572.2385	1.0031119
7572.6822	1.0323749	7572.5412	1.0041975
7572.9796	1.0302042	7572.8386	1.0065304
7573.2823	1.028535	7573.1413	1.0091908
7573.5797	1.0272471	7573.4387	1.0111048
7573.8771	1.0257616	7573.7361	1.0127488
7574.1803	1.024556	7574.0393	1.0142938
7574.4777	1.0224639	7574.3367	1.0156735
7574.7809	1.0206998	7574.6399	1.0172937
7575.0782	1.0184977	7574.9372	1.0191977
7575.381	1.0162536	7575.24	1.0198867
7575.6788	1.0148073	7575.5378	1.0225209
7575.9821	1.0123015	7575.8411	1.0233094
7576.2794	1.0103891	7576.1384	1.0246991
7576.5826	1.008262	7576.4416	1.0257009
7576.8805	1.0062556	7576.7395	1.0261979
7577.1779	1.003578	7577.0369	1.028132
7577.4811	1.0009007	7577.3401	1.0283839
7577.7789	0.99858655	7577.6379	1.0295651
7578.0821	0.99714812	7577.9411	1.0296228
7578.38	0.99565839	7578.239	1.0304641

7578.6779	0.99353144	7578.5369	1.031576
7578.9811	0.99084385	7578.8401	1.0322799
7579.2789	0.98981138	7579.1379	1.0316237
7579.5826	0.98778912	7579.4416	1.0321234
7579.8805	0.98627235	7579.7395	1.0320824
7580.1783	0.98425426	7580.0373	1.0334135
7580.4816	0.98192402	7580.3406	1.0343963
7580.7799	0.98007454	7580.6389	1.0344531
7581.0778	0.9790635	7580.9368	1.0330554
7581.3815	0.9777126	7581.2405	1.0328999
7581.6793	0.97556058	7581.5383	1.0324836
7581.9777	0.9739666	7581.8367	1.0323362
7582.2814	0.97258473	7582.1404	1.0328708
7582.5792	0.97042002	7582.4382	1.0311388
7582.8776	0.9686069	7582.7366	1.0306695
7583.1813	0.96647464	7583.0403	1.0297246
7583.4791	0.96432214	7583.3381	1.0286314
7583.7775	0.96295962	7583.6365	1.0268879
7583.879	0.96220752	7583.738	1.0251051
7586.8795	0.94929252	7586.7385	1.0142837
7589.8824	0.9430213	7589.7414	1.0005576
7592.8771	0.94377819	7592.7361	0.98599938
7595.88	0.95316537	7595.739	0.97468168
7598.88	0.96995796	7598.739	0.9695277
7601.8824	0.99043035	7601.7414	0.96732475
7604.882	1.0088139	7604.741	0.96936374
7607.878	1.0207365	7607.737	0.97449185
7610.8771	1.0248177	7610.7361	0.97976657
7613.879	1.0229164	7613.738	0.98533739
7616.8776	1.0169858	7616.7366	0.99093219
7619.8785	1.0093078	7619.7375	0.99637947
7622.8824	1.0042466	7622.7414	0.99896115
7625.8776	0.99959328	7625.7366	0.9993623
7628.881	0.99865943	7628.74	0.99879948
7631.8815	0.99993057	7631.7405	0.99784632
7634.8785	1.0009963	7634.7375	0.9963892
7637.8785	1.0029607	7637.7375	0.99409793
7640.881	1.0052532	7640.74	0.99420305
7643.88	1.0055443	7643.739	0.99639264
7646.882	1.0040485	7646.741	0.99948428

7649.881	1.0008905	7649.74	1.0023974
7652.8824	0.99571656	7652.7414	1.0042431
7655.8805	0.99220426	7655.7395	1.0070493
7658.8815	0.98607904	7658.7405	1.0088895
7661.8795	0.98251586	7661.7385	1.0093054
7664.8795	0.97906421	7664.7385	1.0089872
7667.8829	0.97943997	7667.7419	1.008506
7670.8824	0.9810659	7670.7414	1.0048496
7673.879	0.9831566	7673.738	1.0023478
7676.8785	0.9871666	7676.7375	0.9986941
7679.88	0.99136303	7679.739	0.99398361
7682.8785	0.9969684	7682.7375	0.98862868
7685.88	1.0042949	7685.739	0.98455648
7688.878	1.0096051	7688.737	0.98322102
7691.8785	1.0139013	7691.7375	0.98377264
7694.882	1.0164343	7694.741	0.98562834
7697.882	1.0169004	7697.741	0.98836796
7700.8785	1.0156125	7700.7375	0.99216435
7703.878	1.012999	7703.737	0.99805353
7706.88	1.0098877	7706.739	1.0021028
7709.8785	1.0050824	7709.7375	1.0059935
7712.8795	1.0017944	7712.7385	1.0076026
7715.8776	0.99916699	7715.7366	1.0081792
7718.878	0.99681931	7718.737	1.0072188
7721.8815	0.99577727	7721.7405	1.0060874
7724.8815	0.99693938	7724.7405	1.0055544
7727.878	0.99801872	7727.737	1.0035093
7730.8829	1.0001259	7730.7419	1.0020947
7733.8785	1.0017632	7733.7375	1.0015461
7736.8771	1.0033517	7736.7361	1.0007281
7739.878	1.0048569	7739.737	0.99940022
7742.882	1.0060323	7742.741	1.0004599
7745.882	1.0063572	7745.741	1.0012938
7748.879	1.005461	7748.738	1.0020457
7751.8785	1.0035384	7751.7375	1.0028771
7754.8805	1.0025569	7754.7395	1.0037886
7757.879	1.000308	7757.738	1.0056596
7760.8805	0.99905217	7760.7395	1.006762
7763.8785	0.9976104	7763.7375	1.0075286
7766.879	0.99622857	7766.738	1.0078874

7769.882	0.99569474	7769.741	1.0082497
7772.8815	0.9952441	7772.7405	1.0071455
7775.878	0.99549392	7775.737	1.0039343
7778.8824	0.99544367	7778.7414	1.0026313
7781.878	0.99561124	7781.737	0.99926025
7784.882	0.99746538	7784.741	0.99785774
7787.8824	0.9998162	7787.7414	0.9958213
7790.8795	1.0015968	7790.7385	0.99477349
7793.879	1.0036103	7793.738	0.99345683
7796.8815	1.0055887	7796.7405	0.99222738
7799.88	1.0066781	7799.739	0.99140566
7802.8815	1.0080855	7802.7405	0.9909589
7805.8795	1.0077103	7805.7385	0.99221035
7808.88	1.0074915	7808.739	0.99277038
7811.8829	1.0057753	7811.7419	0.9929021
7814.8824	1.0047209	7814.7414	0.99440182
7817.8785	1.0023955	7817.7375	0.99612765
7820.8829	0.99985395	7820.7419	0.99408239
7823.878	0.99832155	7823.737	0.99665632
7826.8815	0.99647537	7826.7405	0.99775597
7829.8815	0.9946095	7829.7405	0.99982917
7832.8785	0.99268542	7832.7375	0.99935692
7835.8776	0.99066683	7835.7366	0.99925242
7838.879	0.99011772	7838.738	0.99954224
7841.8771	0.99167916	7841.7361	0.99809218
7844.878	0.99004968	7844.737	0.99644937
7847.8815	0.99077638	7847.7405	0.99420839
7850.881	0.99102906	7850.74	0.99429148
7853.8771	0.99079883	7853.7361	0.99231181
7856.882	0.99338686	7856.741	0.99160576
7859.8829	0.99279659	7859.7419	0.98899501
7862.8805	0.99346395	7862.7395	0.98944143
7865.8805	0.99400957	7865.7395	0.98923994

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