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Steric Control on the Redox Chemistry of (η^5 - C_9H_7)₂Yb^{II}(THF)₂ by 6-Aryl substituted Iminopyridines

Alexander A. Trifonov,^{,§} Boris G. Shestakov,[§] Ivan D. Gudilenkov,[§] Georgy K. Fukin[§]*

Giuliano Giambastiani,^{,†} Andrea Rossin,[†] Claudio Bianchini,[†] Jonathan Filippi,[†]*

Lapo Luconi[†] and Lorenzo Sorace^ξ

[§] *G.A. Razuvaev Institute of Organometallic Chemistry of Russian Academy of Sciences*

Tropinina 49, GSP-445, 603950 Nizhny Novgorod (Russia). Fax:(+7) 8314621497

[†] *Istituto di Chimica dei Composti Organometallici (ICCOM - CNR), Via Madonna*

del Piano 10, 50019, Sesto Fiorentino, (Italy). Fax:(+39) 0555225203

^ξ *Dipartimento di Chimica, Università degli Studi di Firenze, Via della Lastruccia, 13, 50019*

Sesto Fiorentino (Firenze), Italy.

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Crystallographic data and tables for 4 (CCDC: 794890)

Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
C(1)	5690(1)	429(2)	-2490(1)	18(1)
C(2)	5569(1)	1723(2)	-2544(1)	21(1)
C(3)	5893(1)	2481(2)	-3078(1)	22(1)
C(4)	6322(1)	1929(2)	-3549(1)	22(1)
C(5)	6422(1)	610(2)	-3465(1)	17(1)
C(6)	6868(1)	-12(2)	-3947(1)	23(1)
C(7)	7322(1)	494(2)	-4354(2)	44(1)
C(8)	7673(1)	-448(3)	-4725(2)	55(1)
C(9)	7480(1)	-1657(2)	-4604(2)	38(1)
C(10)	5320(1)	-380(2)	-1975(1)	18(1)
C(11)	4932(1)	-2213(2)	-1447(1)	17(1)
C(12)	4436(1)	-2294(2)	-1930(2)	24(1)
C(13)	3962(1)	-2808(2)	-1540(2)	31(1)
C(14)	3975(1)	-3271(2)	-717(2)	32(1)
C(15)	4477(1)	-3277(2)	-274(1)	26(1)
C(16)	4966(1)	-2759(2)	-623(1)	21(1)
C(17)	4394(1)	-1928(3)	-2870(2)	27(1)
C(18)	3990(1)	-817(3)	-3027(2)	41(1)
C(19)	4206(1)	-3096(3)	-3407(2)	37(1)
C(20)	5511(1)	-2760(2)	-112(1)	26(1)
C(21)	5667(1)	-4124(2)	155(2)	38(1)
C(22)	5469(1)	-1920(3)	684(2)	40(1)
C(23)	6340(1)	-4475(2)	-3471(1)	20(1)
C(24)	5786(1)	-4147(2)	-3188(1)	21(1)
C(25)	5754(1)	-4450(1)	-2319(2)	22(1)
C(26)	6280(1)	-4887(2)	-2021(1)	22(1)
C(27)	6655(1)	-4917(2)	-2738(1)	21(1)
C(28)	7213(1)	-5340(2)	-2853(2)	29(1)
C(29)	7447(1)	-5356(2)	-3649(2)	35(1)
C(30)	7137(1)	-4930(2)	-4374(2)	31(1)
C(31)	6598(1)	-4495(2)	-4288(1)	26(1)
C(32)	7185(1)	-530(2)	-1640(1)	24(1)

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C(33)	7486(1)	-1593(2)	-1951(2)	30(1)
C(34)	7359(1)	-2641(2)	-1434(2)	29(1)
C(35)	6953(1)	-2272(2)	-819(1)	25(1)
C(36)	6849(1)	-948(2)	-937(1)	23(1)
C(37)	6504(1)	-63(2)	-499(1)	26(1)
C(38)	6504(1)	1191(2)	-739(2)	33(1)
C(39)	6848(1)	1619(2)	-1415(2)	36(1)
C(40)	7178(1)	799(2)	-1864(1)	33(1)
C(41)	6011(2)	-2283(6)	-6301(3)	128(2)
C(42)	5532(2)	-3013(4)	-5984(3)	76(1)
C(43)	5193(3)	-2617(4)	-5453(3)	92(2)
C(44)	5256(2)	-1435(4)	-5112(2)	79(1)
C(45)	5654(2)	-637(4)	-5317(2)	72(1)
C(46)	6069(2)	-993(5)	-5930(3)	96(2)
C(47)	6320(4)	-3029(10)	-6944(5)	358(4)
N(1)	6112(1)	-140(2)	-2941(1)	16(1)
N(2)	5414(1)	-1564(2)	-1813(1)	16(1)
S(1)	6860(1)	-1647(1)	-4050(1)	22(1)
Yb(1)	6400(1)	-2331(1)	-2322(1)	15(1)

Table S2. Bond lengths [\AA] and angles [$^\circ$] for **4**.

C(1)-N(1)	1.360(2)
C(1)-C(2)	1.386(3)
C(1)-C(10)	1.459(3)
C(2)-C(3)	1.383(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.382(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.406(3)
C(4)-H(4)	0.9500
C(5)-N(1)	1.352(3)
C(5)-C(6)	1.451(3)
C(6)-C(7)	1.359(3)
C(6)-S(1)	1.717(2)

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C(7)-C(8)	1.412(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.357(4)
C(8)-H(8)	0.9500
C(9)-S(1)	1.706(2)
C(9)-H(9)	0.9500
C(10)-N(2)	1.283(3)
C(10)-H(10)	0.9500
C(11)-C(12)	1.398(3)
C(11)-C(16)	1.413(3)
C(11)-N(2)	1.447(2)
C(12)-C(13)	1.386(3)
C(12)-C(17)	1.524(3)
C(13)-C(14)	1.378(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.376(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.389(3)
C(15)-H(15)	0.9500
C(16)-C(20)	1.520(3)
C(17)-C(18)	1.525(4)
C(17)-C(19)	1.548(4)
C(17)-H(17)	1.0000
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(22)	1.528(3)
C(20)-C(21)	1.532(3)
C(20)-H(20)	1.0000
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800

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C(23)-C(31)	1.417(3)
C(23)-C(24)	1.427(3)
C(23)-C(27)	1.444(3)
C(23)-Yb(1)	2.877(2)
C(24)-C(25)	1.400(4)
C(24)-Yb(1)	2.7486(19)
C(24)-H(24)	0.9500
C(25)-C(26)	1.406(3)
C(25)-Yb(1)	2.6917(15)
C(25)-H(25)	0.9500
C(26)-C(27)	1.432(3)
C(26)-Yb(1)	2.729(2)
C(26)-H(26)	0.9500
C(27)-C(28)	1.407(3)
C(27)-Yb(1)	2.8458(19)
C(28)-C(29)	1.364(3)
C(28)-H(28)	0.9500
C(29)-C(30)	1.423(3)
C(29)-H(29)	0.9500
C(30)-C(31)	1.361(3)
C(30)-H(30)	0.9500
C(31)-H(31)	0.9500
C(32)-C(33)	1.408(3)
C(32)-C(36)	1.426(3)
C(32)-C(40)	1.433(3)
C(32)-Yb(1)	2.854(2)
C(33)-C(34)	1.396(3)
C(33)-Yb(1)	2.747(2)
C(33)-H(33)	0.9500
C(34)-C(35)	1.414(3)
C(34)-Yb(1)	2.683(2)
C(34)-H(34)	0.9500
C(35)-C(36)	1.418(3)
C(35)-Yb(1)	2.693(2)
C(35)-H(35)	0.9500
C(36)-C(37)	1.412(3)
C(36)-Yb(1)	2.816(2)
C(37)-C(38)	1.364(3)

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C(37)-H(37)	0.9500
C(38)-C(39)	1.408(4)
C(38)-H(38)	0.9500
C(39)-C(40)	1.357(3)
C(39)-H(39)	0.9500
C(40)-H(40)	0.9500
C(41)-C(42)	1.454(7)
C(41)-C(46)	1.475(8)
C(41)-C(47)	1.470(9)
C(42)-C(43)	1.228(7)
C(42)-H(42)	0.9500
C(43)-C(44)	1.355(6)
C(43)-H(43)	0.9500
C(44)-C(45)	1.300(6)
C(44)-H(44)	0.9500
C(45)-C(46)	1.423(6)
C(45)-H(45)	0.9500
C(46)-H(46)	0.9500
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
N(1)-Yb(1)	2.5804(16)
N(2)-Yb(1)	2.5956(15)
S(1)-Yb(1)	3.0020(5)
N(1)-C(1)-C(2)	123.12(16)
N(1)-C(1)-C(10)	118.28(16)
C(2)-C(1)-C(10)	118.43(16)
C(3)-C(2)-C(1)	118.80(18)
C(3)-C(2)-H(2)	120.6
C(1)-C(2)-H(2)	120.6
C(4)-C(3)-C(2)	119.42(18)
C(4)-C(3)-H(3)	120.3
C(2)-C(3)-H(3)	120.3
C(3)-C(4)-C(5)	118.94(19)
C(3)-C(4)-H(4)	120.5
C(5)-C(4)-H(4)	120.5
N(1)-C(5)-C(4)	122.24(18)

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N(1)-C(5)-C(6)	116.82(17)
C(4)-C(5)-C(6)	120.94(18)
C(7)-C(6)-C(5)	130.2(2)
C(7)-C(6)-S(1)	110.61(17)
C(5)-C(6)-S(1)	119.17(15)
C(6)-C(7)-C(8)	112.8(2)
C(6)-C(7)-H(7)	123.6
C(8)-C(7)-H(7)	123.6
C(9)-C(8)-C(7)	113.3(2)
C(9)-C(8)-H(8)	123.4
C(7)-C(8)-H(8)	123.4
C(8)-C(9)-S(1)	110.74(19)
C(8)-C(9)-H(9)	124.6
S(1)-C(9)-H(9)	124.6
N(2)-C(10)-C(1)	124.41(17)
N(2)-C(10)-H(10)	117.8
C(1)-C(10)-H(10)	117.8
C(12)-C(11)-C(16)	121.07(19)
C(12)-C(11)-N(2)	118.49(17)
C(16)-C(11)-N(2)	120.44(18)
C(13)-C(12)-C(11)	117.8(2)
C(13)-C(12)-C(17)	117.9(2)
C(11)-C(12)-C(17)	124.2(2)
C(14)-C(13)-C(12)	121.9(2)
C(14)-C(13)-H(13)	119.0
C(12)-C(13)-H(13)	119.0
C(15)-C(14)-C(13)	119.5(2)
C(15)-C(14)-H(14)	120.3
C(13)-C(14)-H(14)	120.3
C(14)-C(15)-C(16)	121.3(2)
C(14)-C(15)-H(15)	119.3
C(16)-C(15)-H(15)	119.3
C(15)-C(16)-C(11)	118.01(19)
C(15)-C(16)-C(20)	120.06(19)
C(11)-C(16)-C(20)	121.91(19)
C(12)-C(17)-C(18)	112.9(2)
C(12)-C(17)-C(19)	110.2(2)
C(18)-C(17)-C(19)	109.4(2)

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C(12)-C(17)-H(17)	108.1
C(18)-C(17)-H(17)	108.1
C(19)-C(17)-H(17)	108.1
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-C(22)	111.91(19)
C(16)-C(20)-C(21)	110.46(18)
C(22)-C(20)-C(21)	109.1(2)
C(16)-C(20)-H(20)	108.4
C(22)-C(20)-H(20)	108.4
C(21)-C(20)-H(20)	108.4
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(31)-C(23)-C(24)	132.86(19)
C(31)-C(23)-C(27)	119.33(18)
C(24)-C(23)-C(27)	107.73(18)
C(31)-C(23)-Yb(1)	123.70(14)
C(24)-C(23)-Yb(1)	70.36(11)

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C(27)-C(23)-Yb(1)	74.19(11)
C(25)-C(24)-C(23)	107.28(17)
C(25)-C(24)-Yb(1)	72.85(10)
C(23)-C(24)-Yb(1)	80.36(11)
C(25)-C(24)-H(24)	126.4
C(23)-C(24)-H(24)	126.4
Yb(1)-C(24)-H(24)	113.0
C(24)-C(25)-C(26)	110.39(19)
C(24)-C(25)-Yb(1)	77.36(10)
C(26)-C(25)-Yb(1)	76.43(10)
C(24)-C(25)-H(25)	124.8
C(26)-C(25)-H(25)	124.8
Yb(1)-C(25)-H(25)	113.4
C(25)-C(26)-C(27)	107.25(19)
C(25)-C(26)-Yb(1)	73.52(10)
C(27)-C(26)-Yb(1)	79.71(11)
C(25)-C(26)-H(26)	126.4
C(27)-C(26)-H(26)	126.4
Yb(1)-C(26)-H(26)	112.9
C(28)-C(27)-C(26)	133.7(2)
C(28)-C(27)-C(23)	118.99(19)
C(26)-C(27)-C(23)	107.22(17)
C(28)-C(27)-Yb(1)	121.84(13)
C(26)-C(27)-Yb(1)	70.62(11)
C(23)-C(27)-Yb(1)	76.58(11)
C(29)-C(28)-C(27)	120.1(2)
C(29)-C(28)-H(28)	119.9
C(27)-C(28)-H(28)	119.9
C(28)-C(29)-C(30)	121.0(2)
C(28)-C(29)-H(29)	119.5
C(30)-C(29)-H(29)	119.5
C(31)-C(30)-C(29)	120.7(2)
C(31)-C(30)-H(30)	119.7
C(29)-C(30)-H(30)	119.7
C(30)-C(31)-C(23)	119.8(2)
C(30)-C(31)-H(31)	120.1
C(23)-C(31)-H(31)	120.1
C(33)-C(32)-C(36)	107.88(19)

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C(33)-C(32)-C(40)	133.3(2)
C(36)-C(32)-C(40)	118.7(2)
C(33)-C(32)-Yb(1)	71.29(12)
C(36)-C(32)-Yb(1)	73.97(11)
C(40)-C(32)-Yb(1)	122.81(14)
C(34)-C(33)-C(32)	108.1(2)
C(34)-C(33)-Yb(1)	72.55(13)
C(32)-C(33)-Yb(1)	79.68(12)
C(34)-C(33)-H(33)	126.0
C(32)-C(33)-H(33)	126.0
Yb(1)-C(33)-H(33)	114.1
C(33)-C(34)-C(35)	109.1(2)
C(33)-C(34)-Yb(1)	77.68(13)
C(35)-C(34)-Yb(1)	75.16(13)
C(33)-C(34)-H(34)	125.5
C(35)-C(34)-H(34)	125.5
Yb(1)-C(34)-H(34)	113.9
C(34)-C(35)-C(36)	107.22(19)
C(34)-C(35)-Yb(1)	74.35(13)
C(36)-C(35)-Yb(1)	79.95(12)
C(34)-C(35)-H(35)	126.4
C(36)-C(35)-H(35)	126.4
Yb(1)-C(35)-H(35)	112.0
C(37)-C(36)-C(35)	132.6(2)
C(37)-C(36)-C(32)	119.7(2)
C(35)-C(36)-C(32)	107.66(19)
C(37)-C(36)-Yb(1)	119.45(13)
C(35)-C(36)-Yb(1)	70.33(12)
C(32)-C(36)-Yb(1)	76.91(11)
C(38)-C(37)-C(36)	119.8(2)
C(38)-C(37)-H(37)	120.1
C(36)-C(37)-H(37)	120.1
C(37)-C(38)-C(39)	120.8(2)
C(37)-C(38)-H(38)	119.6
C(39)-C(38)-H(38)	119.6
C(40)-C(39)-C(38)	121.5(2)
C(40)-C(39)-H(39)	119.3
C(38)-C(39)-H(39)	119.3

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C(39)-C(40)-C(32)	119.4(2)
C(39)-C(40)-H(40)	120.3
C(32)-C(40)-H(40)	120.3
C(42)-C(41)-C(46)	114.7(4)
C(42)-C(41)-C(47)	110.1(6)
C(46)-C(41)-C(47)	135.1(6)
C(43)-C(42)-C(41)	124.4(5)
C(43)-C(42)-H(42)	117.8
C(41)-C(42)-H(42)	117.8
C(42)-C(43)-C(44)	120.1(5)
C(42)-C(43)-H(43)	120.0
C(44)-C(43)-H(43)	120.0
C(45)-C(44)-C(43)	124.6(5)
C(45)-C(44)-H(44)	117.7
C(43)-C(44)-H(44)	117.7
C(44)-C(45)-C(46)	120.0(4)
C(44)-C(45)-H(45)	120.0
C(46)-C(45)-H(45)	120.0
C(45)-C(46)-C(41)	116.1(4)
C(45)-C(46)-H(46)	121.9
C(41)-C(46)-H(46)	121.9
C(41)-C(47)-H(47A)	109.5
C(41)-C(47)-H(47B)	109.4
H(47A)-C(47)-H(47B)	109.5
C(41)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(5)-N(1)-C(1)	117.48(16)
C(5)-N(1)-Yb(1)	126.75(12)
C(1)-N(1)-Yb(1)	112.79(12)
C(10)-N(2)-C(11)	113.29(16)
C(10)-N(2)-Yb(1)	113.13(12)
C(11)-N(2)-Yb(1)	133.36(11)
C(9)-S(1)-C(6)	92.58(11)
C(9)-S(1)-Yb(1)	140.31(9)
C(6)-S(1)-Yb(1)	99.02(7)
N(1)-Yb(1)-N(2)	66.56(5)
N(1)-Yb(1)-C(34)	121.75(6)

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N(2)-Yb(1)-C(34)	129.80(6)
N(1)-Yb(1)-C(25)	125.53(6)
N(2)-Yb(1)-C(25)	75.08(5)
C(34)-Yb(1)-C(25)	112.36(7)
N(1)-Yb(1)-C(35)	115.87(6)
N(2)-Yb(1)-C(35)	99.34(6)
C(34)-Yb(1)-C(35)	30.49(7)
C(25)-Yb(1)-C(35)	107.06(8)
N(1)-Yb(1)-C(26)	155.11(6)
N(2)-Yb(1)-C(26)	98.98(6)
C(34)-Yb(1)-C(26)	83.13(7)
C(25)-Yb(1)-C(26)	30.05(6)
C(35)-Yb(1)-C(26)	85.55(6)
N(1)-Yb(1)-C(33)	94.46(6)
N(2)-Yb(1)-C(33)	133.69(6)
C(34)-Yb(1)-C(33)	29.76(7)
C(25)-Yb(1)-C(33)	139.70(7)
C(35)-Yb(1)-C(33)	49.74(7)
C(26)-Yb(1)-C(33)	109.66(7)
N(1)-Yb(1)-C(24)	106.74(5)
N(2)-Yb(1)-C(24)	83.61(5)
C(34)-Yb(1)-C(24)	128.33(6)
C(25)-Yb(1)-C(24)	29.79(8)
C(35)-Yb(1)-C(24)	134.75(6)
C(26)-Yb(1)-C(24)	49.73(6)
C(33)-Yb(1)-C(24)	142.52(6)
N(1)-Yb(1)-C(36)	86.16(6)
N(2)-Yb(1)-C(36)	86.84(5)
C(34)-Yb(1)-C(36)	48.91(6)
C(25)-Yb(1)-C(36)	129.49(8)
C(35)-Yb(1)-C(36)	29.72(6)
C(26)-Yb(1)-C(36)	114.18(6)
C(33)-Yb(1)-C(36)	48.62(6)
C(24)-Yb(1)-C(36)	159.16(6)
N(1)-Yb(1)-C(27)	144.49(6)
N(2)-Yb(1)-C(27)	123.71(5)
C(34)-Yb(1)-C(27)	79.89(6)
C(25)-Yb(1)-C(27)	48.63(5)

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C(35)-Yb(1)-C(27)	96.82(6)
C(26)-Yb(1)-C(27)	29.67(6)
C(33)-Yb(1)-C(27)	96.71(6)
C(24)-Yb(1)-C(27)	48.95(6)
C(36)-Yb(1)-C(27)	125.75(6)
N(1)-Yb(1)-C(32)	74.14(5)
N(2)-Yb(1)-C(32)	105.49(5)
C(34)-Yb(1)-C(32)	48.27(6)
C(25)-Yb(1)-C(32)	155.85(8)
C(35)-Yb(1)-C(32)	48.79(6)
C(26)-Yb(1)-C(32)	130.53(6)
C(33)-Yb(1)-C(32)	29.04(7)
C(24)-Yb(1)-C(32)	170.06(6)
C(36)-Yb(1)-C(32)	29.13(6)
C(27)-Yb(1)-C(32)	125.08(6)
N(1)-Yb(1)-C(23)	116.35(5)
N(2)-Yb(1)-C(23)	112.86(5)
C(34)-Yb(1)-C(23)	105.77(6)
C(25)-Yb(1)-C(23)	48.12(7)
C(35)-Yb(1)-C(23)	126.02(6)
C(26)-Yb(1)-C(23)	48.70(6)
C(33)-Yb(1)-C(23)	113.40(6)
C(24)-Yb(1)-C(23)	29.28(6)
C(36)-Yb(1)-C(23)	154.20(6)
C(27)-Yb(1)-C(23)	29.23(6)
C(32)-Yb(1)-C(23)	141.28(6)

Table S3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	17(1)	16(1)	19(1)	-1(1)	-3(1)	1(1)
C(2)	22(1)	16(1)	25(1)	-3(1)	-3(1)	1(1)
C(3)	26(1)	13(1)	26(1)	0(1)	-7(1)	-1(1)
C(4)	25(1)	17(1)	23(1)	3(1)	-2(1)	-4(1)

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C(5)	19(1)	13(1)	18(1)	2(1)	-3(1)	-2(1)
C(6)	27(1)	19(1)	23(1)	2(1)	5(1)	-4(1)
C(7)	50(1)	23(1)	59(2)	-4(1)	28(1)	-7(1)
C(8)	48(1)	36(1)	79(2)	-9(1)	44(1)	-12(1)
C(9)	39(1)	30(1)	45(1)	-4(1)	23(1)	0(1)
C(10)	17(1)	19(1)	18(1)	-5(1)	-1(1)	1(1)
C(11)	17(1)	15(1)	19(1)	0(1)	3(1)	2(1)
C(12)	19(1)	23(1)	30(1)	3(1)	0(1)	0(1)
C(13)	19(1)	43(1)	32(1)	3(1)	0(1)	-6(1)
C(14)	25(1)	33(1)	37(1)	5(1)	7(1)	-7(1)
C(15)	33(1)	24(1)	23(1)	4(1)	8(1)	0(1)
C(16)	25(1)	16(1)	20(1)	0(1)	2(1)	0(1)
C(17)	19(1)	36(1)	26(1)	1(1)	-2(1)	-5(1)
C(18)	42(1)	45(1)	36(1)	14(1)	-10(1)	-2(1)
C(19)	30(1)	52(2)	30(1)	-1(1)	-1(1)	-10(1)
C(20)	23(1)	30(1)	23(1)	4(1)	2(1)	-1(1)
C(21)	37(1)	39(1)	39(1)	14(1)	0(1)	2(1)
C(22)	35(1)	46(2)	38(1)	-2(1)	7(1)	-8(1)
C(23)	25(1)	10(1)	24(1)	-3(1)	3(1)	-1(1)
C(24)	19(1)	12(1)	31(1)	-4(1)	-3(1)	0(1)
C(25)	22(1)	12(1)	33(1)	-6(2)	11(1)	-2(1)
C(26)	34(1)	9(1)	24(1)	1(1)	1(1)	-1(1)
C(27)	20(1)	12(1)	29(1)	-4(1)	-1(1)	0(1)
C(28)	25(1)	22(1)	39(1)	-6(1)	-6(1)	1(1)
C(29)	22(1)	28(1)	54(1)	-15(1)	8(1)	0(1)
C(30)	31(1)	26(1)	35(1)	-12(1)	13(1)	-9(1)
C(31)	32(1)	19(1)	26(1)	-5(1)	2(1)	-6(1)
C(32)	18(1)	29(1)	26(1)	0(1)	-9(1)	-5(1)
C(33)	15(1)	43(1)	32(1)	-3(1)	-3(1)	-2(1)
C(34)	19(1)	32(1)	36(1)	-7(1)	-12(1)	10(1)
C(35)	22(1)	32(1)	22(1)	9(1)	-12(1)	-3(1)
C(36)	22(1)	25(1)	21(1)	-2(1)	-10(1)	-4(1)
C(37)	25(1)	29(1)	24(1)	-6(1)	-6(1)	-4(1)
C(38)	33(1)	26(1)	40(1)	-10(1)	-11(1)	2(1)
C(39)	45(1)	20(1)	43(1)	0(1)	-19(1)	-9(1)
C(40)	33(1)	35(1)	29(1)	8(1)	-10(1)	-17(1)
C(41)	104(2)	224(4)	56(3)	17(3)	-8(2)	129(3)
C(42)	64(2)	87(2)	76(2)	35(2)	-14(2)	11(2)

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C(43)	105(4)	92(3)	78(3)	23(2)	-10(3)	21(3)
C(44)	121(3)	65(2)	52(2)	20(2)	-20(2)	0(2)
C(45)	84(2)	72(2)	62(2)	7(2)	-35(2)	18(2)
C(46)	57(2)	145(4)	86(3)	48(3)	-28(2)	16(2)
C(47)	429(7)	553(10)	90(5)	25(5)	18(5)	429(7)
N(1)	16(1)	14(1)	17(1)	-1(1)	0(1)	-2(1)
N(2)	19(1)	13(1)	16(1)	0(1)	1(1)	-1(1)
S(1)	25(1)	17(1)	26(1)	1(1)	6(1)	0(1)
Yb(1)	14(1)	13(1)	17(1)	0(1)	-1(1)	1(1)

Table S4. (Selected) torsion angles [°] for **4**.

N(1)-C(5)-C(6)-S(1)	16.8(2)
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Crystallographic data and tables for **5** (CCDC: 795224)

Table S5. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **5**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
C(1)	11749(9)	8075(3)	6413(7)	32(2)
C(2)	12935(7)	7849(3)	6658(7)	29(2)
C(3)	13891(7)	7963(3)	5971(7)	37(2)
C(4)	13700(7)	8294(3)	5080(6)	36(2)
C(5)	12434(6)	8494(2)	4845(6)	20(2)
C(6)	12112(7)	8836(2)	3862(6)	23(2)
C(7)	12825(8)	9052(3)	3103(7)	36(2)
C(8)	11946(8)	9324(3)	2305(8)	42(2)
C(9)	10758(8)	9248(3)	2618(7)	35(2)
C(10)	10634(8)	7936(3)	7028(7)	31(2)

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C(11)	8446(7)	7856(3)	7284(6)	24(2)
C(12)	8081(8)	7401(3)	6823(7)	29(2)
C(13)	7015(13)	7175(5)	7207(12)	33(4)
C(14)	6340(8)	7396(3)	8056(8)	38(2)
C(15)	6729(13)	7840(5)	8507(13)	38(4)
C(16)	7763(7)	8085(3)	8141(7)	28(2)
C(17)	8804(8)	7136(3)	5914(6)	37(2)
C(18)	7875(9)	6903(3)	4939(7)	53(3)
C(19)	9759(8)	6760(3)	6467(8)	51(2)
C(20)	8214(8)	8568(3)	8675(7)	41(2)
C(21)	9057(12)	8487(3)	9851(7)	77(4)
C(22)	7085(10)	8913(3)	8806(10)	80(3)
C(23)	10489(7)	9454(3)	7076(7)	29(2)
C(24)	9151(8)	9577(2)	6835(7)	31(2)
C(25)	8906(12)	9799(4)	5730(10)	35(3)
C(26)	10071(14)	9806(4)	5219(10)	42(3)
C(27)	11075(8)	9610(3)	6043(7)	32(2)
C(28)	12474(10)	9564(4)	6065(11)	48(3)
C(29)	13168(9)	9381(3)	7032(10)	48(3)
C(30)	12608(10)	9232(3)	8033(9)	48(3)
C(31)	11278(13)	9277(4)	8046(13)	43(4)
C(32)	6676(7)	8897(3)	4437(7)	38(2)
C(33)	7007(12)	8431(5)	4848(12)	37(4)
C(34)	7713(10)	8202(4)	4110(9)	41(3)
C(35)	7949(7)	8510(3)	3200(8)	46(2)
C(36)	7277(8)	8945(3)	3343(7)	37(2)
C(37)	7055(13)	9380(5)	2659(13)	61(5)
C(38)	6277(12)	9733(4)	3037(14)	81(4)
C(39)	5701(12)	9693(5)	4091(16)	73(5)
C(40)	5890(8)	9290(4)	4797(9)	50(3)
N(1)	11481(10)	8393(3)	5498(8)	22(2)
N(2)	9478(6)	8112(2)	6830(5)	28(2)
O(1)	10829(4)	8941(2)	3571(4)	29(1)
Yb(1)	9349(1)	8856(1)	5250(1)	26(1)

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Table S6. Bond lengths [Å] and angles [°] for **5**.

C(1)-N(1)	1.360(12)
C(1)-C(2)	1.370(11)
C(1)-C(10)	1.466(12)
C(2)-C(3)	1.365(10)
C(2)-H(2)	0.9500
C(3)-C(4)	1.356(10)
C(3)-H(3)	0.9500
C(4)-C(5)	1.412(9)
C(4)-H(4)	0.9500
C(5)-N(1)	1.329(12)
C(5)-C(6)	1.467(9)
C(6)-C(7)	1.337(10)
C(6)-O(1)	1.354(8)
C(7)-C(8)	1.416(11)
C(7)-H(7)	0.9500
C(8)-C(9)	1.332(10)
C(8)-H(8)	0.9500
C(9)-O(1)	1.367(8)
C(9)-H(9)	0.9500
C(10)-N(2)	1.281(9)
C(10)-H(10)	0.9500
C(11)-C(12)	1.390(10)
C(11)-C(16)	1.416(10)
C(11)-N(2)	1.424(8)
C(12)-C(13)	1.378(15)
C(12)-C(17)	1.528(10)
C(13)-C(14)	1.395(16)
C(13)-H(13)	0.9500
C(14)-C(15)	1.366(16)
C(14)-H(14)	0.9500
C(15)-C(16)	1.367(15)
C(15)-H(15)	0.9500
C(16)-C(20)	1.510(10)
C(17)-C(19)	1.513(10)
C(17)-C(18)	1.515(10)
C(17)-H(17)	1.0000

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C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(21)	1.518(10)
C(20)-C(22)	1.524(11)
C(20)-H(20)	1.0000
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-C(31)	1.377(15)
C(23)-C(24)	1.414(10)
C(23)-C(27)	1.447(11)
C(23)-Yb(1)	2.791(7)
C(24)-C(25)	1.390(13)
C(24)-Yb(1)	2.701(7)
C(24)-H(24)	0.9500
C(25)-C(26)	1.395(10)
C(25)-Yb(1)	2.701(12)
C(25)-H(25)	0.9500
C(26)-C(27)	1.415(14)
C(26)-Yb(1)	2.719(12)
C(26)-H(26)	0.9500
C(27)-C(28)	1.444(13)
C(27)-Yb(1)	2.810(7)
C(28)-C(29)	1.333(14)
C(28)-H(28)	0.9500
C(29)-C(30)	1.397(13)
C(29)-H(29)	0.9500
C(30)-C(31)	1.379(16)
C(30)-H(30)	0.9500
C(31)-H(31)	0.9500
C(32)-C(33)	1.393(14)

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C(32)-C(40)	1.440(11)
C(32)-C(36)	1.459(11)
C(32)-Yb(1)	2.800(7)
C(33)-C(34)	1.332(17)
C(33)-Yb(1)	2.672(12)
C(33)-H(33)	0.9500
C(34)-C(35)	1.381(12)
C(34)-Yb(1)	2.689(9)
C(34)-H(34)	0.9500
C(35)-C(36)	1.401(10)
C(35)-Yb(1)	2.754(8)
C(35)-H(35)	0.9500
C(36)-C(37)	1.430(15)
C(36)-Yb(1)	2.860(7)
C(37)-C(38)	1.362(18)
C(37)-H(37)	0.9500
C(38)-C(39)	1.403(18)
C(38)-H(38)	0.9500
C(39)-C(40)	1.368(15)
C(39)-H(39)	0.9500
C(40)-H(40)	0.9500
N(1)-Yb(1)	2.527(10)
N(2)-Yb(1)	2.714(6)
O(1)-Yb(1)	2.592(5)
N(1)-C(1)-C(2)	122.7(9)
N(1)-C(1)-C(10)	115.7(9)
C(2)-C(1)-C(10)	121.1(8)
C(3)-C(2)-C(1)	117.9(7)
C(3)-C(2)-H(2)	121.0
C(1)-C(2)-H(2)	121.0
C(4)-C(3)-C(2)	122.0(7)
C(4)-C(3)-H(3)	119.0
C(2)-C(3)-H(3)	119.0
C(3)-C(4)-C(5)	116.7(7)
C(3)-C(4)-H(4)	121.6
C(5)-C(4)-H(4)	121.6
N(1)-C(5)-C(4)	122.8(7)

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N(1)-C(5)-C(6)	116.3(7)
C(4)-C(5)-C(6)	120.9(6)
C(7)-C(6)-O(1)	110.2(6)
C(7)-C(6)-C(5)	133.1(7)
O(1)-C(6)-C(5)	116.5(6)
C(6)-C(7)-C(8)	106.7(7)
C(6)-C(7)-H(7)	126.6
C(8)-C(7)-H(7)	126.6
C(9)-C(8)-C(7)	106.5(7)
C(9)-C(8)-H(8)	126.8
C(7)-C(8)-H(8)	126.8
C(8)-C(9)-O(1)	110.2(7)
C(8)-C(9)-H(9)	124.9
O(1)-C(9)-H(9)	124.9
N(2)-C(10)-C(1)	125.7(8)
N(2)-C(10)-H(10)	117.1
C(1)-C(10)-H(10)	117.1
C(12)-C(11)-C(16)	121.6(7)
C(12)-C(11)-N(2)	119.3(7)
C(16)-C(11)-N(2)	118.9(7)
C(13)-C(12)-C(11)	118.5(9)
C(13)-C(12)-C(17)	118.1(9)
C(11)-C(12)-C(17)	123.4(7)
C(12)-C(13)-C(14)	120.3(11)
C(12)-C(13)-H(13)	119.8
C(14)-C(13)-H(13)	119.8
C(15)-C(14)-C(13)	120.0(12)
C(15)-C(14)-H(14)	120.0
C(13)-C(14)-H(14)	120.0
C(14)-C(15)-C(16)	122.1(13)
C(14)-C(15)-H(15)	118.9
C(16)-C(15)-H(15)	118.9
C(15)-C(16)-C(11)	117.4(9)
C(15)-C(16)-C(20)	121.6(10)
C(11)-C(16)-C(20)	120.9(7)
C(19)-C(17)-C(18)	109.5(7)
C(19)-C(17)-C(12)	113.1(6)
C(18)-C(17)-C(12)	112.2(7)

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C(19)-C(17)-H(17)	107.2
C(18)-C(17)-H(17)	107.2
C(12)-C(17)-H(17)	107.2
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-C(21)	109.9(7)
C(16)-C(20)-C(22)	112.7(7)
C(21)-C(20)-C(22)	111.6(8)
C(16)-C(20)-H(20)	107.4
C(21)-C(20)-H(20)	107.4
C(22)-C(20)-H(20)	107.4
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(31)-C(23)-C(24)	135.0(9)
C(31)-C(23)-C(27)	119.2(9)
C(24)-C(23)-C(27)	105.5(7)
C(31)-C(23)-Yb(1)	122.6(6)
C(24)-C(23)-Yb(1)	71.6(4)

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C(27)-C(23)-Yb(1)	75.7(4)
C(25)-C(24)-C(23)	110.2(8)
C(25)-C(24)-Yb(1)	75.1(6)
C(23)-C(24)-Yb(1)	78.7(4)
C(25)-C(24)-H(24)	124.9
C(23)-C(24)-H(24)	124.9
Yb(1)-C(24)-H(24)	113.3
C(24)-C(25)-C(26)	108.1(10)
C(24)-C(25)-Yb(1)	75.1(6)
C(26)-C(25)-Yb(1)	75.8(9)
C(24)-C(25)-H(25)	126.0
C(26)-C(25)-H(25)	126.0
Yb(1)-C(25)-H(25)	115.4
C(25)-C(26)-C(27)	108.5(11)
C(25)-C(26)-Yb(1)	74.4(9)
C(27)-C(26)-Yb(1)	78.8(6)
C(25)-C(26)-H(26)	125.7
C(27)-C(26)-H(26)	125.7
Yb(1)-C(26)-H(26)	113.4
C(26)-C(27)-C(28)	134.0(10)
C(26)-C(27)-C(23)	107.7(9)
C(28)-C(27)-C(23)	118.3(8)
C(26)-C(27)-Yb(1)	71.7(6)
C(28)-C(27)-Yb(1)	122.1(6)
C(23)-C(27)-Yb(1)	74.3(4)
C(29)-C(28)-C(27)	118.9(10)
C(29)-C(28)-H(28)	120.6
C(27)-C(28)-H(28)	120.6
C(28)-C(29)-C(30)	123.1(10)
C(28)-C(29)-H(29)	118.4
C(30)-C(29)-H(29)	118.4
C(31)-C(30)-C(29)	119.5(10)
C(31)-C(30)-H(30)	120.3
C(29)-C(30)-H(30)	120.3
C(23)-C(31)-C(30)	121.0(12)
C(23)-C(31)-H(31)	119.5
C(30)-C(31)-H(31)	119.5
C(33)-C(32)-C(40)	136.1(10)

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C(33)-C(32)-C(36)	104.8(8)
C(40)-C(32)-C(36)	119.0(8)
C(33)-C(32)-Yb(1)	70.2(6)
C(40)-C(32)-Yb(1)	120.1(5)
C(36)-C(32)-Yb(1)	77.3(4)
C(34)-C(33)-C(32)	110.8(11)
C(34)-C(33)-Yb(1)	76.3(7)
C(32)-C(33)-Yb(1)	80.4(6)
C(34)-C(33)-H(33)	124.6
C(32)-C(33)-H(33)	124.6
Yb(1)-C(33)-H(33)	110.8
C(33)-C(34)-C(35)	109.8(10)
C(33)-C(34)-Yb(1)	74.9(7)
C(35)-C(34)-Yb(1)	77.9(5)
C(33)-C(34)-H(34)	125.1
C(35)-C(34)-H(34)	125.1
Yb(1)-C(34)-H(34)	114.1
C(34)-C(35)-C(36)	107.6(8)
C(34)-C(35)-Yb(1)	72.7(5)
C(36)-C(35)-Yb(1)	79.8(5)
C(34)-C(35)-H(35)	126.2
C(36)-C(35)-H(35)	126.2
Yb(1)-C(35)-H(35)	113.7
C(35)-C(36)-C(37)	134.4(10)
C(35)-C(36)-C(32)	106.8(7)
C(37)-C(36)-C(32)	118.7(9)
C(35)-C(36)-Yb(1)	71.4(4)
C(37)-C(36)-Yb(1)	122.5(7)
C(32)-C(36)-Yb(1)	72.8(4)
C(38)-C(37)-C(36)	119.2(12)
C(38)-C(37)-H(37)	120.4
C(36)-C(37)-H(37)	120.4
C(37)-C(38)-C(39)	122.6(11)
C(37)-C(38)-H(38)	118.7
C(39)-C(38)-H(38)	118.7
C(40)-C(39)-C(38)	121.2(12)
C(40)-C(39)-H(39)	119.4
C(38)-C(39)-H(39)	119.4

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C(39)-C(40)-C(32)	119.2(11)
C(39)-C(40)-H(40)	120.4
C(32)-C(40)-H(40)	120.4
C(5)-N(1)-C(1)	117.7(9)
C(5)-N(1)-Yb(1)	121.6(6)
C(1)-N(1)-Yb(1)	120.2(7)
C(10)-N(2)-C(11)	118.0(6)
C(10)-N(2)-Yb(1)	111.8(5)
C(11)-N(2)-Yb(1)	129.4(4)
C(6)-O(1)-C(9)	106.4(6)
C(6)-O(1)-Yb(1)	116.5(4)
C(9)-O(1)-Yb(1)	131.0(4)
N(1)-Yb(1)-O(1)	62.9(2)
N(1)-Yb(1)-C(33)	123.6(2)
O(1)-Yb(1)-C(33)	120.9(3)
N(1)-Yb(1)-C(34)	101.6(3)
O(1)-Yb(1)-C(34)	95.6(3)
C(33)-Yb(1)-C(34)	28.8(4)
N(1)-Yb(1)-C(24)	115.6(3)
O(1)-Yb(1)-C(24)	121.5(2)
C(33)-Yb(1)-C(24)	107.2(4)
C(34)-Yb(1)-C(24)	135.9(3)
N(1)-Yb(1)-C(25)	128.9(3)
O(1)-Yb(1)-C(25)	101.0(3)
C(33)-Yb(1)-C(25)	106.5(4)
C(34)-Yb(1)-C(25)	129.0(3)
C(24)-Yb(1)-C(25)	29.8(3)
N(1)-Yb(1)-N(2)	64.8(2)
O(1)-Yb(1)-N(2)	124.54(17)
C(33)-Yb(1)-N(2)	75.7(3)
C(34)-Yb(1)-N(2)	77.9(2)
C(24)-Yb(1)-N(2)	96.7(2)
C(25)-Yb(1)-N(2)	126.0(3)
N(1)-Yb(1)-C(26)	104.5(4)
O(1)-Yb(1)-C(26)	73.6(3)
C(33)-Yb(1)-C(26)	131.5(4)
C(34)-Yb(1)-C(26)	142.6(3)
C(24)-Yb(1)-C(26)	49.2(3)

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C(25)-Yb(1)-C(26)	29.8(2)
N(2)-Yb(1)-C(26)	137.9(3)
N(1)-Yb(1)-C(35)	106.2(3)
O(1)-Yb(1)-C(35)	72.8(2)
C(33)-Yb(1)-C(35)	48.3(4)
C(34)-Yb(1)-C(35)	29.4(3)
C(24)-Yb(1)-C(35)	137.9(2)
C(25)-Yb(1)-C(35)	114.7(3)
N(2)-Yb(1)-C(35)	106.0(2)
C(26)-Yb(1)-C(35)	115.9(3)
N(1)-Yb(1)-C(23)	86.2(3)
O(1)-Yb(1)-C(23)	105.1(2)
C(33)-Yb(1)-C(23)	132.5(4)
C(34)-Yb(1)-C(23)	159.2(3)
C(24)-Yb(1)-C(23)	29.8(2)
C(25)-Yb(1)-C(23)	49.5(3)
N(2)-Yb(1)-C(23)	88.4(2)
C(26)-Yb(1)-C(23)	49.6(3)
C(35)-Yb(1)-C(23)	163.9(2)
N(1)-Yb(1)-C(32)	149.8(3)
O(1)-Yb(1)-C(32)	113.4(2)
C(33)-Yb(1)-C(32)	29.4(3)
C(34)-Yb(1)-C(32)	48.2(3)
C(24)-Yb(1)-C(32)	92.2(2)
C(25)-Yb(1)-C(32)	81.1(3)
N(2)-Yb(1)-C(32)	102.4(2)
C(26)-Yb(1)-C(32)	102.6(3)
C(35)-Yb(1)-C(32)	48.8(2)
C(23)-Yb(1)-C(32)	122.0(2)
N(1)-Yb(1)-C(27)	80.1(3)
O(1)-Yb(1)-C(27)	76.3(2)
C(33)-Yb(1)-C(27)	154.5(4)
C(34)-Yb(1)-C(27)	169.9(3)
C(24)-Yb(1)-C(27)	48.8(2)
C(25)-Yb(1)-C(27)	48.8(3)
N(2)-Yb(1)-C(27)	111.6(2)
C(26)-Yb(1)-C(27)	29.6(3)
C(35)-Yb(1)-C(27)	140.6(3)

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C(23)-Yb(1)-C(27)	29.9(2)
C(32)-Yb(1)-C(27)	129.5(2)

Table S7. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	36(6)	41(6)	18(5)	-3(4)	2(4)	-13(5)
C(2)	18(5)	40(5)	28(5)	2(4)	3(4)	7(4)
C(3)	22(5)	29(5)	63(6)	8(4)	13(4)	6(4)
C(4)	53(5)	30(4)	28(5)	10(4)	20(5)	26(4)
C(5)	16(4)	22(4)	24(4)	0(3)	5(3)	0(3)
C(6)	24(4)	16(4)	29(4)	-9(4)	3(3)	-2(4)
C(7)	38(5)	36(5)	38(5)	-1(4)	24(4)	2(4)
C(8)	53(6)	22(5)	57(6)	11(4)	30(5)	2(4)
C(9)	45(6)	34(5)	24(5)	9(4)	-1(4)	12(4)
C(10)	26(5)	38(5)	31(5)	0(4)	9(4)	0(4)
C(11)	16(4)	36(5)	22(4)	16(4)	2(3)	3(4)
C(12)	29(5)	32(5)	24(5)	4(4)	-2(4)	-9(4)
C(13)	40(9)	25(7)	35(8)	7(5)	7(6)	5(6)
C(14)	26(5)	43(6)	46(6)	22(5)	9(4)	2(5)
C(15)	29(8)	51(9)	34(7)	19(6)	1(6)	7(6)
C(16)	16(4)	39(5)	28(5)	6(4)	6(4)	0(4)
C(17)	49(6)	39(5)	23(5)	2(4)	9(4)	-5(4)
C(18)	75(7)	41(5)	44(6)	-2(5)	18(5)	-29(5)
C(19)	62(6)	36(5)	61(6)	4(5)	28(5)	8(5)
C(20)	44(5)	45(5)	39(6)	1(4)	27(4)	-6(4)
C(21)	132(12)	75(7)	26(6)	-13(5)	23(7)	-31(8)
C(22)	76(8)	48(6)	128(10)	-10(7)	64(7)	2(6)
C(23)	25(5)	25(4)	35(5)	-5(4)	-4(4)	-7(4)
C(24)	39(5)	20(4)	37(5)	-11(4)	12(4)	-2(4)
C(25)	45(7)	26(6)	34(7)	-1(5)	8(6)	10(5)
C(26)	85(9)	16(5)	27(7)	-6(5)	8(7)	-3(6)
C(27)	40(5)	16(4)	41(6)	-15(4)	9(4)	-9(4)
C(28)	32(8)	42(7)	72(9)	-31(6)	15(6)	-16(6)

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C(29)	32(6)	43(6)	68(8)	-30(6)	3(6)	-1(5)
C(30)	47(7)	38(6)	54(7)	-16(5)	-21(6)	4(5)
C(31)	47(8)	25(6)	56(8)	-10(5)	-1(6)	7(5)
C(32)	25(4)	31(5)	57(6)	-8(5)	1(4)	-12(4)
C(33)	16(6)	57(9)	37(8)	37(6)	0(6)	-3(6)
C(34)	38(7)	39(6)	45(7)	-3(5)	-2(6)	4(5)
C(35)	25(5)	73(7)	38(6)	-22(5)	2(4)	-2(5)
C(36)	27(5)	48(6)	33(5)	11(4)	-11(4)	-2(4)
C(37)	41(9)	81(12)	54(9)	43(8)	-23(7)	-22(8)
C(38)	37(7)	53(8)	143(13)	46(8)	-32(8)	-9(6)
C(39)	20(7)	50(9)	144(15)	-18(9)	-8(8)	3(6)
C(40)	20(5)	58(7)	71(8)	-6(6)	8(5)	6(5)
N(1)	28(5)	18(5)	18(5)	5(4)	-3(4)	2(4)
N(2)	34(4)	31(4)	20(4)	0(3)	10(3)	1(3)
O(1)	29(3)	37(3)	21(3)	1(2)	12(2)	5(3)
Yb(1)	24(1)	26(1)	29(1)	-2(1)	5(1)	0(1)

Table S8. Torsion angles [°] for **5**.

N(1)-C(5)-C(6)-O(1)	-12.6(9)
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Crystallographic data and tables for **6** (CCDC: 794891)

Table S9. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **6**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
C(1)	4090(5)	1179(1)	-207(5)	15(1)
C(2)	2716(5)	1168(1)	-1455(5)	18(1)
C(3)	1579(6)	1431(1)	-1700(5)	20(1)
C(4)	1873(5)	1695(1)	-687(5)	19(1)
C(5)	3296(5)	1698(1)	530(5)	14(1)

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C(6)	3597(5)	1971(1)	1655(5)	16(1)
C(7)	4341(5)	1875(1)	3095(5)	19(1)
C(8)	4541(5)	2120(1)	4156(5)	21(1)
C(9)	4008(5)	2463(1)	3803(5)	22(1)
C(10)	3287(5)	2566(1)	2391(5)	24(1)
C(11)	3080(5)	2320(1)	1320(5)	22(1)
C(12)	5234(6)	887(1)	161(5)	18(1)
C(13)	7426(5)	553(1)	1572(5)	16(1)
C(14)	7046(5)	308(1)	2386(5)	20(1)
C(15)	7865(5)	-17(1)	2721(5)	22(1)
C(16)	9057(5)	-85(1)	2311(5)	23(1)
C(17)	9452(6)	169(1)	1536(5)	24(1)
C(18)	8665(5)	493(1)	1155(5)	19(1)
C(19)	5739(5)	370(1)	2890(5)	23(1)
C(20)	6306(6)	292(1)	4485(5)	32(1)
C(21)	4274(6)	150(2)	2040(6)	40(2)
C(22)	9064(5)	763(1)	269(5)	21(1)
C(23)	8164(6)	680(1)	-1327(5)	30(1)
C(24)	10837(6)	790(2)	677(6)	33(1)
C(25)	9495(5)	1127(1)	4787(5)	19(1)
C(26)	8099(5)	1199(1)	4985(5)	22(1)
C(27)	8054(6)	1575(1)	5164(5)	25(1)
C(28)	9328(5)	1737(1)	5015(4)	21(1)
C(29)	10242(5)	1466(1)	4785(4)	19(1)
C(30)	11691(6)	1468(1)	4617(5)	22(1)
C(31)	12368(6)	1150(2)	4525(5)	26(1)
C(32)	11649(6)	820(2)	4557(5)	26(1)
C(33)	10237(6)	805(1)	4671(5)	24(1)
C(34)	7784(5)	1765(1)	-70(5)	19(1)
C(35)	9292(6)	1780(1)	1141(5)	20(1)
C(36)	9208(5)	2054(1)	2028(5)	23(1)
C(37)	7689(6)	2204(1)	1478(5)	21(1)
C(38)	6775(5)	2028(1)	133(5)	19(1)
C(39)	5233(5)	2084(1)	-945(5)	23(1)
C(40)	4713(6)	1887(1)	-2169(5)	25(1)
C(41)	5700(6)	1623(1)	-2362(5)	24(1)
C(42)	7213(6)	1566(1)	-1351(5)	21(1)
N(1)	4411(4)	1445(1)	774(4)	12(1)

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N(2)	6593(5)	890(1)	1222(4)	16(1)
Yb(1)	7422(1)	1521(1)	2344(1)	17(1)

Table S10. Bond lengths [Å] and angles [°] for **6**.

C(1)-N(1)	1.359(5)
C(1)-C(2)	1.380(6)
C(1)-C(12)	1.458(6)
C(2)-C(3)	1.388(6)
C(2)-H(2)	0.9500
C(3)-C(4)	1.378(6)
C(3)-H(3)	0.9500
C(4)-C(5)	1.388(6)
C(4)-H(4)	0.9500
C(5)-N(1)	1.346(5)
C(5)-C(6)	1.482(6)
C(6)-C(11)	1.384(6)
C(6)-C(7)	1.396(6)
C(7)-C(8)	1.377(6)
C(7)-H(7)	0.9500
C(8)-C(9)	1.371(6)
C(8)-H(8)	0.9500
C(9)-C(10)	1.377(6)
C(9)-H(9)	0.9500
C(10)-C(11)	1.387(6)
C(10)-H(10)	0.9500
C(11)-H(11)	0.9500
C(12)-N(2)	1.276(6)
C(12)-H(12)	0.9500
C(13)-C(14)	1.385(6)
C(13)-C(18)	1.406(6)
C(13)-N(2)	1.443(5)
C(14)-C(15)	1.398(6)
C(14)-C(19)	1.527(6)
C(15)-C(16)	1.366(6)
C(15)-H(15)	0.9500

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C(16)-C(17)	1.385(6)
C(16)-H(16)	0.9500
C(17)-C(18)	1.385(6)
C(17)-H(17)	0.9500
C(18)-C(22)	1.510(6)
C(19)-C(21)	1.516(6)
C(19)-C(20)	1.529(6)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(24)	1.522(6)
C(22)-C(23)	1.532(6)
C(22)-H(22)	1.0000
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-C(33)	1.417(7)
C(25)-C(26)	1.422(6)
C(25)-C(29)	1.445(6)
C(25)-Yb(1)	2.853(5)
C(26)-C(27)	1.420(7)
C(26)-Yb(1)	2.796(5)
C(26)-H(26)	0.9500
C(27)-C(28)	1.394(6)
C(27)-Yb(1)	2.722(5)
C(27)-H(27)	0.9500
C(28)-C(29)	1.404(6)
C(28)-Yb(1)	2.696(4)
C(28)-H(28)	0.9500
C(29)-C(30)	1.428(6)
C(29)-Yb(1)	2.773(4)

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C(30)-C(31)	1.365(7)
C(30)-H(30)	0.9500
C(31)-C(32)	1.412(7)
C(31)-H(31)	0.9500
C(32)-C(33)	1.368(7)
C(32)-H(32)	0.9500
C(33)-H(33)	0.9500
C(34)-C(42)	1.411(6)
C(34)-C(35)	1.433(6)
C(34)-C(38)	1.434(6)
C(34)-Yb(1)	2.802(5)
C(35)-C(36)	1.398(7)
C(35)-Yb(1)	2.703(5)
C(35)-H(35)	0.9500
C(36)-C(37)	1.398(6)
C(36)-Yb(1)	2.699(5)
C(36)-H(36)	0.9500
C(37)-C(38)	1.445(6)
C(37)-Yb(1)	2.751(5)
C(37)-H(37)	0.9500
C(38)-C(39)	1.412(6)
C(38)-Yb(1)	2.829(5)
C(39)-C(40)	1.364(7)
C(39)-H(39)	0.9500
C(40)-C(41)	1.417(7)
C(40)-H(40)	0.9500
C(41)-C(42)	1.369(6)
C(41)-H(41)	0.9500
C(42)-H(42)	0.9500
N(1)-Yb(1)	2.592(4)
N(2)-Yb(1)	2.597(4)
N(1)-C(1)-C(2)	122.9(4)
N(1)-C(1)-C(12)	116.5(4)
C(2)-C(1)-C(12)	120.5(4)
C(1)-C(2)-C(3)	118.9(4)
C(1)-C(2)-H(2)	120.6
C(3)-C(2)-H(2)	120.6

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C(4)-C(3)-C(2)	118.5(4)
C(4)-C(3)-H(3)	120.8
C(2)-C(3)-H(3)	120.8
C(3)-C(4)-C(5)	120.1(4)
C(3)-C(4)-H(4)	120.0
C(5)-C(4)-H(4)	120.0
N(1)-C(5)-C(4)	121.9(4)
N(1)-C(5)-C(6)	117.5(4)
C(4)-C(5)-C(6)	120.5(4)
C(11)-C(6)-C(7)	118.1(4)
C(11)-C(6)-C(5)	121.6(4)
C(7)-C(6)-C(5)	120.1(4)
C(8)-C(7)-C(6)	121.1(5)
C(8)-C(7)-H(7)	119.5
C(6)-C(7)-H(7)	119.5
C(9)-C(8)-C(7)	119.9(5)
C(9)-C(8)-H(8)	120.0
C(7)-C(8)-H(8)	120.0
C(8)-C(9)-C(10)	120.2(5)
C(8)-C(9)-H(9)	119.9
C(10)-C(9)-H(9)	119.9
C(9)-C(10)-C(11)	120.0(5)
C(9)-C(10)-H(10)	120.0
C(11)-C(10)-H(10)	120.0
C(6)-C(11)-C(10)	120.7(4)
C(6)-C(11)-H(11)	119.7
C(10)-C(11)-H(11)	119.7
N(2)-C(12)-C(1)	124.5(5)
N(2)-C(12)-H(12)	117.7
C(1)-C(12)-H(12)	117.7
C(14)-C(13)-C(18)	121.9(4)
C(14)-C(13)-N(2)	118.9(4)
C(18)-C(13)-N(2)	119.1(4)
C(13)-C(14)-C(15)	118.3(4)
C(13)-C(14)-C(19)	123.2(4)
C(15)-C(14)-C(19)	118.4(4)
C(16)-C(15)-C(14)	121.0(5)
C(16)-C(15)-H(15)	119.5

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C(14)-C(15)-H(15)	119.5
C(15)-C(16)-C(17)	119.7(5)
C(15)-C(16)-H(16)	120.1
C(17)-C(16)-H(16)	120.1
C(18)-C(17)-C(16)	121.8(5)
C(18)-C(17)-H(17)	119.1
C(16)-C(17)-H(17)	119.1
C(17)-C(18)-C(13)	117.2(4)
C(17)-C(18)-C(22)	121.5(4)
C(13)-C(18)-C(22)	121.3(4)
C(21)-C(19)-C(14)	111.7(4)
C(21)-C(19)-C(20)	109.7(4)
C(14)-C(19)-C(20)	112.0(4)
C(21)-C(19)-H(19)	107.8
C(14)-C(19)-H(19)	107.8
C(20)-C(19)-H(19)	107.8
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(18)-C(22)-C(24)	113.0(4)
C(18)-C(22)-C(23)	110.6(4)
C(24)-C(22)-C(23)	110.4(4)
C(18)-C(22)-H(22)	107.5
C(24)-C(22)-H(22)	107.5
C(23)-C(22)-H(22)	107.5
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5

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H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(33)-C(25)-C(26)	132.7(5)
C(33)-C(25)-C(29)	119.6(4)
C(26)-C(25)-C(29)	107.6(4)
C(33)-C(25)-Yb(1)	122.4(3)
C(26)-C(25)-Yb(1)	73.2(3)
C(29)-C(25)-Yb(1)	72.1(2)
C(27)-C(26)-C(25)	106.5(4)
C(27)-C(26)-Yb(1)	72.2(3)
C(25)-C(26)-Yb(1)	77.7(3)
C(27)-C(26)-H(26)	126.7
C(25)-C(26)-H(26)	126.7
Yb(1)-C(26)-H(26)	115.8
C(28)-C(27)-C(26)	110.0(4)
C(28)-C(27)-Yb(1)	74.1(3)
C(26)-C(27)-Yb(1)	78.0(3)
C(28)-C(27)-H(27)	125.0
C(26)-C(27)-H(27)	125.0
Yb(1)-C(27)-H(27)	114.8
C(27)-C(28)-C(29)	107.9(5)
C(27)-C(28)-Yb(1)	76.1(3)
C(29)-C(28)-Yb(1)	78.2(3)
C(27)-C(28)-H(28)	126.0
C(29)-C(28)-H(28)	126.0
Yb(1)-C(28)-H(28)	112.2
C(28)-C(29)-C(30)	133.3(5)
C(28)-C(29)-C(25)	107.9(4)
C(30)-C(29)-C(25)	118.8(4)
C(28)-C(29)-Yb(1)	72.1(2)
C(30)-C(29)-Yb(1)	117.9(3)
C(25)-C(29)-Yb(1)	78.2(2)

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C(31)-C(30)-C(29)	119.4(5)
C(31)-C(30)-H(30)	120.3
C(29)-C(30)-H(30)	120.3
C(30)-C(31)-C(32)	121.5(5)
C(30)-C(31)-H(31)	119.2
C(32)-C(31)-H(31)	119.2
C(33)-C(32)-C(31)	121.2(5)
C(33)-C(32)-H(32)	119.4
C(31)-C(32)-H(32)	119.4
C(32)-C(33)-C(25)	119.4(5)
C(32)-C(33)-H(33)	120.3
C(25)-C(33)-H(33)	120.3
C(42)-C(34)-C(35)	132.9(5)
C(42)-C(34)-C(38)	119.2(4)
C(35)-C(34)-C(38)	107.8(4)
C(42)-C(34)-Yb(1)	121.5(3)
C(35)-C(34)-Yb(1)	71.1(3)
C(38)-C(34)-Yb(1)	76.3(3)
C(36)-C(35)-C(34)	107.2(4)
C(36)-C(35)-Yb(1)	74.8(3)
C(34)-C(35)-Yb(1)	78.7(3)
C(36)-C(35)-H(35)	126.4
C(34)-C(35)-H(35)	126.4
Yb(1)-C(35)-H(35)	112.6
C(35)-C(36)-C(37)	110.7(4)
C(35)-C(36)-Yb(1)	75.2(3)
C(37)-C(36)-Yb(1)	77.2(3)
C(35)-C(36)-H(36)	124.6
C(37)-C(36)-H(36)	124.6
Yb(1)-C(36)-H(36)	114.8
C(36)-C(37)-C(38)	107.0(4)
C(36)-C(37)-Yb(1)	73.1(3)
C(38)-C(37)-Yb(1)	78.0(3)
C(36)-C(37)-H(37)	126.5
C(38)-C(37)-H(37)	126.5
Yb(1)-C(37)-H(37)	114.8
C(39)-C(38)-C(34)	119.8(4)
C(39)-C(38)-C(37)	132.8(5)

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C(34)-C(38)-C(37)	107.3(4)
C(39)-C(38)-Yb(1)	122.4(3)
C(34)-C(38)-Yb(1)	74.2(3)
C(37)-C(38)-Yb(1)	72.0(3)
C(40)-C(39)-C(38)	119.6(5)
C(40)-C(39)-H(39)	120.2
C(38)-C(39)-H(39)	120.2
C(39)-C(40)-C(41)	120.6(4)
C(39)-C(40)-H(40)	119.7
C(41)-C(40)-H(40)	119.7
C(42)-C(41)-C(40)	121.3(5)
C(42)-C(41)-H(41)	119.3
C(40)-C(41)-H(41)	119.3
C(41)-C(42)-C(34)	119.4(5)
C(41)-C(42)-H(42)	120.3
C(34)-C(42)-H(42)	120.3
C(5)-N(1)-C(1)	117.7(4)
C(5)-N(1)-Yb(1)	125.6(3)
C(1)-N(1)-Yb(1)	112.7(3)
C(12)-N(2)-C(13)	116.1(4)
C(12)-N(2)-Yb(1)	113.0(3)
C(13)-N(2)-Yb(1)	130.9(3)
N(1)-Yb(1)-N(2)	65.27(12)
N(1)-Yb(1)-C(28)	138.02(13)
N(2)-Yb(1)-C(28)	132.16(14)
N(1)-Yb(1)-C(36)	124.25(13)
N(2)-Yb(1)-C(36)	134.33(13)
C(28)-Yb(1)-C(36)	74.32(15)
N(1)-Yb(1)-C(35)	119.08(13)
N(2)-Yb(1)-C(35)	104.36(13)
C(28)-Yb(1)-C(35)	95.12(15)
C(36)-Yb(1)-C(35)	29.99(14)
N(1)-Yb(1)-C(27)	111.48(13)
N(2)-Yb(1)-C(27)	115.70(14)
C(28)-Yb(1)-C(27)	29.83(14)
C(36)-Yb(1)-C(27)	101.96(15)
C(35)-Yb(1)-C(27)	124.94(15)
N(1)-Yb(1)-C(37)	96.93(12)

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N(2)-Yb(1)-C(37)	138.48(13)
C(28)-Yb(1)-C(37)	86.78(14)
C(36)-Yb(1)-C(37)	29.71(13)
C(35)-Yb(1)-C(37)	49.88(14)
C(27)-Yb(1)-C(37)	105.65(15)
N(1)-Yb(1)-C(29)	156.62(12)
N(2)-Yb(1)-C(29)	109.08(13)
C(28)-Yb(1)-C(29)	29.72(13)
C(36)-Yb(1)-C(29)	76.72(14)
C(35)-Yb(1)-C(29)	84.20(14)
C(27)-Yb(1)-C(29)	48.64(14)
C(37)-Yb(1)-C(29)	100.58(14)
N(1)-Yb(1)-C(26)	107.58(12)
N(2)-Yb(1)-C(26)	86.91(13)
C(28)-Yb(1)-C(26)	49.61(15)
C(36)-Yb(1)-C(26)	122.53(14)
C(35)-Yb(1)-C(26)	132.58(14)
C(27)-Yb(1)-C(26)	29.80(14)
C(37)-Yb(1)-C(26)	134.57(14)
C(29)-Yb(1)-C(26)	49.08(14)
N(1)-Yb(1)-C(34)	88.99(12)
N(2)-Yb(1)-C(34)	91.35(13)
C(28)-Yb(1)-C(34)	122.54(14)
C(36)-Yb(1)-C(34)	48.90(14)
C(35)-Yb(1)-C(34)	30.11(13)
C(27)-Yb(1)-C(34)	150.82(15)
C(37)-Yb(1)-C(34)	49.33(14)
C(29)-Yb(1)-C(34)	114.20(14)
C(26)-Yb(1)-C(34)	160.71(14)
N(1)-Yb(1)-C(38)	76.28(12)
N(2)-Yb(1)-C(38)	109.07(13)
C(28)-Yb(1)-C(38)	116.65(14)
C(36)-Yb(1)-C(38)	48.76(14)
C(35)-Yb(1)-C(38)	49.44(14)
C(27)-Yb(1)-C(38)	133.54(15)
C(37)-Yb(1)-C(38)	29.98(13)
C(29)-Yb(1)-C(38)	125.48(14)
C(26)-Yb(1)-C(38)	163.33(14)

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C(34)-Yb(1)-C(38)	29.50(13)
N(1)-Yb(1)-C(25)	130.15(12)
N(2)-Yb(1)-C(25)	83.58(13)
C(28)-Yb(1)-C(25)	48.95(15)
C(36)-Yb(1)-C(25)	105.47(14)
C(35)-Yb(1)-C(25)	105.34(14)
C(27)-Yb(1)-C(25)	48.17(15)
C(37)-Yb(1)-C(25)	130.26(14)
C(29)-Yb(1)-C(25)	29.72(13)
C(26)-Yb(1)-C(25)	29.13(13)
C(34)-Yb(1)-C(25)	131.59(14)
C(38)-Yb(1)-C(25)	153.28(14)

Table S11. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	20(3)	10(3)	19(3)	2(2)	13(2)	2(2)
C(2)	23(3)	20(3)	9(3)	-3(2)	7(2)	0(2)
C(3)	20(3)	26(3)	12(3)	3(2)	3(2)	0(2)
C(4)	18(3)	19(3)	20(3)	7(2)	8(2)	3(2)
C(5)	16(3)	14(3)	15(3)	6(2)	8(2)	-2(2)
C(6)	18(3)	14(3)	16(3)	-3(2)	7(2)	-2(2)
C(7)	17(3)	16(3)	23(3)	1(2)	9(2)	1(2)
C(8)	22(3)	24(3)	17(3)	-1(2)	7(2)	-1(2)
C(9)	17(3)	26(3)	23(3)	-9(2)	8(2)	-1(2)
C(10)	24(3)	21(3)	26(3)	0(2)	10(2)	6(2)
C(11)	20(3)	21(3)	21(3)	3(2)	6(2)	6(2)
C(12)	27(3)	11(3)	20(3)	-2(2)	16(3)	0(2)
C(13)	17(3)	15(3)	14(3)	0(2)	4(2)	2(2)
C(14)	22(3)	24(3)	13(3)	6(2)	8(2)	10(2)
C(15)	27(3)	16(3)	23(3)	4(2)	10(2)	-5(2)
C(16)	22(3)	19(3)	27(3)	5(2)	8(2)	3(2)
C(17)	25(3)	20(3)	26(3)	-1(2)	12(2)	3(2)
C(18)	22(3)	15(3)	17(3)	1(2)	6(2)	3(2)

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C(19)	25(3)	14(3)	35(3)	7(2)	17(2)	2(2)
C(20)	38(3)	25(4)	45(4)	5(3)	30(3)	-3(3)
C(21)	24(3)	45(4)	54(4)	0(3)	17(3)	0(3)
C(22)	31(3)	12(3)	25(3)	3(2)	17(2)	5(2)
C(23)	47(4)	18(3)	33(3)	4(2)	24(3)	9(3)
C(24)	39(4)	27(4)	42(4)	3(3)	26(3)	2(3)
C(25)	20(3)	16(3)	14(3)	3(2)	1(2)	-3(2)
C(26)	20(3)	25(3)	16(3)	3(2)	5(2)	-3(2)
C(27)	19(3)	39(4)	12(3)	2(2)	2(2)	7(2)
C(28)	25(3)	20(3)	12(3)	-2(2)	4(2)	-1(2)
C(29)	13(3)	27(3)	10(2)	1(2)	-1(2)	-1(2)
C(30)	23(3)	24(3)	16(3)	3(2)	4(2)	-3(2)
C(31)	19(3)	39(4)	22(3)	0(3)	10(2)	0(3)
C(32)	32(3)	26(3)	16(3)	-2(2)	7(2)	12(3)
C(33)	27(3)	18(3)	22(3)	2(2)	6(2)	1(2)
C(34)	23(3)	20(3)	17(3)	3(2)	12(2)	0(2)
C(35)	21(3)	17(3)	23(3)	8(2)	9(2)	0(2)
C(36)	21(3)	23(3)	24(3)	5(2)	8(2)	-7(2)
C(37)	32(3)	16(3)	18(3)	-4(2)	13(2)	-4(2)
C(38)	26(3)	12(3)	22(3)	8(2)	12(2)	1(2)
C(39)	22(3)	22(3)	28(3)	11(2)	14(2)	6(2)
C(40)	21(3)	29(3)	18(3)	9(2)	3(2)	-3(2)
C(41)	33(3)	23(3)	14(3)	0(2)	9(2)	-7(2)
C(42)	33(3)	14(3)	18(3)	2(2)	14(2)	-1(2)
N(1)	11(2)	10(2)	15(2)	1(2)	7(2)	-2(2)
N(2)	20(2)	12(2)	18(2)	2(2)	12(2)	1(2)
Yb(1)	18(1)	17(1)	14(1)	0(1)	6(1)	-1(1)

Crystallographic data and tables for **7** (CCDC: 794889)

Table S12. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **7**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

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C(1)	4310(2)	9556(5)	6694(3)	18(1)
C(2)	4422(2)	8253(5)	6629(3)	20(1)
C(3)	4104(2)	7504(5)	6095(3)	24(1)
C(4)	3677(2)	8095(6)	5632(3)	23(1)
C(5)	3576(2)	9412(5)	5726(3)	19(1)
C(6)	3112(2)	10057(6)	5264(3)	23(1)
C(7)	3101(2)	11379(6)	5096(3)	24(1)
C(8)	2581(2)	11774(5)	4644(3)	16(1)
C(9)	2643(3)	9440(6)	4969(4)	40(2)
C(10)	4686(2)	10349(5)	7214(3)	18(1)
C(11)	5074(2)	12184(5)	7758(3)	20(1)
C(12)	5572(3)	12283(6)	7274(5)	21(2)
C(13)	6044(2)	12822(6)	7663(4)	31(1)
C(14)	6028(2)	13278(6)	8478(4)	31(1)
C(15)	5527(2)	13284(5)	8918(3)	25(1)
C(16)	5042(2)	12733(5)	8573(3)	21(1)
C(17)	5618(3)	11889(7)	6339(4)	29(2)
C(18)	5796(3)	13079(7)	5806(4)	36(2)
C(19)	6022(3)	10815(7)	6170(4)	45(2)
C(20)	4496(2)	12729(5)	9089(3)	29(1)
C(21)	4547(3)	11871(8)	9859(4)	44(2)
C(22)	4336(3)	14102(6)	9374(4)	46(2)
C(23)	3660(2)	14428(5)	5729(3)	20(1)
C(24)	4215(2)	14097(4)	5999(3)	21(1)
C(25)	4251(2)	14416(4)	6884(5)	25(1)
C(26)	3733(2)	14862(5)	7165(3)	24(1)
C(27)	3351(2)	14891(5)	6461(3)	21(1)
C(28)	2788(2)	15345(5)	6353(4)	29(1)
C(29)	2563(2)	15378(6)	5562(4)	36(2)
C(30)	2872(3)	14939(6)	4852(4)	37(2)
C(31)	3402(2)	14470(5)	4919(3)	29(1)
C(32)	3145(2)	10914(6)	8273(3)	24(1)
C(33)	3031(2)	12236(6)	8368(4)	29(1)
C(34)	2638(2)	12592(6)	7745(4)	34(1)
C(35)	2514(2)	11529(6)	7231(4)	31(1)
C(36)	2819(2)	10469(6)	7557(3)	25(1)
C(37)	2839(2)	9127(6)	7348(3)	32(1)
C(38)	3161(3)	8320(6)	7815(4)	35(1)

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C(39)	3490(2)	8773(6)	8496(4)	33(1)
C(40)	3478(3)	10027(6)	8721(3)	29(1)
C(41)	4314(4)	10741(9)	13868(5)	69(2)
C(42)	4745(4)	11497(11)	14057(6)	84(3)
C(43)	4808(5)	12694(9)	13702(6)	84(3)
C(44)	4470(4)	13124(8)	13167(5)	65(2)
C(45)	4014(5)	12442(9)	12908(7)	85(3)
C(46)	3917(4)	11139(10)	13269(6)	90(3)
C(47)	3735(8)	13130(20)	12116(18)	276(11)
N(1)	3893(2)	10136(4)	6258(3)	16(1)
N(2)	4590(2)	11539(4)	7398(2)	16(1)
S(1)	2198(1)	10447(2)	4476(2)	64(1)
Yb(1)	3603(1)	12289(1)	6887(1)	17(1)

Table S13. Bond lengths [\AA] and angles [$^\circ$] for **7**.

C(1)-N(1)	1.344(6)
C(1)-C(2)	1.382(7)
C(1)-C(10)	1.462(6)
C(2)-C(3)	1.369(7)
C(2)-H(2)	0.9500
C(3)-C(4)	1.387(8)
C(3)-H(3)	0.9500
C(4)-C(5)	1.395(8)
C(4)-H(4)	0.9500
C(5)-N(1)	1.351(6)
C(5)-C(6)	1.478(7)
C(6)-C(9)	1.363(7)
C(6)-C(7)	1.397(8)
C(7)-C(8)	1.479(7)
C(7)-Yb(1)	3.194(5)
C(7)-H(7)	0.9500
C(8)-S(1)	1.671(5)
C(8)-H(8)	0.9500
C(9)-S(1)	1.675(6)
C(9)-H(9)	0.9500

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C(10)-N(2)	1.289(6)
C(10)-H(10)	0.9500
C(11)-C(16)	1.402(7)
C(11)-C(12)	1.407(9)
C(11)-N(2)	1.444(6)
C(12)-C(13)	1.390(9)
C(12)-C(17)	1.526(7)
C(13)-C(14)	1.364(8)
C(13)-H(13)	0.9500
C(14)-C(15)	1.371(7)
C(14)-H(14)	0.9500
C(15)-C(16)	1.394(7)
C(15)-H(15)	0.9500
C(16)-C(20)	1.526(8)
C(17)-C(19)	1.492(9)
C(17)-C(18)	1.550(10)
C(17)-H(17)	1.0000
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(21)	1.506(8)
C(20)-C(22)	1.540(8)
C(20)-H(20)	1.0000
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-C(31)	1.410(7)
C(23)-C(24)	1.423(7)
C(23)-C(27)	1.444(7)
C(23)-Yb(1)	2.872(5)
C(24)-C(25)	1.430(9)
C(24)-Yb(1)	2.751(5)

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C(24)-H(24)	0.9500
C(25)-C(26)	1.383(7)
C(25)-Yb(1)	2.688(4)
C(25)-H(25)	0.9500
C(26)-C(27)	1.429(7)
C(26)-Yb(1)	2.723(5)
C(26)-H(26)	0.9500
C(27)-C(28)	1.424(7)
C(27)-Yb(1)	2.845(5)
C(28)-C(29)	1.350(8)
C(28)-H(28)	0.9500
C(29)-C(30)	1.407(9)
C(29)-H(29)	0.9500
C(30)-C(31)	1.353(8)
C(30)-H(30)	0.9500
C(31)-H(31)	0.9500
C(32)-C(40)	1.402(8)
C(32)-C(33)	1.407(8)
C(32)-C(36)	1.438(7)
C(32)-Yb(1)	2.818(6)
C(33)-C(34)	1.400(8)
C(33)-Yb(1)	2.690(5)
C(33)-H(33)	0.9500
C(34)-C(35)	1.399(8)
C(34)-Yb(1)	2.673(5)
C(34)-H(34)	0.9500
C(35)-C(36)	1.412(8)
C(35)-Yb(1)	2.751(5)
C(35)-H(35)	0.9500
C(36)-C(37)	1.432(8)
C(36)-Yb(1)	2.850(5)
C(37)-C(38)	1.349(8)
C(37)-H(37)	0.9500
C(38)-C(39)	1.405(8)
C(38)-H(38)	0.9500
C(39)-C(40)	1.349(9)
C(39)-H(39)	0.9500
C(40)-H(40)	0.9500

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C(41)-C(42)	1.322(12)
C(41)-C(46)	1.393(12)
C(41)-H(41)	0.9500
C(42)-C(43)	1.370(14)
C(42)-H(42)	0.9500
C(43)-C(44)	1.243(12)
C(43)-H(43)	0.9500
C(44)-C(45)	1.354(12)
C(44)-H(44)	0.9500
C(45)-C(46)	1.484(13)
C(45)-C(47)	1.58(3)
C(46)-H(46)	0.9500
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
N(1)-Yb(1)	2.538(4)
N(2)-Yb(1)	2.591(4)

N(1)-C(1)-C(2)	122.8(4)
N(1)-C(1)-C(10)	118.6(4)
C(2)-C(1)-C(10)	118.4(4)
C(3)-C(2)-C(1)	119.6(5)
C(3)-C(2)-H(2)	120.2
C(1)-C(2)-H(2)	120.2
C(2)-C(3)-C(4)	118.1(5)
C(2)-C(3)-H(3)	121.0
C(4)-C(3)-H(3)	121.0
C(3)-C(4)-C(5)	120.2(5)
C(3)-C(4)-H(4)	119.9
C(5)-C(4)-H(4)	119.9
N(1)-C(5)-C(4)	121.0(5)
N(1)-C(5)-C(6)	117.7(4)
C(4)-C(5)-C(6)	121.3(5)
C(9)-C(6)-C(7)	112.4(5)
C(9)-C(6)-C(5)	124.1(5)
C(7)-C(6)-C(5)	123.5(5)
C(6)-C(7)-C(8)	112.2(5)
C(6)-C(7)-Yb(1)	96.8(4)

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C(8)-C(7)-Yb(1)	130.5(3)
C(6)-C(7)-H(7)	123.9
C(8)-C(7)-H(7)	123.9
Yb(1)-C(7)-H(7)	46.5
C(7)-C(8)-S(1)	107.5(4)
C(7)-C(8)-H(8)	126.3
S(1)-C(8)-H(8)	126.3
C(6)-C(9)-S(1)	112.2(5)
C(6)-C(9)-H(9)	123.9
S(1)-C(9)-H(9)	123.9
N(2)-C(10)-C(1)	123.8(4)
N(2)-C(10)-H(10)	118.1
C(1)-C(10)-H(10)	118.1
C(16)-C(11)-C(12)	120.5(5)
C(16)-C(11)-N(2)	120.1(4)
C(12)-C(11)-N(2)	119.3(5)
C(13)-C(12)-C(11)	117.8(6)
C(13)-C(12)-C(17)	118.2(8)
C(11)-C(12)-C(17)	123.9(7)
C(14)-C(13)-C(12)	121.9(6)
C(14)-C(13)-H(13)	119.0
C(12)-C(13)-H(13)	119.0
C(13)-C(14)-C(15)	119.8(5)
C(13)-C(14)-H(14)	120.1
C(15)-C(14)-H(14)	120.1
C(14)-C(15)-C(16)	121.1(5)
C(14)-C(15)-H(15)	119.4
C(16)-C(15)-H(15)	119.4
C(15)-C(16)-C(11)	118.4(5)
C(15)-C(16)-C(20)	119.7(5)
C(11)-C(16)-C(20)	122.0(5)
C(19)-C(17)-C(12)	114.6(6)
C(19)-C(17)-C(18)	108.9(6)
C(12)-C(17)-C(18)	108.9(6)
C(19)-C(17)-H(17)	108.1
C(12)-C(17)-H(17)	108.1
C(18)-C(17)-H(17)	108.1
C(17)-C(18)-H(18A)	109.5

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C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(21)-C(20)-C(16)	111.0(5)
C(21)-C(20)-C(22)	109.5(5)
C(16)-C(20)-C(22)	111.1(5)
C(21)-C(20)-H(20)	108.4
C(16)-C(20)-H(20)	108.4
C(22)-C(20)-H(20)	108.4
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(31)-C(23)-C(24)	132.5(5)
C(31)-C(23)-C(27)	119.0(5)
C(24)-C(23)-C(27)	108.2(4)
C(31)-C(23)-Yb(1)	125.0(3)
C(24)-C(23)-Yb(1)	70.7(3)
C(27)-C(23)-Yb(1)	74.3(3)
C(23)-C(24)-C(25)	106.7(4)
C(23)-C(24)-Yb(1)	80.1(3)
C(25)-C(24)-Yb(1)	72.3(2)

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C(23)-C(24)-H(24)	126.7
C(25)-C(24)-H(24)	126.7
Yb(1)-C(24)-H(24)	113.4
C(26)-C(25)-C(24)	109.5(5)
C(26)-C(25)-Yb(1)	76.6(3)
C(24)-C(25)-Yb(1)	77.2(3)
C(26)-C(25)-H(25)	125.2
C(24)-C(25)-H(25)	125.2
Yb(1)-C(25)-H(25)	113.1
C(25)-C(26)-C(27)	108.9(5)
C(25)-C(26)-Yb(1)	73.8(3)
C(27)-C(26)-Yb(1)	80.0(3)
C(25)-C(26)-H(26)	125.6
C(27)-C(26)-H(26)	125.6
Yb(1)-C(26)-H(26)	113.0
C(28)-C(27)-C(26)	133.8(5)
C(28)-C(27)-C(23)	119.4(5)
C(26)-C(27)-C(23)	106.6(4)
C(28)-C(27)-Yb(1)	122.6(4)
C(26)-C(27)-Yb(1)	70.4(3)
C(23)-C(27)-Yb(1)	76.4(3)
C(29)-C(28)-C(27)	119.1(5)
C(29)-C(28)-H(28)	120.5
C(27)-C(28)-H(28)	120.5
C(28)-C(29)-C(30)	121.0(5)
C(28)-C(29)-H(29)	119.5
C(30)-C(29)-H(29)	119.5
C(31)-C(30)-C(29)	122.5(5)
C(31)-C(30)-H(30)	118.8
C(29)-C(30)-H(30)	118.8
C(30)-C(31)-C(23)	118.9(6)
C(30)-C(31)-H(31)	120.5
C(23)-C(31)-H(31)	120.5
C(40)-C(32)-C(33)	134.0(6)
C(40)-C(32)-C(36)	118.9(6)
C(33)-C(32)-C(36)	107.1(5)
C(40)-C(32)-Yb(1)	120.2(3)
C(33)-C(32)-Yb(1)	70.2(3)

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C(36)-C(32)-Yb(1)	76.5(3)
C(34)-C(33)-C(32)	108.1(5)
C(34)-C(33)-Yb(1)	74.2(3)
C(32)-C(33)-Yb(1)	80.3(3)
C(34)-C(33)-H(33)	125.9
C(32)-C(33)-H(33)	125.9
Yb(1)-C(33)-H(33)	112.1
C(35)-C(34)-C(33)	109.5(5)
C(35)-C(34)-Yb(1)	78.2(3)
C(33)-C(34)-Yb(1)	75.5(3)
C(35)-C(34)-H(34)	125.3
C(33)-C(34)-H(34)	125.3
Yb(1)-C(34)-H(34)	113.2
C(34)-C(35)-C(36)	107.4(5)
C(34)-C(35)-Yb(1)	72.0(3)
C(36)-C(35)-Yb(1)	79.3(3)
C(34)-C(35)-H(35)	126.3
C(36)-C(35)-H(35)	126.3
Yb(1)-C(35)-H(35)	114.7
C(35)-C(36)-C(37)	133.7(5)
C(35)-C(36)-C(32)	107.9(5)
C(37)-C(36)-C(32)	118.3(5)
C(35)-C(36)-Yb(1)	71.6(3)
C(37)-C(36)-Yb(1)	122.7(3)
C(32)-C(36)-Yb(1)	74.1(3)
C(38)-C(37)-C(36)	119.9(5)
C(38)-C(37)-H(37)	120.1
C(36)-C(37)-H(37)	120.1
C(37)-C(38)-C(39)	121.3(6)
C(37)-C(38)-H(38)	119.4
C(39)-C(38)-H(38)	119.4
C(40)-C(39)-C(38)	120.7(6)
C(40)-C(39)-H(39)	119.6
C(38)-C(39)-H(39)	119.6
C(39)-C(40)-C(32)	120.9(6)
C(39)-C(40)-H(40)	119.5
C(32)-C(40)-H(40)	119.5
C(42)-C(41)-C(46)	119.8(10)

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C(42)-C(41)-H(41)	120.1
C(46)-C(41)-H(41)	120.1
C(41)-C(42)-C(43)	122.2(11)
C(41)-C(42)-H(42)	118.9
C(43)-C(42)-H(42)	118.9
C(44)-C(43)-C(42)	122.0(11)
C(44)-C(43)-H(43)	119.0
C(42)-C(43)-H(43)	119.0
C(43)-C(44)-C(45)	121.9(10)
C(43)-C(44)-H(44)	119.1
C(45)-C(44)-H(44)	119.1
C(44)-C(45)-C(46)	119.1(10)
C(44)-C(45)-C(47)	109.5(11)
C(46)-C(45)-C(47)	130.4(13)
C(41)-C(46)-C(45)	115.0(10)
C(41)-C(46)-H(46)	122.5
C(45)-C(46)-H(46)	122.5
C(45)-C(47)-H(47A)	109.5
C(45)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(45)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(1)-N(1)-C(5)	118.2(4)
C(1)-N(1)-Yb(1)	113.3(3)
C(5)-N(1)-Yb(1)	125.4(3)
C(10)-N(2)-C(11)	113.0(4)
C(10)-N(2)-Yb(1)	112.3(3)
C(11)-N(2)-Yb(1)	134.3(3)
C(8)-S(1)-C(9)	95.7(3)
N(1)-Yb(1)-N(2)	67.12(13)
N(1)-Yb(1)-C(34)	122.08(16)
N(2)-Yb(1)-C(34)	130.71(15)
N(1)-Yb(1)-C(25)	124.60(16)
N(2)-Yb(1)-C(25)	74.47(13)
C(34)-Yb(1)-C(25)	113.13(19)
N(1)-Yb(1)-C(33)	117.01(16)
N(2)-Yb(1)-C(33)	100.49(16)

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C(34)-Yb(1)-C(33)	30.26(18)
C(25)-Yb(1)-C(33)	107.8(2)
N(1)-Yb(1)-C(26)	153.52(15)
N(2)-Yb(1)-C(26)	98.25(15)
C(34)-Yb(1)-C(26)	84.31(18)
C(25)-Yb(1)-C(26)	29.61(15)
C(33)-Yb(1)-C(26)	86.52(17)
N(1)-Yb(1)-C(24)	105.12(14)
N(2)-Yb(1)-C(24)	83.44(14)
C(34)-Yb(1)-C(24)	128.76(17)
C(25)-Yb(1)-C(24)	30.5(2)
C(33)-Yb(1)-C(24)	135.83(17)
C(26)-Yb(1)-C(24)	49.64(15)
N(1)-Yb(1)-C(35)	94.44(15)
N(2)-Yb(1)-C(35)	134.39(15)
C(34)-Yb(1)-C(35)	29.84(18)
C(25)-Yb(1)-C(35)	140.46(16)
C(33)-Yb(1)-C(35)	49.64(17)
C(26)-Yb(1)-C(35)	110.85(17)
C(24)-Yb(1)-C(35)	142.11(16)
N(1)-Yb(1)-C(32)	87.59(16)
N(2)-Yb(1)-C(32)	87.56(14)
C(34)-Yb(1)-C(32)	48.81(17)
C(25)-Yb(1)-C(32)	129.6(2)
C(33)-Yb(1)-C(32)	29.48(17)
C(26)-Yb(1)-C(32)	114.67(17)
C(24)-Yb(1)-C(32)	159.99(16)
C(35)-Yb(1)-C(32)	48.87(16)
N(1)-Yb(1)-C(27)	143.23(15)
N(2)-Yb(1)-C(27)	123.20(14)
C(34)-Yb(1)-C(27)	80.03(17)
C(25)-Yb(1)-C(27)	48.73(14)
C(33)-Yb(1)-C(27)	96.70(17)
C(26)-Yb(1)-C(27)	29.63(14)
C(24)-Yb(1)-C(27)	49.03(15)
C(35)-Yb(1)-C(27)	96.95(16)
C(32)-Yb(1)-C(27)	125.54(17)
N(1)-Yb(1)-C(36)	74.68(14)

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N(2)-Yb(1)-C(36)	105.97(14)
C(34)-Yb(1)-C(36)	48.30(17)
C(25)-Yb(1)-C(36)	156.5(2)
C(33)-Yb(1)-C(36)	48.69(16)
C(26)-Yb(1)-C(36)	131.68(16)
C(24)-Yb(1)-C(36)	169.26(15)
C(35)-Yb(1)-C(36)	29.14(16)
C(32)-Yb(1)-C(36)	29.40(15)
C(27)-Yb(1)-C(36)	125.36(16)
N(1)-Yb(1)-C(23)	114.95(14)
N(2)-Yb(1)-C(23)	112.65(13)
C(34)-Yb(1)-C(23)	105.54(16)
C(25)-Yb(1)-C(23)	48.49(18)
C(33)-Yb(1)-C(23)	125.87(17)
C(26)-Yb(1)-C(23)	48.52(15)
C(24)-Yb(1)-C(23)	29.22(14)
C(35)-Yb(1)-C(23)	112.94(15)
C(32)-Yb(1)-C(23)	153.87(17)
C(27)-Yb(1)-C(23)	29.26(14)
C(36)-Yb(1)-C(23)	140.92(15)

Table S14. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **7**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	17(2)	20(2)	15(3)	-1(2)	5(2)	-1(2)
C(2)	19(2)	17(2)	23(3)	1(2)	6(2)	2(2)
C(3)	24(3)	19(3)	29(3)	-2(2)	6(2)	-1(2)
C(4)	25(3)	22(3)	22(3)	-3(2)	3(2)	-8(2)
C(5)	16(2)	15(3)	24(2)	-7(2)	4(2)	-4(2)
C(6)	18(3)	22(3)	28(3)	-4(2)	-1(2)	-4(2)
C(7)	21(3)	24(3)	27(3)	-3(3)	-7(2)	4(2)
C(8)	25(3)	8(2)	17(2)	-1(2)	-13(2)	-3(2)
C(9)	32(3)	32(4)	56(4)	-3(3)	-18(3)	-8(3)
C(10)	15(2)	22(3)	17(2)	2(2)	-1(2)	1(2)

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C(11)	21(3)	17(3)	20(2)	5(2)	-6(2)	-1(2)
C(12)	15(3)	22(3)	25(3)	-1(3)	-1(2)	0(2)
C(13)	14(3)	45(4)	33(3)	0(3)	0(2)	-7(3)
C(14)	22(3)	35(3)	35(3)	-4(3)	-9(3)	-6(3)
C(15)	26(3)	28(3)	22(2)	-7(2)	-9(2)	-2(2)
C(16)	19(2)	20(3)	25(3)	1(2)	-3(2)	5(2)
C(17)	24(4)	41(4)	22(3)	-6(3)	1(3)	-7(3)
C(18)	21(3)	54(4)	32(3)	2(3)	-3(3)	-6(3)
C(19)	47(4)	52(4)	36(3)	-18(3)	13(3)	-2(3)
C(20)	25(3)	32(3)	28(3)	-12(3)	-2(2)	-2(3)
C(21)	37(4)	63(5)	31(3)	15(3)	-8(3)	-7(4)
C(22)	34(4)	56(4)	49(4)	-24(3)	4(3)	12(3)
C(23)	22(3)	14(3)	24(2)	4(2)	-4(2)	-2(2)
C(24)	19(3)	12(2)	33(3)	5(2)	5(2)	1(2)
C(25)	21(2)	18(2)	37(2)	15(5)	-16(4)	-5(2)
C(26)	36(3)	15(3)	21(3)	-3(2)	-3(2)	0(2)
C(27)	18(3)	16(3)	30(3)	3(2)	-1(2)	-1(2)
C(28)	22(3)	22(3)	41(3)	10(3)	9(3)	4(2)
C(29)	19(3)	34(4)	57(4)	16(3)	-6(3)	-2(3)
C(30)	34(3)	32(3)	44(4)	22(3)	-24(3)	-12(3)
C(31)	34(3)	23(3)	29(3)	9(2)	-1(3)	-7(2)
C(32)	13(3)	35(4)	23(3)	-2(3)	7(2)	-3(3)
C(33)	26(3)	30(3)	30(3)	-9(3)	12(2)	-3(3)
C(34)	21(3)	40(4)	41(3)	8(3)	13(3)	11(3)
C(35)	16(3)	42(4)	37(3)	2(3)	-4(2)	2(3)
C(36)	17(3)	32(3)	27(3)	-4(2)	5(2)	-8(2)
C(37)	33(3)	32(4)	31(3)	-7(3)	10(3)	-12(3)
C(38)	41(4)	20(3)	43(3)	4(3)	23(3)	-3(3)
C(39)	34(4)	27(4)	37(3)	8(3)	8(3)	3(3)
C(40)	33(4)	32(4)	20(3)	5(2)	11(2)	-7(3)
N(1)	17(2)	19(2)	13(2)	-1(2)	0(2)	-4(2)
N(2)	17(2)	18(2)	13(2)	0(2)	-1(2)	-1(2)
S(1)	48(1)	48(1)	97(2)	2(1)	-34(1)	-6(1)
Yb(1)	15(1)	16(1)	20(1)	-1(1)	1(1)	1(1)

Electronic Supporting Information

UV-VIS spectra

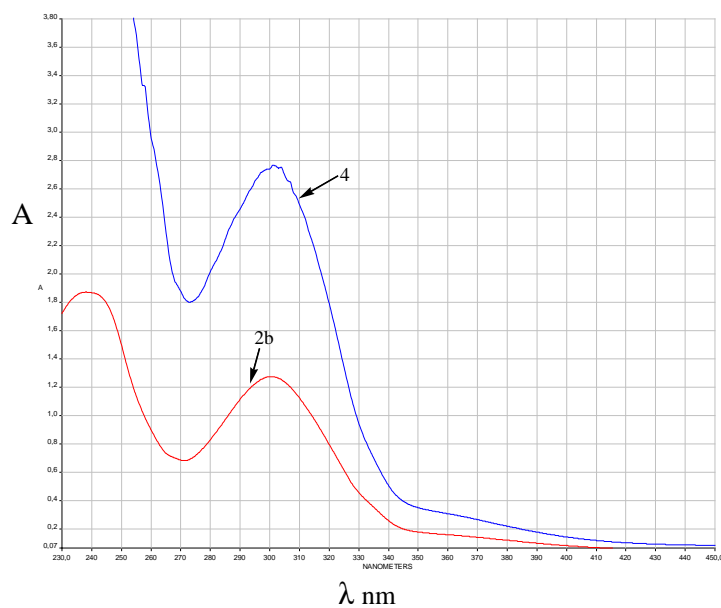


Fig S1. UV-VIS spectra of **2b** (red line) and **4** (blue line) in *n*-hexane.

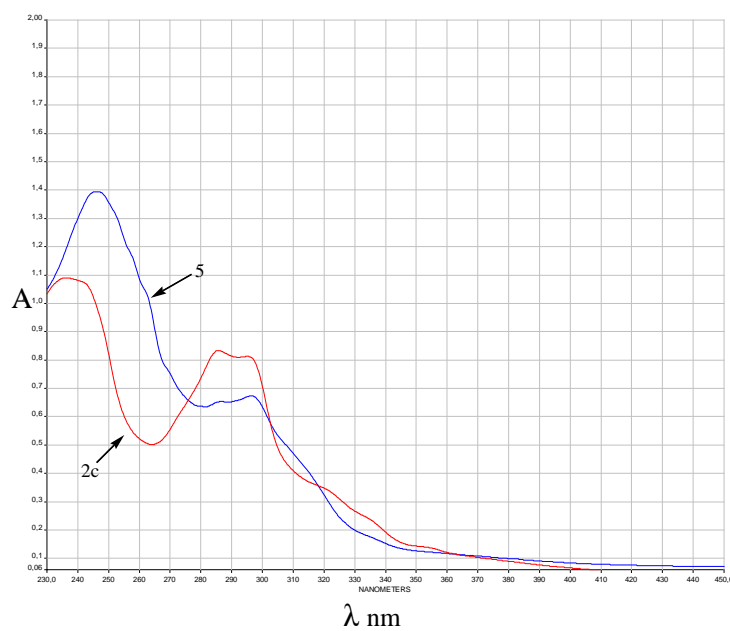


Fig S2. UV-VIS spectra of **2c** (red line) and **5** (blue line) in *n*-hexane.

Electronic Supporting Information

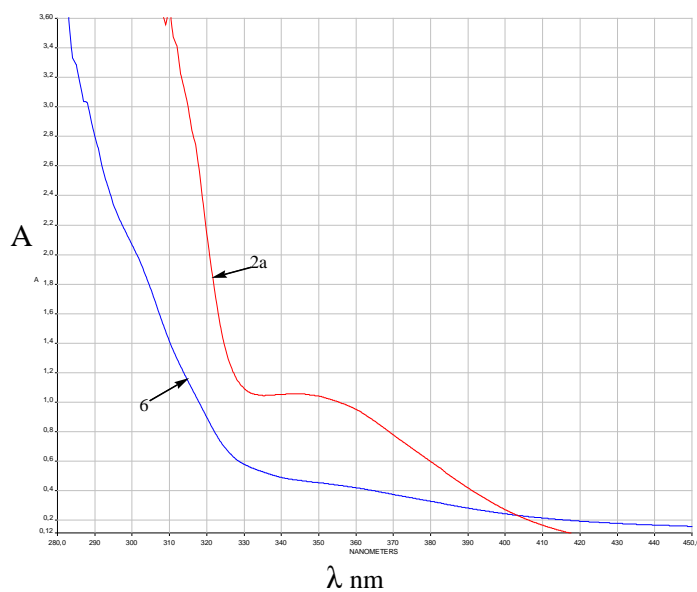


Fig S3. UV-VIS spectra of **2a** (red line) and **6** (blue line) in *n*-hexane.

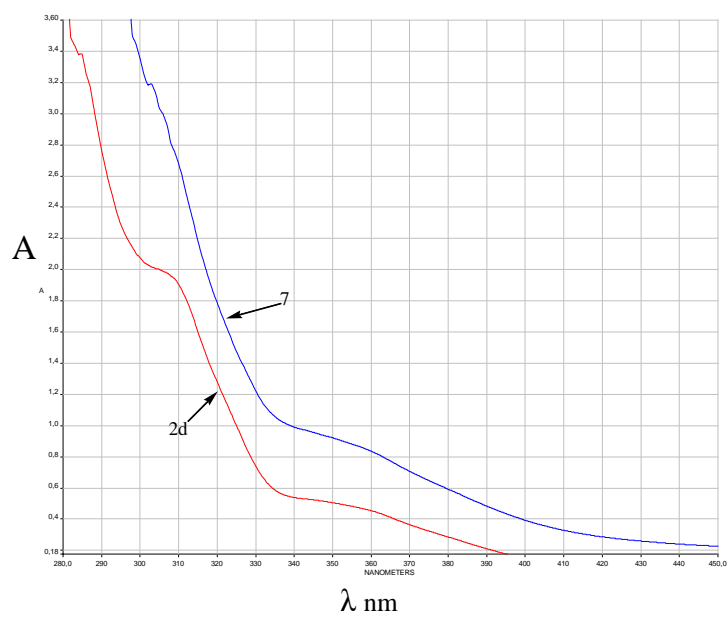


Fig S4. UV-VIS spectra of **2d** (red line) and **7** (blue line) in *n*-hexane.