

Table 1. Crystal data and structure refinement for $[(C_5Me_5)Yb]_2(\mu-\eta^8:\eta^8-C_8H_8)$, 2.

Identification code	maj5
Empirical formula	$C_{28}H_{38}Yb_2$
Formula weight	720.66
Temperature	163 K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	$a = 13.338(2)$ Å $\alpha = 114.772(7)^\circ$ $b = 13.549(2)$ Å $\beta = 93.948(11)^\circ$ $c = 15.815(2)$ Å $\gamma = 90.803(14)^\circ$
Volume, Z	$2585.9(7)$ Å ³ , 4
Density (calculated)	1.851 Mg/m ³
Absorption coefficient	7.200 mm ⁻¹
F(000)	1384
Crystal size	0.46 x 0.43 x 0.10 mm
θ range for data collection	2.00 to 27.50°
Limiting indices	$0 \leq h \leq 17$, $-15 \leq k \leq 15$, $-20 \leq l \leq 20$
Reflections collected	11704
Independent reflections	11224 ($R_{int} = 0.0178$)
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.9696 and 0.1352
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11224 / 0 / 542
Goodness-of-fit on F^2	1.032
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0604$, $wR2 = 0.1607$
R indices (all data)	$R1 = 0.0798$, $wR2 = 0.1777$
Extinction coefficient	$0.0006(2)$
Largest diff. peak and hole	2.966 and -4.280 eÅ ⁻³

Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Yb(1)	5233(1)	5964(1)	7622(1)	22(1)
Yb(2)	3112(1)	4371(1)	8097(1)	21(1)
C(1)	5515(7)	7189(8)	6739(6)	21(2)
C(2)	5416(7)	7947(8)	7688(6)	20(2)
C(3)	6273(6)	7837(8)	8234(6)	21(2)
C(4)	6885(7)	7043(8)	7634(6)	19(2)
C(5)	6420(8)	6669(8)	6706(6)	23(2)
C(6)	4790(8)	7077(11)	5936(7)	36(3)
C(7)	4573(8)	8644(9)	8056(8)	30(2)
C(8)	6474(8)	8477(10)	9272(7)	32(2)
C(9)	7925(8)	6784(11)	7897(8)	35(3)
C(10)	6864(9)	5854(11)	5843(7)	39(3)
C(11)	2757(7)	2463(8)	8129(6)	22(2)
C(12)	2429(8)	2344(9)	7213(7)	25(2)
C(13)	1569(7)	2974(9)	7285(7)	25(2)
C(14)	1377(7)	3484(9)	8224(7)	25(2)
C(15)	2108(7)	3199(8)	8759(6)	22(2)
C(16)	3666(8)	1969(9)	8392(7)	30(2)
C(17)	2889(9)	1620(9)	6335(7)	32(2)
C(18)	933(9)	2999(10)	6454(8)	39(3)
C(19)	474(9)	4158(10)	8597(9)	42(3)
C(20)	2127(9)	3473(10)	9796(7)	36(3)
C(21)	4008(9)	4261(10)	6608(8)	39(3)
C(22)	3391(8)	5158(10)	6851(7)	30(2)
C(23)	3259(8)	6070(10)	7682(8)	32(2)
C(24)	3644(9)	6462(9)	8615(8)	34(3)
C(25)	4364(9)	6085(10)	9115(7)	34(3)
C(26)	4963(7)	5182(12)	8879(8)	37(3)
C(27)	5094(8)	4267(11)	8048(10)	37(3)
C(28)	4724(9)	3882(10)	7107(9)	41(3)
Yb(3)	8207(1)	10998(1)	7282(1)	24(1)

ID (4)	3306 (1)	8753 (1)	7188 (1)	24 (1)
C (29)	6262 (6)	11160 (9)	7113 (6)	22 (2)
C (30)	6545 (7)	11664 (8)	8081 (6)	21 (2)
C (31)	7140 (7)	12601 (8)	8265 (7)	22 (2)
C (32)	7219 (7)	12707 (8)	7424 (7)	24 (2)
C (33)	6669 (7)	11822 (9)	6706 (7)	27 (2)
C (34)	5603 (8)	10110 (9)	6601 (7)	31 (2)
C (35)	6269 (8)	11252 (9)	8796 (7)	28 (2)
C (36)	7597 (8)	13429 (9)	9226 (7)	28 (2)
C (37)	7680 (9)	13654 (10)	7289 (9)	40 (3)
C (38)	6513 (10)	11590 (11)	5674 (7)	40 (3)
C (39)	11068 (7)	7621 (9)	7854 (6)	25 (2)
C (40)	11689 (7)	8528 (9)	7948 (7)	27 (2)
C (41)	11876 (7)	8385 (8)	7012 (6)	21 (2)
C (42)	11353 (8)	7393 (9)	6376 (7)	28 (2)
C (43)	10859 (7)	6923 (8)	6896 (7)	22 (2)
C (44)	10755 (9)	7413 (12)	8673 (8)	41 (3)
C (45)	12088 (9)	9431 (10)	8831 (7)	39 (3)
C (46)	12445 (8)	9146 (9)	6750 (8)	29 (2)
C (47)	11360 (10)	6911 (11)	5324 (7)	42 (3)
C (48)	10297 (10)	5838 (10)	6489 (9)	45 (3)
C (49)	8015 (8)	8931 (9)	7003 (10)	40 (3)
C (50)	8361 (10)	8929 (10)	6180 (8)	47 (3)
C (51)	9158 (11)	9446 (10)	5977 (8)	43 (3)
C (52)	9900 (10)	10233 (12)	6484 (10)	48 (4)
C (53)	10173 (8)	10832 (10)	7463 (12)	47 (4)
C (54)	9814 (11)	10842 (10)	8297 (8)	47 (3)
C (55)	9026 (10)	10322 (11)	8493 (8)	41 (3)
C (56)	8294 (9)	9515 (11)	7953 (10)	44 (3)

Table 3. Selected bond lengths [Å] and angles [°] for $[(C_5Me_5)Yb]_2(\mu-\eta^8:\eta^8-C_8H_8)$, 2.

Yb(1) - C(1)	2.615(9)	Yb(1) - C(4)	2.621(9)
Yb(1) - C(5)	2.636(9)	Yb(1) - C(3)	2.638(9)
Yb(1) - C(23)	2.644(10)	Yb(1) - C(25)	2.646(10)
Yb(1) - C(21)	2.645(12)	Yb(1) - C(24)	2.650(10)
Yb(1) - C(2)	2.651(10)	Yb(1) - C(28)	2.652(12)
Yb(1) - C(26)	2.657(10)	Yb(1) - C(27)	2.661(11)
Yb(1) - C(22)	2.667(10)	Yb(2) - C(12)	2.620(11)
Yb(2) - C(15)	2.633(9)	Yb(2) - C(13)	2.637(9)
Yb(2) - C(11)	2.643(10)	Yb(2) - C(22)	2.648(10)
Yb(2) - C(14)	2.651(10)	Yb(2) - C(27)	2.654(10)
Yb(2) - C(23)	2.652(11)	Yb(2) - C(21)	2.664(11)
Yb(2) - C(24)	2.668(11)	Yb(2) - C(28)	2.673(11)
Yb(2) - C(25)	2.676(11)	Yb(2) - C(26)	2.683(10)
Yb(1) - Cnt1	1.909	Yb(1) - Cnt2	2.338
Yb(2) - Cnt1	1.926	Yb(2) - Cnt3	2.346
C(1) - C(5)	1.399(14)	C(1) - C(2)	1.437(13)
C(1) - C(6)	1.496(12)	C(2) - C(3)	1.432(12)
C(2) - C(7)	1.469(14)	C(3) - C(4)	1.414(14)
C(3) - C(8)	1.502(13)	C(4) - C(5)	1.428(13)
C(4) - C(9)	1.508(13)	C(5) - C(10)	1.517(14)
C(11) - C(15)	1.430(14)	C(11) - C(12)	1.425(12)
C(11) - C(16)	1.509(13)	C(12) - C(13)	1.421(14)
C(12) - C(17)	1.503(14)	C(13) - C(14)	1.394(14)
C(13) - C(18)	1.528(13)	C(14) - C(15)	1.410(14)
C(14) - C(19)	1.519(15)	C(15) - C(20)	1.521(13)
C(21) - C(22)	1.41(2)	C(21) - C(28)	1.43(2)
C(22) - C(23)	1.40(2)	C(23) - C(24)	1.40(2)
C(24) - C(25)	1.43(2)	C(25) - C(26)	1.40(2)
C(26) - C(27)	1.40(2)	C(27) - C(28)	1.40(2)
Yb(3) - C(31)	2.592(9)	Yb(3) - C(30)	2.610(9)
Yb(3) - C(29)	2.611(9)	Yb(3) - C(32)	2.616(10)
Yb(3) - C(50)	2.629(12)	Yb(3) - C(55)	2.628(12)
Yb(3) - C(33)	2.635(10)	Yb(3) - C(56)	2.638(11)

Cnt1-Yb(1)-Cnt2	161.2	Cnt1-Yb(2)-Cnt3	159.2
Cnt4-Yb(3)-Cnt5	159.5	Cnt4-Yb(4)-Cnt6	163.8
C(5)-C(1)-C(2)	108.6(8)	C(5)-C(1)-C(6)	127.6(9)
C(2)-C(1)-C(6)	123.7(10)	C(3)-C(2)-C(1)	106.6(9)
C(3)-C(2)-C(7)	125.7(9)	C(1)-C(2)-C(7)	127.6(9)
C(4)-C(3)-C(2)	108.7(8)	C(4)-C(3)-C(8)	126.6(8)
C(2)-C(3)-C(8)	124.7(9)	C(3)-C(4)-C(5)	107.5(8)
C(3)-C(4)-C(9)	126.0(9)	C(5)-C(4)-C(9)	125.7(9)
C(1)-C(5)-C(4)	108.6(8)	C(1)-C(5)-C(10)	127.0(9)
C(4)-C(5)-C(10)	124.4(10)	C(15)-C(11)-C(12)	107.3(8)
C(15)-C(11)-C(16)	126.4(8)	C(12)-C(11)-C(16)	126.2(9)
C(13)-C(12)-C(11)	107.7(9)	C(13)-C(12)-C(17)	127.3(9)
C(11)-C(12)-C(17)	124.9(9)	C(14)-C(13)-C(12)	108.3(8)
C(14)-C(13)-C(18)	126.9(10)	C(12)-C(13)-C(18)	124.6(10)
C(13)-C(14)-C(15)	109.0(9)	C(13)-C(14)-C(19)	125.4(10)
C(15)-C(14)-C(19)	125.5(9)	C(14)-C(15)-C(11)	107.7(8)
C(14)-C(15)-C(20)	126.9(9)	C(11)-C(15)-C(20)	124.9(9)
C(22)-C(21)-C(28)	135.1(10)	C(21)-C(22)-C(23)	134.3(10)
C(24)-C(23)-C(22)	136.3(11)	C(23)-C(24)-C(25)	134.2(10)
C(26)-C(25)-C(24)	135.3(9)	C(25)-C(26)-C(27)	134.3(9)
C(26)-C(27)-C(28)	136.3(11)	C(27)-C(28)-C(21)	134.1(11)
C(30)-C(29)-C(33)	107.6(9)	C(30)-C(29)-C(34)	125.9(9)
C(33)-C(29)-C(34)	126.4(9)	C(31)-C(30)-C(29)	108.0(9)
C(31)-C(30)-C(35)	125.9(9)	C(29)-C(30)-C(35)	126.1(9)
C(30)-C(31)-C(32)	108.8(9)	C(30)-C(31)-C(36)	126.7(9)
C(32)-C(31)-C(36)	124.4(9)	C(33)-C(32)-C(31)	107.8(9)
C(33)-C(32)-C(37)	123.6(9)	C(31)-C(32)-C(37)	128.1(10)
C(32)-C(33)-C(29)	107.7(8)	C(32)-C(33)-C(38)	127.5(10)
C(29)-C(33)-C(38)	124.8(10)	C(43)-C(39)-C(40)	109.6(9)
C(43)-C(39)-C(44)	126.3(10)	C(40)-C(39)-C(44)	124.0(9)
C(39)-C(40)-C(41)	107.0(9)	C(39)-C(40)-C(45)	126.6(10)
C(41)-C(40)-C(45)	126.4(10)	C(42)-C(41)-C(40)	107.0(9)
C(42)-C(41)-C(46)	125.9(9)	C(40)-C(41)-C(46)	127.0(9)
C(43)-C(42)-C(41)	108.9(8)	C(43)-C(42)-C(47)	125.9(10)
C(41)-C(42)-C(47)	125.2(10)	C(39)-C(43)-C(42)	107.5(9)
C(39)-C(43)-C(48)	127.1(10)	C(42)-C(43)-C(48)	125.2(10)
C(56)-C(49)-C(50)	134.4(11)	C(51)-C(50)-C(49)	135.0(10)
C(52)-C(51)-C(50)	136.3(11)	C(51)-C(52)-C(53)	133.5(11)

Yb(3) - C(53)	2.641 (11)	Yb(3) - C(49)	2.652 (12)
Yb(3) - C(54)	2.653 (12)	Yb(3) - C(51)	2.662 (11)
Yb(3) - C(52)	2.670 (12)	Yb(4) - C(40)	2.601 (10)
Yb(4) - C(39)	2.613 (10)	Yb(4) - C(41)	2.613 (9)
Yb(4) - C(56)	2.626 (11)	Yb(4) - C(49)	2.625 (10)
Yb(4) - C(42)	2.627 (10)	Yb(4) - C(51)	2.637 (11)
Yb(4) - C(43)	2.641 (9)	Yb(4) - C(54)	2.652 (12)
Yb(4) - C(50)	2.654 (11)	Yb(4) - C(55)	2.666 (11)
Yb(4) - C(52)	2.670 (12)	Yb(4) - C(53)	2.671 (12)
Yb(3) - Cnt4	1.911	Yb(3) - Cnt5	2.321
Yb(4) - Cnt4	1.916	Yb(4) - Cnt6	2.321
C(29) - C(30)	1.410 (13)	C(29) - C(33)	1.426 (15)
C(29) - C(34)	1.534 (14)	C(30) - C(31)	1.399 (14)
C(30) - C(35)	1.518 (13)	C(31) - C(32)	1.406 (13)
C(31) - C(36)	1.538 (13)	C(32) - C(33)	1.409 (15)
C(32) - C(37)	1.515 (15)	C(33) - C(38)	1.524 (13)
C(39) - C(43)	1.414 (13)	C(39) - C(40)	1.42 (2)
C(39) - C(44)	1.520 (14)	C(40) - C(41)	1.451 (14)
C(40) - C(45)	1.476 (14)	C(41) - C(42)	1.431 (14)
C(41) - C(46)	1.479 (14)	C(42) - C(43)	1.421 (14)
C(42) - C(47)	1.512 (14)	C(43) - C(48)	1.499 (15)
C(49) - C(56)	1.39 (2)	C(49) - C(50)	1.41 (2)
C(50) - C(51)	1.39 (2)	C(51) - C(52)	1.38 (2)
C(52) - C(53)	1.43 (2)	C(53) - C(54)	1.43 (2)
C(54) - C(55)	1.38 (2)	C(55) - C(56)	1.40 (2)

* Cnt1 is the centroid of the C(21)-C(28) ring.

* Cnt2 is the centroid of the C(1)-C(5) ring.

* Cnt3 is the centroid of the C(11)-C(15) ring.

* Cnt4 is the centroid of the C(49)-C(56) ring.

* Cnt5 is the centroid of the C(29)-C(33) ring.

* Cnt6 is the centroid of the C(39)-C(43) ring.

E

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(h a^*)^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Yb(1)	14(1)	26(1)	31(1)	17(1)	5(1)	-5(1)
Yb(2)	14(1)	24(1)	29(1)	14(1)	4(1)	-5(1)
C(1)	22(5)	22(5)	23(4)	13(4)	-5(3)	-11(4)
C(2)	12(4)	23(5)	28(4)	15(4)	1(3)	-9(4)
C(3)	9(4)	28(5)	30(5)	18(4)	-3(3)	-8(4)
C(4)	14(4)	21(5)	27(4)	15(4)	1(3)	-4(4)
C(5)	28(5)	17(5)	23(4)	7(4)	6(4)	-9(4)
C(6)	32(6)	54(8)	31(5)	28(5)	-14(4)	-11(5)
C(7)	20(5)	24(6)	50(6)	18(5)	8(4)	3(4)
C(8)	24(5)	49(7)	28(5)	21(5)	-1(4)	0(5)
C(9)	16(5)	53(8)	48(6)	33(6)	2(4)	6(5)
C(10)	39(7)	49(8)	28(5)	14(5)	10(4)	-1(6)
C(11)	19(5)	22(5)	30(5)	19(4)	-6(3)	-6(4)
C(12)	24(5)	26(6)	29(5)	14(4)	3(4)	1(4)
C(13)	20(5)	25(5)	34(5)	20(4)	-9(4)	-10(4)
C(14)	15(5)	25(5)	38(5)	15(4)	7(4)	1(4)
C(15)	22(5)	17(5)	29(5)	12(4)	2(4)	-9(4)
C(16)	26(5)	35(6)	34(5)	18(5)	-5(4)	-1(5)
C(17)	45(7)	21(5)	29(5)	11(4)	0(4)	2(5)
C(18)	43(7)	39(7)	40(6)	23(5)	-13(5)	-2(6)
C(19)	32(6)	34(7)	57(7)	16(5)	15(5)	9(5)
C(20)	37(6)	38(7)	31(5)	13(5)	5(4)	-5(5)
C(21)	40(7)	41(7)	28(5)	6(5)	9(4)	-10(6)
C(22)	22(5)	41(7)	33(5)	20(5)	-4(4)	-12(5)
C(23)	14(5)	45(7)	48(6)	31(5)	8(4)	-1(5)
C(24)	33(6)	20(5)	43(6)	5(4)	22(5)	1(5)
C(25)	36(6)	47(7)	17(4)	12(4)	-3(4)	-15(5)
C(26)	9(5)	77(10)	42(6)	44(6)	-7(4)	-16(5)
C(27)	10(5)	51(8)	78(9)	53(7)	15(5)	11(5)
C(28)	38(7)	28(6)	60(7)	15(5)	32(6)	4(5)
Yb(3)	17(1)	24(1)	38(1)	18(1)	8(1)	6(1)
Yb(4)	16(1)	21(1)	36(1)	13(1)	2(1)	3(1)
C(29)	4(4)	31(6)	27(4)	9(4)	3(3)	0(4)
C(30)	16(4)	19(5)	29(5)	11(4)	6(3)	6(4)
C(31)	16(5)	16(5)	34(5)	12(4)	6(4)	2(4)
C(32)	22(5)	21(5)	35(5)	16(4)	11(4)	10(4)
C(33)	18(5)	38(6)	26(5)	15(4)	2(4)	7(4)
C(34)	22(5)	30(6)	29(5)	2(4)	0(4)	-4(4)
C(35)	28(5)	29(6)	30(5)	16(4)	3(4)	-3(4)
C(36)	24(5)	28(6)	31(5)	11(4)	-2(4)	-6(4)
C(37)	36(7)	37(7)	57(7)	27(6)	17(5)	4(5)
C(38)	50(8)	44(7)	30(5)	20(5)	-1(5)	4(6)
C(39)	22(5)	33(6)	24(4)	15(4)	4(4)	8(4)
C(40)	17(5)	32(6)	33(5)	13(4)	1(4)	5(4)
C(41)	8(4)	24(5)	30(5)	9(4)	-3(3)	-4(4)
C(42)	20(5)	31(6)	31(5)	9(4)	4(4)	1(4)
C(43)	12(4)	11(4)	39(5)	5(4)	3(3)	5(3)

C(50)-C(51)-Yb(4)	75.4(7)	C(52)-C(51)-Yb(3)	75.3(7)
C(50)-C(51)-Yb(3)	73.4(7)	Yb(4)-C(51)-Yb(3)	92.5(3)
C(51)-C(52)-C(53)	133.5(11)	C(51)-C(52)-Yb(3)	74.7(7)
C(53)-C(52)-Yb(3)	73.3(6)	C(51)-C(52)-Yb(4)	73.6(7)
C(53)-C(52)-Yb(4)	74.5(7)	Yb(3)-C(52)-Yb(4)	91.6(3)
C(52)-C(53)-C(54)	134.9(11)	C(52)-C(53)-Yb(3)	75.4(7)
C(54)-C(53)-Yb(3)	74.8(7)	C(52)-C(53)-Yb(4)	74.4(7)
C(54)-C(53)-Yb(4)	73.7(7)	Yb(3)-C(53)-Yb(4)	92.2(3)
C(55)-C(54)-C(53)	134.9(11)	C(55)-C(54)-Yb(4)	75.5(7)
C(53)-C(54)-Yb(4)	75.2(7)	C(55)-C(54)-Yb(3)	73.8(7)
C(53)-C(54)-Yb(3)	73.9(6)	Yb(4)-C(54)-Yb(3)	92.3(3)
C(54)-C(55)-C(56)	134.7(11)	C(54)-C(55)-Yb(3)	75.9(7)
C(56)-C(55)-Yb(3)	75.0(7)	C(54)-C(55)-Yb(4)	74.4(7)
C(56)-C(55)-Yb(4)	73.1(7)	Yb(3)-C(55)-Yb(4)	92.6(3)
C(49)-C(56)-C(55)	136.0(11)	C(49)-C(56)-Yb(4)	74.6(7)
C(55)-C(56)-Yb(4)	76.3(7)	C(49)-C(56)-Yb(3)	75.3(7)
C(55)-C(56)-Yb(3)	74.2(7)	Yb(4)-C(56)-Yb(3)	93.3(3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H(6A)	4222 (8)	7539 (11)	6170 (7)	55
H(6B)	4542 (8)	6317 (11)	5600 (7)	55
H(6C)	5130 (8)	7302 (11)	5511 (7)	55
H(7A)	4085 (8)	8571 (9)	7538 (8)	45
H(7B)	4824 (8)	9404 (9)	8385 (8)	45
H(7C)	4245 (8)	8424 (9)	8490 (8)	45
H(8A)	5928 (8)	8971 (10)	9511 (7)	49
H(8B)	7113 (8)	8902 (10)	9406 (7)	49
H(8C)	6512 (8)	7977 (10)	9574 (7)	49
H(9A)	8181 (8)	6202 (11)	7352 (8)	53
H(9B)	7895 (8)	6547 (11)	8401 (8)	53
H(9C)	8374 (8)	7435 (11)	8108 (8)	53
H(10A)	7504 (9)	5623 (11)	6026 (7)	58
H(10B)	6980 (9)	6194 (11)	5417 (7)	58
H(10C)	6396 (9)	5220 (11)	5527 (7)	58
H(16A)	3973 (8)	1495 (9)	7825 (7)	46
H(16B)	3459 (8)	1542 (9)	8725 (7)	46
H(16C)	4155 (8)	2550 (9)	8796 (7)	46
H(17A)	3477 (9)	1289 (9)	6497 (7)	47
H(17B)	3097 (9)	2053 (9)	6007 (7)	47
H(17C)	2394 (9)	1047 (9)	5931 (7)	47
H(18A)	1245 (9)	2570 (10)	5876 (8)	59
H(18B)	891 (9)	3753 (10)	6530 (8)	59
H(18C)	256 (9)	2690 (10)	6422 (8)	59
H(19A)	514 (9)	4426 (10)	9279 (9)	62
H(19B)	-146 (9)	3706 (10)	8325 (9)	62
H(19C)	473 (9)	4776 (10)	8429 (9)	62
H(20A)	2721 (9)	3173 (10)	9984 (7)	54
H(20B)	1518 (9)	3159 (10)	9918 (7)	54
H(20C)	2155 (9)	4265 (10)	10154 (7)	54
H(21)	3933 (9)	3798 (10)	5958 (8)	47
H(22)	2969 (8)	5141 (10)	6335 (7)	37
H(23)	2789 (8)	6541 (10)	7588 (8)	38
H(24)	3366 (9)	7126 (9)	9004 (8)	41
H(25)	4457 (9)	6562 (10)	9760 (7)	41
H(26)	5372 (7)	5190 (12)	9399 (8)	45
H(27)	5549 (8)	3785 (11)	8147 (10)	44
H(28)	5011 (9)	3225 (10)	6716 (9)	49
H(34A)	5523 (8)	9936 (9)	5932 (7)	47
H(34B)	4942 (8)	10212 (9)	6851 (7)	47
H(34C)	5925 (8)	9512 (9)	6692 (7)	47
H(35A)	5845 (8)	10582 (9)	8484 (7)	42
H(35B)	5900 (8)	11805 (9)	9273 (7)	42
H(35C)	6883 (8)	11105 (9)	9091 (7)	42
H(36A)	7980 (8)	14006 (9)	9151 (7)	43
H(36B)	8045 (8)	13061 (9)	9507 (7)	43
H(36C)	7056 (8)	13748 (9)	9633 (7)	43
H(37A)	8025 (9)	14171 (10)	7880 (9)	60

H(37B)	7148 (9)	14019 (10)	7086 (9)	60
H(37C)	8164 (9)	13385 (10)	6812 (9)	60
H(38A)	6097 (10)	10917 (11)	5340 (7)	61
H(38B)	7167 (10)	11508 (11)	5411 (7)	61
H(38C)	6175 (10)	12195 (11)	5610 (7)	61
H(44A)	10997 (9)	8026 (12)	9260 (8)	62
H(44B)	11047 (9)	6743 (12)	8651 (8)	62
H(44C)	10020 (9)	7335 (12)	8637 (8)	62
H(45A)	12493 (9)	9947 (10)	8693 (7)	59
H(45B)	12509 (9)	9142 (10)	9200 (7)	59
H(45C)	11528 (9)	9804 (10)	9187 (7)	59
H(46A)	12729 (8)	9761 (9)	7317 (8)	44
H(46B)	11992 (8)	9414 (9)	6386 (8)	44
H(46C)	12990 (8)	8767 (9)	6374 (8)	44
H(47A)	11756 (10)	7397 (11)	5144 (7)	63
H(47B)	10668 (10)	6825 (11)	5041 (7)	63
H(47C)	11660 (10)	6199 (11)	5104 (7)	63
H(48A)	10265 (10)	5536 (10)	5806 (9)	68
H(48B)	9613 (10)	5927 (10)	6692 (9)	68
H(48C)	10645 (10)	5342 (10)	6704 (9)	68
H(49)	7469 (8)	8420 (9)	6882 (10)	48
H(50)	7955 (10)	8466 (10)	5635 (8)	57
H(51)	9203 (11)	9192 (10)	5323 (8)	51
H(52)	10317 (10)	10417 (12)	6103 (10)	58
H(53)	10721 (8)	11342 (10)	7587 (12)	57
H(54)	10210 (11)	11317 (10)	8844 (8)	57
H(55)	8967 (10)	10571 (11)	9144 (8)	50
H(56)	7884 (9)	9312 (11)	8328 (10)	52

Table 6. Bond lengths [Å] and angles [°] for 1.

Yb(1)-C(1)	2.615(9)	Yb(1)-C(4)	2.621(9)
Yb(1)-C(5)	2.636(9)	Yb(1)-C(3)	2.638(9)
Yb(1)-C(23)	2.644(10)	Yb(1)-C(25)	2.646(10)
Yb(1)-C(21)	2.645(12)	Yb(1)-C(24)	2.650(10)
Yb(1)-C(2)	2.651(10)	Yb(1)-C(28)	2.652(12)
Yb(1)-C(26)	2.657(10)	Yb(1)-C(27)	2.661(11)
Yb(1)-C(22)	2.667(10)	Yb(2)-C(12)	2.620(11)
Yb(2)-C(15)	2.633(9)	Yb(2)-C(13)	2.637(9)
Yb(2)-C(11)	2.643(10)	Yb(2)-C(22)	2.648(10)
Yb(2)-C(14)	2.651(10)	Yb(2)-C(27)	2.654(10)
Yb(2)-C(23)	2.652(11)	Yb(2)-C(21)	2.664(11)
Yb(2)-C(24)	2.668(11)	Yb(2)-C(28)	2.673(11)
Yb(2)-C(25)	2.676(11)	Yb(2)-C(26)	2.683(10)
Yb(1)-Cnt1	1.909	Yb(1)-Cnt2	2.338
Yb(2)-Cnt1	1.926	Yb(2)-Cnt3	2.346
C(1)-C(5)	1.399(14)	C(1)-C(2)	1.437(13)
C(1)-C(6)	1.496(12)	C(2)-C(3)	1.432(12)
C(2)-C(7)	1.469(14)	C(3)-C(4)	1.414(14)
C(3)-C(8)	1.502(13)	C(4)-C(5)	1.428(13)
C(4)-C(9)	1.508(13)	C(5)-C(10)	1.517(14)
C(11)-C(15)	1.430(14)	C(11)-C(12)	1.425(12)
C(11)-C(16)	1.509(13)	C(12)-C(13)	1.421(14)
C(12)-C(17)	1.503(14)	C(13)-C(14)	1.394(14)
C(13)-C(18)	1.528(13)	C(14)-C(15)	1.410(14)
C(14)-C(19)	1.519(15)	C(15)-C(20)	1.521(13)
C(21)-C(22)	1.41(2)	C(21)-C(28)	1.43(2)
C(22)-C(23)	1.40(2)	C(23)-C(24)	1.40(2)
C(24)-C(25)	1.43(2)	C(25)-C(26)	1.40(2)
C(26)-C(27)	1.40(2)	C(27)-C(28)	1.40(2)
Yb(3)-C(31)	2.592(9)	Yb(3)-C(30)	2.610(9)
Yb(3)-C(29)	2.611(9)	Yb(3)-C(32)	2.616(10)
Yb(3)-C(50)	2.629(12)	Yb(3)-C(55)	2.628(12)
Yb(3)-C(33)	2.635(10)	Yb(3)-C(56)	2.638(11)
Yb(3)-C(53)	2.641(11)	Yb(3)-C(49)	2.652(12)
Yb(3)-C(54)	2.653(12)	Yb(3)-C(51)	2.662(11)

Yb(3) - C(52)	2.670(12)	Yb(4) - C(40)	2.601(10)
Yb(4) - C(39)	2.613(10)	Yb(4) - C(41)	2.613(9)
Yb(4) - C(56)	2.626(11)	Yb(4) - C(49)	2.625(10)
Yb(4) - C(42)	2.627(10)	Yb(4) - C(51)	2.637(11)
Yb(4) - C(43)	2.641(9)	Yb(4) - C(54)	2.652(12)
Yb(4) - C(50)	2.654(11)	Yb(4) - C(55)	2.666(11)
Yb(4) - C(52)	2.670(12)	Yb(4) - C(53)	2.671(12)
Yb(3) - Cnt4	1.911	Yb(3) - Cnt5	2.321
Yb(4) - Cnt4	1.916	Yb(4) - Cnt6	2.321
C(29) - C(30)	1.410(13)	C(29) - C(33)	1.426(15)
C(29) - C(34)	1.534(14)	C(30) - C(31)	1.399(14)
C(30) - C(35)	1.518(13)	C(31) - C(32)	1.406(13)
C(31) - C(36)	1.538(13)	C(32) - C(33)	1.409(15)
C(32) - C(37)	1.515(15)	C(33) - C(38)	1.524(13)
C(39) - C(43)	1.414(13)	C(39) - C(40)	1.42(2)
C(39) - C(44)	1.520(14)	C(40) - C(41)	1.451(14)
C(40) - C(45)	1.476(14)	C(41) - C(42)	1.431(14)
C(41) - C(46)	1.479(14)	C(42) - C(43)	1.421(14)
C(42) - C(47)	1.512(14)	C(43) - C(48)	1.499(15)
C(49) - C(56)	1.39(2)	C(49) - C(50)	1.41(2)
C(50) - C(51)	1.39(2)	C(51) - C(52)	1.38(2)
C(52) - C(53)	1.43(2)	C(53) - C(54)	1.43(2)
C(54) - C(55)	1.38(2)	C(55) - C(56)	1.40(2)
Cnt1-Yb(1) - Cnt2	161.2	Cnt1-Yb(2) - Cnt3	159.2
Cnt4-Yb(3) - Cnt5	159.5	Cnt4-Yb(4) - Cnt6	163.8
C(1) - Yb(1) - C(4)	52.0(3)	C(1) - Yb(1) - C(5)	30.9(3)
C(4) - Yb(1) - C(5)	31.5(3)	C(1) - Yb(1) - C(3)	51.9(3)
C(4) - Yb(1) - C(3)	31.2(3)	C(5) - Yb(1) - C(3)	51.5(3)
C(1) - Yb(1) - C(23)	98.9(3)	C(4) - Yb(1) - C(23)	144.1(3)
C(5) - Yb(1) - C(23)	128.7(3)	C(3) - Yb(1) - C(23)	116.4(3)
C(1) - Yb(1) - C(25)	138.1(4)	C(4) - Yb(1) - C(25)	125.8(3)
C(5) - Yb(1) - C(25)	154.7(3)	C(3) - Yb(1) - C(25)	103.2(3)
C(23) - Yb(1) - C(25)	59.1(3)	C(1) - Yb(1) - C(21)	111.2(3)
C(4) - Yb(1) - C(21)	144.6(3)	C(5) - Yb(1) - C(21)	116.7(3)
C(3) - Yb(1) - C(21)	162.8(3)	C(23) - Yb(1) - C(21)	58.6(4)
C(25) - Yb(1) - C(21)	88.2(3)	C(1) - Yb(1) - C(24)	113.5(3)
C(4) - Yb(1) - C(24)	134.1(3)	C(5) - Yb(1) - C(24)	142.9(3)
C(3) - Yb(1) - C(24)	103.2(3)	C(23) - Yb(1) - C(24)	30.6(4)

C(23)-Yb(1)-C(24)	31.4(4)	C(21)-Yb(1)-C(24)	79.8(3)
C(1)-Yb(1)-C(2)	31.7(3)	C(4)-Yb(1)-C(2)	52.0(3)
C(5)-Yb(1)-C(2)	51.6(3)	C(3)-Yb(1)-C(2)	31.4(3)
C(23)-Yb(1)-C(2)	92.0(3)	C(25)-Yb(1)-C(2)	108.7(3)
C(21)-Yb(1)-C(2)	132.6(3)	C(24)-Yb(1)-C(2)	92.2(3)
C(1)-Yb(1)-C(28)	134.9(4)	C(4)-Yb(1)-C(28)	134.7(3)
C(5)-Yb(1)-C(28)	123.7(3)	C(3)-Yb(1)-C(28)	162.7(4)
C(23)-Yb(1)-C(28)	80.0(4)	C(25)-Yb(1)-C(28)	79.7(4)
C(21)-Yb(1)-C(28)	31.4(4)	C(24)-Yb(1)-C(28)	88.2(3)
C(2)-Yb(1)-C(28)	163.4(4)	C(1)-Yb(1)-C(26)	166.1(4)
C(4)-Yb(1)-C(26)	122.8(3)	C(5)-Yb(1)-C(26)	151.0(3)
C(3)-Yb(1)-C(26)	116.1(3)	C(23)-Yb(1)-C(26)	79.9(3)
C(25)-Yb(1)-C(26)	30.6(4)	C(21)-Yb(1)-C(26)	80.2(4)
C(24)-Yb(1)-C(26)	59.2(4)	C(2)-Yb(1)-C(26)	134.5(4)
C(28)-Yb(1)-C(26)	58.7(4)	C(1)-Yb(1)-C(27)	163.1(4)
C(4)-Yb(1)-C(27)	126.8(3)	C(5)-Yb(1)-C(27)	137.5(3)
C(3)-Yb(1)-C(27)	138.1(3)	C(23)-Yb(1)-C(27)	87.4(3)
C(25)-Yb(1)-C(27)	58.3(4)	C(21)-Yb(1)-C(27)	58.9(4)
C(24)-Yb(1)-C(27)	79.6(3)	C(2)-Yb(1)-C(27)	164.7(4)
C(28)-Yb(1)-C(27)	30.6(4)	C(26)-Yb(1)-C(27)	30.6(4)
C(1)-Yb(1)-C(22)	98.0(3)	C(4)-Yb(1)-C(22)	149.2(3)
C(5)-Yb(1)-C(22)	118.9(3)	C(3)-Yb(1)-C(22)	138.1(3)
C(23)-Yb(1)-C(22)	30.6(4)	C(25)-Yb(1)-C(22)	79.9(3)
C(21)-Yb(1)-C(22)	30.7(4)	C(24)-Yb(1)-C(22)	58.5(3)
C(2)-Yb(1)-C(22)	107.4(3)	C(28)-Yb(1)-C(22)	59.1(4)
C(26)-Yb(1)-C(22)	88.0(3)	C(27)-Yb(1)-C(22)	79.5(3)
C(12)-Yb(2)-C(15)	51.9(3)	C(12)-Yb(2)-C(13)	31.4(3)
C(15)-Yb(2)-C(13)	51.3(3)	C(12)-Yb(2)-C(11)	31.4(3)
C(15)-Yb(2)-C(11)	31.4(3)	C(13)-Yb(2)-C(11)	51.6(3)
C(12)-Yb(2)-C(22)	108.6(3)	C(15)-Yb(2)-C(22)	153.0(3)
C(13)-Yb(2)-C(22)	102.0(3)	C(11)-Yb(2)-C(22)	138.4(3)
C(12)-Yb(2)-C(14)	51.3(3)	C(15)-Yb(2)-C(14)	30.9(3)
C(13)-Yb(2)-C(14)	30.6(3)	C(11)-Yb(2)-C(14)	51.3(3)
C(22)-Yb(2)-C(14)	123.7(3)	C(12)-Yb(2)-C(27)	104.4(4)
C(15)-Yb(2)-C(27)	120.3(3)	C(13)-Yb(2)-C(27)	134.7(4)
C(11)-Yb(2)-C(27)	97.3(3)	C(22)-Yb(2)-C(27)	80.0(3)
C(14)-Yb(2)-C(27)	148.5(3)	C(12)-Yb(2)-C(23)	135.7(3)
C(15)-Yb(2)-C(23)	150.5(3)	C(13)-Yb(2)-C(23)	117.3(3)
C(11)-Yb(2)-C(23)	167.1(3)	C(22)-Yb(2)-C(23)	30.7(3)

C(12)-Yb(2)-C(21)	91.4(3)	C(15)-Yb(2)-C(21)	143.1(3)
C(13)-Yb(2)-C(21)	100.7(3)	C(11)-Yb(2)-C(21)	114.2(3)
C(22)-Yb(2)-C(21)	30.7(4)	C(14)-Yb(2)-C(21)	130.7(3)
C(27)-Yb(2)-C(21)	58.8(4)	C(23)-Yb(2)-C(21)	58.3(4)
C(12)-Yb(2)-C(24)	166.1(3)	C(15)-Yb(2)-C(24)	137.7(3)
C(13)-Yb(2)-C(24)	140.4(4)	C(11)-Yb(2)-C(24)	162.4(3)
C(22)-Yb(2)-C(24)	58.5(3)	C(14)-Yb(2)-C(24)	129.3(3)
C(27)-Yb(2)-C(24)	79.4(4)	C(23)-Yb(2)-C(24)	30.4(4)
C(21)-Yb(2)-C(24)	79.1(3)	C(12)-Yb(2)-C(28)	89.6(3)
C(15)-Yb(2)-C(28)	129.5(4)	C(13)-Yb(2)-C(28)	113.0(4)
C(11)-Yb(2)-C(28)	98.5(3)	C(22)-Yb(2)-C(28)	59.1(4)
C(14)-Yb(2)-C(28)	140.8(4)	C(27)-Yb(2)-C(28)	30.5(4)
C(23)-Yb(2)-C(28)	79.4(4)	C(21)-Yb(2)-C(28)	31.1(4)
C(24)-Yb(2)-C(28)	87.4(3)	C(12)-Yb(2)-C(25)	159.8(4)
C(15)-Yb(2)-C(25)	125.3(3)	C(13)-Yb(2)-C(25)	167.3(4)
C(11)-Yb(2)-C(25)	133.8(3)	C(22)-Yb(2)-C(25)	79.7(3)
C(14)-Yb(2)-C(25)	139.3(3)	C(27)-Yb(2)-C(25)	58.0(4)
C(23)-Yb(2)-C(25)	58.6(3)	C(21)-Yb(2)-C(25)	87.2(3)
C(24)-Yb(2)-C(25)	31.1(4)	C(28)-Yb(2)-C(25)	78.8(4)
C(12)-Yb(2)-C(26)	129.9(4)	C(15)-Yb(2)-C(26)	118.8(3)
C(13)-Yb(2)-C(26)	160.9(4)	C(11)-Yb(2)-C(26)	110.7(3)
C(22)-Yb(2)-C(26)	87.9(3)	C(14)-Yb(2)-C(26)	147.7(3)
C(27)-Yb(2)-C(26)	30.5(4)	C(23)-Yb(2)-C(26)	79.3(3)
C(21)-Yb(2)-C(26)	79.4(3)	C(24)-Yb(2)-C(26)	58.7(4)
C(28)-Yb(2)-C(26)	58.2(4)	C(25)-Yb(2)-C(26)	30.3(4)
C(5)-C(1)-C(2)	108.6(8)	C(5)-C(1)-C(6)	127.6(9)
C(2)-C(1)-C(6)	123.7(10)	C(5)-C(1)-Yb(1)	75.4(5)
C(2)-C(1)-Yb(1)	75.5(5)	C(6)-C(1)-Yb(1)	119.3(7)
C(3)-C(2)-C(1)	106.6(9)	C(3)-C(2)-C(7)	125.7(9)
C(1)-C(2)-C(7)	127.6(9)	C(3)-C(2)-Yb(1)	73.8(6)
C(1)-C(2)-Yb(1)	72.8(5)	C(7)-C(2)-Yb(1)	115.3(6)
C(4)-C(3)-C(2)	108.7(8)	C(4)-C(3)-C(8)	126.6(8)
C(2)-C(3)-C(8)	124.7(9)	C(4)-C(3)-Yb(1)	73.7(5)
C(2)-C(3)-Yb(1)	74.8(5)	C(8)-C(3)-Yb(1)	118.0(6)
C(3)-C(4)-C(5)	107.5(8)	C(3)-C(4)-C(9)	126.0(9)
C(5)-C(4)-C(9)	125.7(9)	C(3)-C(4)-Yb(1)	75.1(5)
C(5)-C(4)-Yb(1)	74.8(5)	C(9)-C(4)-Yb(1)	124.1(7)
C(1)-C(5)-C(4)	108.6(8)	C(1)-C(5)-C(10)	127.0(9)

14

C(4)-C(5)-Yb(1)	73.7(5)	C(10)-C(5)-Yb(1)	119.4(7)
C(15)-C(11)-C(12)	107.3(8)	C(15)-C(11)-C(16)	126.4(8)
C(12)-C(11)-C(16)	126.2(9)	C(15)-C(11)-Yb(2)	73.9(5)
C(12)-C(11)-Yb(2)	73.4(6)	C(16)-C(11)-Yb(2)	115.1(6)
C(13)-C(12)-C(11)	107.7(9)	C(13)-C(12)-C(17)	127.3(9)
C(11)-C(12)-C(17)	124.9(9)	C(13)-C(12)-Yb(2)	75.0(6)
C(11)-C(12)-Yb(2)	75.2(6)	C(17)-C(12)-Yb(2)	118.6(7)
C(14)-C(13)-C(12)	108.3(8)	C(14)-C(13)-C(18)	126.9(10)
C(12)-C(13)-C(18)	124.6(10)	C(14)-C(13)-Yb(2)	75.3(6)
C(12)-C(13)-Yb(2)	73.7(6)	C(18)-C(13)-Yb(2)	120.8(7)
C(13)-C(14)-C(15)	109.0(9)	C(13)-C(14)-C(19)	125.4(10)
C(15)-C(14)-C(19)	125.5(9)	C(13)-C(14)-Yb(2)	74.1(5)
C(15)-C(14)-Yb(2)	73.8(5)	C(19)-C(14)-Yb(2)	122.2(7)
C(14)-C(15)-C(11)	107.7(8)	C(14)-C(15)-C(20)	126.9(9)
C(11)-C(15)-C(20)	124.9(9)	C(14)-C(15)-Yb(2)	75.2(5)
C(11)-C(15)-Yb(2)	74.6(5)	C(20)-C(15)-Yb(2)	122.9(7)
C(22)-C(21)-C(28)	135.1(10)	C(22)-C(21)-Yb(1)	75.5(6)
C(28)-C(21)-Yb(1)	74.6(7)	C(22)-C(21)-Yb(2)	74.0(6)
C(28)-C(21)-Yb(2)	74.8(6)	Yb(1)-C(21)-Yb(2)	92.5(3)
C(21)-C(22)-C(23)	134.3(10)	C(21)-C(22)-Yb(2)	75.3(6)
C(23)-C(22)-Yb(2)	74.9(6)	C(21)-C(22)-Yb(1)	73.8(6)
C(23)-C(22)-Yb(1)	73.8(6)	Yb(2)-C(22)-Yb(1)	92.4(3)
C(24)-C(23)-C(22)	136.3(11)	C(24)-C(23)-Yb(1)	74.9(6)
C(22)-C(23)-Yb(1)	75.6(6)	C(24)-C(23)-Yb(2)	75.4(7)
C(22)-C(23)-Yb(2)	74.5(7)	Yb(1)-C(23)-Yb(2)	92.8(4)
C(23)-C(24)-C(25)	134.2(10)	C(23)-C(24)-Yb(1)	74.5(6)
C(25)-C(24)-Yb(1)	74.1(6)	C(23)-C(24)-Yb(2)	74.2(7)
C(25)-C(24)-Yb(2)	74.7(6)	Yb(1)-C(24)-Yb(2)	92.3(3)
C(26)-C(25)-C(24)	135.3(9)	C(26)-C(25)-Yb(1)	75.1(6)
C(24)-C(25)-Yb(1)	74.4(6)	C(26)-C(25)-Yb(2)	75.1(6)
C(24)-C(25)-Yb(2)	74.1(6)	Yb(1)-C(25)-Yb(2)	92.2(3)
C(25)-C(26)-C(27)	134.3(9)	C(25)-C(26)-Yb(1)	74.2(6)
C(27)-C(26)-Yb(1)	74.9(6)	C(25)-C(26)-Yb(2)	74.6(6)
C(27)-C(26)-Yb(2)	73.6(6)	Yb(1)-C(26)-Yb(2)	91.8(3)
C(26)-C(27)-C(28)	136.3(11)	C(26)-C(27)-Yb(2)	75.9(6)
C(28)-C(27)-Yb(2)	75.5(7)	C(26)-C(27)-Yb(1)	74.6(7)
C(28)-C(27)-Yb(1)	74.3(7)	Yb(2)-C(27)-Yb(1)	92.4(3)
C(27)-C(28)-C(21)	134.1(11)	C(27)-C(28)-Yb(1)	75.1(7)

C(21)-C(28)-Yb(1)	74.1 (7)	C(27)-C(28)-Yb(2)	74.0 (6)
C(21)-C(28)-Yb(2)	74.1 (6)	Yb(1)-C(28)-Yb(2)	92.1 (4)
C(31)-Yb(3)-C(30)	31.2 (3)	C(31)-Yb(3)-C(29)	51.8 (3)
C(30)-Yb(3)-C(29)	31.3 (3)	C(31)-Yb(3)-C(32)	31.3 (3)
C(30)-Yb(3)-C(32)	51.8 (3)	C(29)-Yb(3)-C(32)	51.9 (3)
C(31)-Yb(3)-C(50)	150.5 (4)	C(30)-Yb(3)-C(50)	119.9 (4)
C(29)-Yb(3)-C(50)	100.5 (4)	C(32)-Yb(3)-C(50)	142.0 (3)
C(31)-Yb(3)-C(55)	104.4 (3)	C(30)-Yb(3)-C(55)	97.6 (3)
C(29)-Yb(3)-C(55)	120.6 (4)	C(32)-Yb(3)-C(55)	134.3 (3)
C(50)-Yb(3)-C(55)	80.1 (4)	C(31)-Yb(3)-C(33)	51.6 (3)
C(30)-Yb(3)-C(33)	51.7 (3)	C(29)-Yb(3)-C(33)	31.5 (3)
C(32)-Yb(3)-C(33)	31.1 (3)	C(50)-Yb(3)-C(33)	111.5 (3)
C(55)-Yb(3)-C(33)	149.3 (3)	C(31)-Yb(3)-C(56)	111.4 (3)
C(30)-Yb(3)-C(56)	89.8 (3)	C(29)-Yb(3)-C(56)	100.3 (4)
C(32)-Yb(3)-C(56)	140.9 (3)	C(50)-Yb(3)-C(56)	58.8 (4)
C(55)-Yb(3)-C(56)	30.8 (4)	C(33)-Yb(3)-C(56)	131.6 (4)
C(31)-Yb(3)-C(53)	128.1 (4)	C(30)-Yb(3)-C(53)	148.4 (4)
C(29)-Yb(3)-C(53)	179.6 (4)	C(32)-Yb(3)-C(53)	128.2 (3)
C(50)-Yb(3)-C(53)	79.6 (4)	C(55)-Yb(3)-C(53)	59.0 (4)
C(33)-Yb(3)-C(53)	148.8 (4)	C(56)-Yb(3)-C(53)	79.4 (4)
C(31)-Yb(3)-C(49)	128.1 (4)	C(30)-Yb(3)-C(49)	98.3 (3)
C(29)-Yb(3)-C(49)	92.4 (3)	C(32)-Yb(3)-C(49)	144.3 (3)
C(50)-Yb(3)-C(49)	31.0 (4)	C(55)-Yb(3)-C(49)	58.7 (4)
C(33)-Yb(3)-C(49)	117.4 (3)	C(56)-Yb(3)-C(49)	30.6 (4)
C(53)-Yb(3)-C(49)	87.5 (3)	C(31)-Yb(3)-C(54)	111.1 (3)
C(30)-Yb(3)-C(54)	119.3 (4)	C(29)-Yb(3)-C(54)	148.3 (4)
C(32)-Yb(3)-C(54)	129.9 (4)	C(50)-Yb(3)-C(54)	87.7 (4)
C(55)-Yb(3)-C(54)	30.3 (4)	C(33)-Yb(3)-C(54)	160.9 (4)
C(56)-Yb(3)-C(54)	58.0 (5)	C(53)-Yb(3)-C(54)	31.3 (5)
C(49)-Yb(3)-C(54)	78.9 (4)	C(31)-Yb(3)-C(51)	168.0 (3)
C(30)-Yb(3)-C(51)	148.6 (4)	C(29)-Yb(3)-C(51)	121.9 (4)
C(32)-Yb(3)-C(51)	137.0 (3)	C(50)-Yb(3)-C(51)	30.5 (4)
C(55)-Yb(3)-C(51)	87.6 (3)	C(33)-Yb(3)-C(51)	117.1 (3)
C(56)-Yb(3)-C(51)	79.0 (4)	C(53)-Yb(3)-C(51)	58.3 (5)
C(49)-Yb(3)-C(51)	58.3 (4)	C(54)-Yb(3)-C(51)	79.3 (4)
C(31)-Yb(3)-C(52)	151.1 (4)	C(30)-Yb(3)-C(52)	177.2 (3)
C(29)-Yb(3)-C(52)	149.0 (4)	C(32)-Yb(3)-C(52)	131.0 (3)
C(50)-Yb(3)-C(52)	58.1 (5)	C(55)-Yb(3)-C(52)	80.3 (4)
C(33)-Yb(3)-C(52)	130.3 (4)	C(56)-Yb(3)-C(52)	87.4 (3)

C(53)-Yb(3)-C(54)	31.3(5)	C(49)-Yb(3)-C(52)	79.1(4)
C(54)-Yb(3)-C(52)	59.5(5)	C(51)-Yb(3)-C(52)	30.0(5)
C(40)-Yb(4)-C(39)	31.6(3)	C(40)-Yb(4)-C(41)	32.3(3)
C(39)-Yb(4)-C(41)	52.4(3)	C(40)-Yb(4)-C(56)	130.1(4)
C(39)-Yb(4)-C(56)	118.7(3)	C(41)-Yb(4)-C(56)	160.5(4)
C(40)-Yb(4)-C(49)	157.8(4)	C(39)-Yb(4)-C(49)	132.6(4)
C(41)-Yb(4)-C(49)	168.7(4)	C(56)-Yb(4)-C(49)	30.8(4)
C(40)-Yb(4)-C(42)	52.6(3)	C(39)-Yb(4)-C(42)	51.7(3)
C(41)-Yb(4)-C(42)	31.7(3)	C(56)-Yb(4)-C(42)	161.1(4)
C(49)-Yb(4)-C(42)	139.5(4)	C(40)-Yb(4)-C(51)	142.3(4)
C(39)-Yb(4)-C(51)	159.5(3)	C(41)-Yb(4)-C(51)	113.0(4)
C(56)-Yb(4)-C(51)	79.6(4)	C(49)-Yb(4)-C(51)	58.9(4)
C(42)-Yb(4)-C(51)	108.0(3)	C(40)-Yb(4)-C(43)	52.5(3)
C(39)-Yb(4)-C(43)	31.2(3)	C(41)-Yb(4)-C(43)	52.4(3)
C(56)-Yb(4)-C(43)	131.3(3)	C(49)-Yb(4)-C(43)	124.9(3)
C(42)-Yb(4)-C(43)	31.3(3)	C(51)-Yb(4)-C(43)	129.9(3)
C(40)-Yb(4)-C(54)	96.5(4)	C(39)-Yb(4)-C(54)	117.0(3)
C(41)-Yb(4)-C(54)	107.9(4)	C(56)-Yb(4)-C(54)	58.1(5)
C(49)-Yb(4)-C(54)	79.4(4)	C(42)-Yb(4)-C(54)	139.3(4)
C(51)-Yb(4)-C(54)	79.7(4)	C(43)-Yb(4)-C(54)	147.4(3)
C(40)-Yb(4)-C(50)	171.1(4)	C(39)-Yb(4)-C(50)	150.8(4)
C(41)-Yb(4)-C(50)	138.8(4)	C(56)-Yb(4)-C(50)	58.6(4)
C(49)-Yb(4)-C(50)	31.0(4)	C(42)-Yb(4)-C(50)	120.1(4)
C(51)-Yb(4)-C(50)	30.5(4)	C(43)-Yb(4)-C(50)	125.1(3)
C(54)-Yb(4)-C(50)	87.2(4)	C(40)-Yb(4)-C(55)	108.1(4)
C(39)-Yb(4)-C(55)	113.1(3)	C(41)-Yb(4)-C(55)	131.6(4)
C(56)-Yb(4)-C(55)	30.6(4)	C(49)-Yb(4)-C(55)	58.5(4)
C(42)-Yb(4)-C(55)	160.7(4)	C(51)-Yb(4)-C(55)	87.3(3)
C(43)-Yb(4)-C(55)	140.7(3)	C(54)-Yb(4)-C(55)	30.1(4)
C(50)-Yb(4)-C(55)	79.0(4)	C(40)-Yb(4)-C(52)	117.3(4)
C(39)-Yb(4)-C(52)	147.8(4)	C(41)-Yb(4)-C(52)	96.5(4)
C(56)-Yb(4)-C(52)	87.7(3)	C(49)-Yb(4)-C(52)	79.6(4)
C(42)-Yb(4)-C(52)	107.7(4)	C(51)-Yb(4)-C(52)	30.1(4)
C(43)-Yb(4)-C(52)	138.5(3)	C(54)-Yb(4)-C(52)	59.5(4)
C(50)-Yb(4)-C(52)	57.8(5)	C(55)-Yb(4)-C(52)	79.6(4)
C(40)-Yb(4)-C(53)	100.4(4)	C(39)-Yb(4)-C(53)	130.6(4)
C(41)-Yb(4)-C(53)	94.7(3)	C(56)-Yb(4)-C(53)	79.1(4)
C(49)-Yb(4)-C(53)	87.4(3)	C(42)-Yb(4)-C(53)	119.8(4)
C(51)-Yb(4)-C(53)	58.2(4)	C(43)-Yb(4)-C(53)	147.1(3)

C(54) - Yb(4) - C(53)	31.1(4)	C(50) - Yb(4) - C(53)	78.6(4)
C(55) - Yb(4) - C(53)	58.2(4)	C(52) - Yb(4) - C(53)	31.1(5)
C(30) - C(29) - C(33)	107.6(9)	C(30) - C(29) - C(34)	125.9(9)
C(33) - C(29) - C(34)	126.4(9)	C(30) - C(29) - Yb(3)	74.3(5)
C(33) - C(29) - Yb(3)	75.2(5)	C(34) - C(29) - Yb(3)	118.2(7)
C(31) - C(30) - C(29)	108.0(9)	C(31) - C(30) - C(35)	125.9(9)
C(29) - C(30) - C(35)	126.1(9)	C(31) - C(30) - Yb(3)	73.7(5)
C(29) - C(30) - Yb(3)	74.4(5)	C(35) - C(30) - Yb(3)	117.0(6)
C(30) - C(31) - C(32)	108.8(9)	C(30) - C(31) - C(36)	126.7(9)
C(32) - C(31) - C(36)	124.4(9)	C(30) - C(31) - Yb(3)	75.1(5)
C(32) - C(31) - Yb(3)	75.2(5)	C(36) - C(31) - Yb(3)	118.6(6)
C(33) - C(32) - C(31)	107.8(9)	C(33) - C(32) - C(37)	123.6(9)
C(31) - C(32) - C(37)	128.1(10)	C(33) - C(32) - Yb(3)	75.2(6)
C(31) - C(32) - Yb(3)	73.4(5)	C(37) - C(32) - Yb(3)	123.3(7)
C(32) - C(33) - C(29)	107.7(8)	C(32) - C(33) - C(38)	127.5(10)
C(29) - C(33) - C(38)	124.8(10)	C(32) - C(33) - Yb(3)	73.7(6)
C(29) - C(33) - Yb(3)	73.3(5)	C(38) - C(33) - Yb(3)	119.1(7)
C(43) - C(39) - C(40)	109.6(9)	C(43) - C(39) - C(44)	126.3(10)
C(40) - C(39) - C(44)	124.0(9)	C(43) - C(39) - Yb(4)	75.5(5)
C(40) - C(39) - Yb(4)	73.7(6)	C(44) - C(39) - Yb(4)	120.9(7)
C(39) - C(40) - C(41)	107.0(9)	C(39) - C(40) - C(45)	126.6(10)
C(41) - C(40) - C(45)	126.4(10)	C(39) - C(40) - Yb(4)	74.7(6)
C(41) - C(40) - Yb(4)	74.3(5)	C(45) - C(40) - Yb(4)	117.8(8)
C(42) - C(41) - C(40)	107.0(9)	C(42) - C(41) - C(46)	125.9(9)
C(40) - C(41) - C(46)	127.0(9)	C(42) - C(41) - Yb(4)	74.7(5)
C(40) - C(41) - Yb(4)	73.4(5)	C(46) - C(41) - Yb(4)	114.8(7)
C(43) - C(42) - C(41)	108.9(8)	C(43) - C(42) - C(47)	125.9(10)
C(41) - C(42) - C(47)	125.2(10)	C(43) - C(42) - Yb(4)	74.9(5)
C(41) - C(42) - Yb(4)	73.6(6)	C(47) - C(42) - Yb(4)	119.4(8)
C(39) - C(43) - C(42)	107.5(9)	C(39) - C(43) - C(48)	127.1(10)
C(42) - C(43) - C(48)	125.2(10)	C(39) - C(43) - Yb(4)	73.3(6)
C(42) - C(43) - Yb(4)	73.8(6)	C(48) - C(43) - Yb(4)	122.5(7)
C(56) - C(49) - C(50)	134.4(11)	C(56) - C(49) - Yb(4)	74.6(6)
C(50) - C(49) - Yb(4)	75.7(7)	C(56) - C(49) - Yb(3)	74.2(7)
C(50) - C(49) - Yb(3)	73.6(7)	Yb(4) - C(49) - Yb(3)	93.0(3)
C(51) - C(50) - C(49)	135.0(10)	C(51) - C(50) - Yb(3)	76.1(7)
C(49) - C(50) - Yb(3)	75.4(7)	C(51) - C(50) - Yb(4)	74.1(7)
C(49) - C(50) - Yb(4)	73.4(6)	Yb(3) - C(50) - Yb(4)	92.8(3)
C(52) - C(51) - C(50)	136.3(11)	C(52) - C(51) - Yb(4)	76.2(7)

Table 1. Crystal data and structure refinement for $[(C_5Me_5)Eu]_2(C_8H_8) \cdot C_7H_8$, 4.

Formula	$C_{35}H_{46}Eu_2$
fw	770.64
a	11.856(6) Å
b	15.220(6) Å
c	17.399(6) Å
α	90°
β	90°
γ	90°
V	3139.9(23) Å ³
Z	4
Space group	$P2_12_12_1$
T	153 K
λ	0.71073 Å
ρ (calcd)	1.630 g/cm ³
μ	3.979 mm ⁻¹
R1, wR2 [I > 2 σ (I)]	0.0526, 0.1519
R1, wR2 (all data)	0.0760, 0.1665

$$R1 = \sum ||F_o| - |F_c|| / \sum |F_o|$$

$$wR2 = [\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{1/2}$$

Table 2. Crystal data and structure refinement for $[(C_5Me_5)Eu]_2(C_8H_8) \cdot C_7H_8$, 4.

Empirical formula	$C_{35}H_{46}Eu_2$
Formula weight	770.64
Temperature	153 K
Wavelength	0.71073 Å
Crystal system, Space Group	Orthorhombic, $P2_1^2 2_1^2 2_1^2$
Unit cell dimensions	$a = 11.856(6)$ Å $\alpha = 90^\circ$ $b = 15.220(6)$ Å $\beta = 90^\circ$ $c = 17.399(6)$ Å $\gamma = 90^\circ$
Volume, Z	3140(2) Å ³ , 4
Density (calculated)	1.630 Mg/m ³
Absorption coefficient	3.979 mm ⁻¹
F(000)	1528
Crystal size	0.23 x 0.16 x 0.1 mm
θ range for data collection	2.08 to 26.00°
Limiting indices	$0 \leq h \leq 14$, $0 \leq k \leq 18$, $0 \leq l \leq 21$
Reflections collected	3456
Independent reflections	3456 ($R_{int} = 0.0000$)
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.1022 and 0.0648
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3455 / 0 / 347
Goodness-of-fit on F^2	1.255
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0526$, $wR2 = 0.1519$
R indices (all data)	$R1 = 0.0760$, $wR2 = 0.1665$
Absolute structure parameter	0.46(8)
Largest diff. peak and hole	2.226 and -1.527 eÅ ⁻³

$$R1 = \sum ||F_o| - |F_c|| / \sum |F_o|$$

$$wR2 = [\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{1/2}$$

Crystal data.

Empirical formula	$C_{35}H_{46}Eu_2$
Formula weight	770.64
Crystal Description	irregular
Crystal Color	orange
Crystal size	0.23 x 0.16 x 0.1 mm
Crystal system	Orthorhombic
Space group	$P2_1^2 2_1^2$
Unit cell dimensions:	$a = 11.856(6) \text{ \AA}$
	$b = 15.220(6) \text{ \AA}$
	$c = 17.399(6) \text{ \AA}$
	$\alpha = 90^\circ$
	$\beta = 90^\circ$
	$\gamma = 90^\circ$
Volume	$3140(2) \text{ \AA}^3$
Z	4
Density (calculated)	1.630 Mg/m^3
Absorption coefficient	3.979 mm^{-1}
F(000)	1528

Data Collection and Reduction.

Diffractometer type	Siemens P4
Radiation source	fine-focus sealed tube
Monochromator type	graphite
Radiation	MoK α
Wavelength	0.71073 Å
Temperature	153 K
Cell measurement reflections	21 ($5.80^{\circ} < \theta < 15.65^{\circ}$)
Intensity measurement method	$2\theta/\omega$ scans
θ range for data collection	2.08 to 26.00°
Limiting indices	$0 \leq h \leq 14, 0 \leq k \leq 18, 0 \leq l \leq 21$
Scan width (in ω)	1.2° plus α_1, α_2 separation
Scan speed (in ω)	$4.0^{\circ}/\text{min}$
Reflections collected	3456
Independent reflections	3456 ($R_{\text{int}} = 0.0000$)
Observed reflections	2762 ($I > 2\sigma(I)$)
Number of standards	1
Interval between standards	99
Decay of standards	<1%
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.1022 and 0.0648

Unit cell refinement and data collection were carried out by use of the Siemens XSCANs system, Version 2.10b. Data were processed with a local version of CARESS (R.W. Broach et al.), which employs a modified version of the Lehman-Larsen algorithm to obtain integrated intensities and standard deviations from the measured 96-step peak profiles.

Structure Solution and Refinement.

Structure solution method	direct methods
Refinement method	Full-matrix least-squares on F^2
Scattering Factor Source	International Tables Vol C Tables 4.2.6.8 and 6.1.1.4
Final refinement: Data	3455
Restraints	0
Parameters	347
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0526$, $wR_2 = 0.1519$
R indices (all data)	$R_1 = 0.0760$, $wR_2 = 0.1665$
Goodness-of-fit on F^2	1.255
Absolute structure parameter	0.46(8)
Largest diff. peak and hole	2.226 and $-1.527 \text{ e}\text{\AA}^{-3}$
Maximum Δ/σ in final cycle	1.310
Mean Δ/σ in final cycle	0.009

Final weighting scheme:

$$\text{calc } w = 1 / [\sigma^2(F_o^2) + (0.0653P)^2 + 33.5493P]$$

$$\text{where } P = (F_o^2 + 2F_c^2) / 3$$

R-factor definitions:

$$R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$$

$$wR_2 = [\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{1/2}$$

Structure solution, refinement, and generation of figures and tables were carried out by use of Version 5.03 of the Siemens SHELXTL program package.

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

	x	y	z	U(eq)
Eu(1)	1470 (1)	-13812 (1)	-8019 (1)	30 (1)
Eu(2)	1782 (1)	-13687 (1)	-5563 (1)	25 (1)
C(1)	-234 (19)	-14308 (15)	-9049 (14)	35 (5)
C(2)	-553 (20)	-13494 (14)	-8779 (11)	32 (5)
C(3)	230 (21)	-12861 (14)	-9049 (14)	38 (6)
C(4)	1025 (20)	-13302 (14)	-9508 (12)	34 (5)
C(5)	750 (17)	-14204 (13)	-9521 (13)	26 (4)
C(6)	-835 (22)	-15179 (18)	-8927 (16)	54 (7)
C(7)	-1599 (25)	-13303 (20)	-8289 (14)	63 (8)
C(8)	232 (30)	-11845 (17)	-8917 (19)	73 (10)
C(9)	2005 (25)	-12870 (18)	-9945 (14)	56 (7)
C(10)	1257 (22)	-14907 (15)	-10012 (15)	48 (7)
C(11)	-7 (18)	-14067 (13)	-4555 (10)	27 (4)
C(12)	43 (20)	-13143 (13)	-4583 (11)	28 (5)
C(13)	1046 (19)	-12855 (13)	-4211 (11)	25 (4)
C(14)	1616 (17)	-13643 (13)	-3961 (10)	29 (4)
C(15)	983 (20)	-14395 (14)	-4170 (11)	27 (5)
C(16)	-993 (17)	-14628 (15)	-4858 (13)	34 (5)
C(17)	-834 (23)	-12539 (17)	-4907 (14)	41 (6)
C(18)	1409 (23)	-11930 (15)	-4045 (14)	46 (6)
C(19)	2672 (19)	-13657 (16)	-3442 (11)	39 (5)
C(20)	1200 (18)	-15333 (15)	-3958 (12)	33 (5)
C(21)	692 (22)	-12818 (16)	-6774 (14)	36 (6)

C(22)	1828 (20)	-12543 (13)	-6842 (13)	34 (5)
C(23)	2871 (22)	-12979 (14)	-6930 (13)	37 (6)
C(24)	3205 (16)	-13887 (14)	-6896 (9)	32 (5)
C(25)	2667 (20)	-14703 (14)	-6829 (13)	31 (5)
C(26)	1540 (20)	-14947 (13)	-6738 (12)	34 (5)
C(27)	490 (20)	-14504 (15)	-6716 (13)	31 (5)
C(28)	122 (19)	-13628 (17)	-6713 (11)	39 (5)
C(29)	-328 (17)	-13456 (14)	-11814 (10)	36 (5)
C(30)	-907 (18)	-13654 (18)	-11141 (10)	43 (6)
C(31)	-1667 (26)	-14306 (18)	-11083 (17)	61 (8)
C(32)	-1919 (28)	-14814 (19)	-11736 (20)	69 (9)
C(33)	-1368 (23)	-14658 (16)	-12440 (16)	53 (7)
C(34)	-565 (18)	-13967 (16)	-12443 (13)	42 (6)
C(35)	470 (26)	-12725 (23)	-11890 (23)	85 (11)

Table 4. Bond lengths [Å] and angles [°] for 3.

Eu(1)-C(3)	2.73(2)	Eu(1)-C(4)	2.76(2)
Eu(1)-C(27)	2.76(2)	Eu(1)-C(2)	2.78(2)
Eu(1)-C(28)	2.79(2)	Eu(1)-C(21)	2.80(2)
Eu(1)-C(1)	2.80(2)	Eu(1)-C(5)	2.81(2)
Eu(1)-C(26)	2.82(2)	Eu(1)-C(23)	2.82(2)
Eu(1)-C(24)	2.84(2)	Eu(1)-C(22)	2.85(2)
Eu(2)-C(14)	2.80(2)	Eu(2)-C(12)	2.80(2)
Eu(2)-C(21)	2.80(2)	Eu(2)-C(28)	2.81(2)
Eu(2)-C(13)	2.81(2)	Eu(2)-C(11)	2.81(2)
Eu(2)-C(27)	2.81(2)	Eu(2)-C(15)	2.82(2)
Eu(2)-C(26)	2.82(2)	Eu(2)-C(22)	2.83(2)
Eu(2)-C(24)	2.88(2)	Eu(2)-C(25)	2.89(2)
C(1)-C(2)	1.38(3)	C(1)-C(5)	1.44(3)
C(1)-C(6)	1.52(3)	C(2)-C(3)	1.42(3)
C(2)-C(7)	1.53(3)	C(3)-C(4)	1.41(3)
C(3)-C(8)	1.56(3)	C(4)-C(5)	1.41(3)
C(4)-C(9)	1.54(3)	C(5)-C(10)	1.50(3)
C(11)-C(12)	1.41(3)	C(11)-C(15)	1.44(3)
C(11)-C(16)	1.54(3)	C(12)-C(13)	1.42(3)
C(12)-C(17)	1.50(3)	C(13)-C(14)	1.44(3)
C(13)-C(18)	1.50(3)	C(14)-C(15)	1.42(3)
C(14)-C(19)	1.54(3)	C(15)-C(20)	1.50(3)
C(21)-C(28)	1.41(4)	C(21)-C(22)	1.41(3)
C(22)-C(23)	1.41(3)	C(23)-C(24)	1.44(3)
C(24)-C(25)	1.40(3)	C(25)-C(26)	1.40(3)
C(26)-C(27)	1.42(3)	C(27)-C(28)	1.40(3)
C(29)-C(30)	1.39	C(29)-C(34)	1.37(3)
C(29)-C(35)	1.47(4)	C(30)-C(31)	1.34(3)
C(31)-C(32)	1.41(4)	C(32)-C(33)	1.41(4)
C(33)-C(34)	1.42(3)		
C(3)-Eu(1)-C(4)	29.7(7)	C(3)-Eu(1)-C(27)	121.0(7)
C(4)-Eu(1)-C(27)	143.2(7)	C(3)-Eu(1)-C(2)	29.8(7)
C(4)-Eu(1)-C(2)	48.6(6)	C(27)-Eu(1)-C(2)	95.4(6)
C(3)-Eu(1)-C(28)	99.9(7)	C(4)-Eu(1)-C(28)	128.8(7)
C(27)-Eu(1)-C(28)	29.3(7)	C(2)-Eu(1)-C(28)	82.9(6)

C(3) -Eu(1) -C(21)	92.5 (7)	C(4) -Eu(1) -C(21)	120.8 (7)
C(27) -Eu(1) -C(21)	55.3 (7)	C(2) -Eu(1) -C(21)	89.4 (6)
C(28) -Eu(1) -C(21)	29.2 (7)	C(3) -Eu(1) -C(1)	48.4 (7)
C(4) -Eu(1) -C(1)	48.5 (7)	C(27) -Eu(1) -C(1)	96.9 (7)
C(2) -Eu(1) -C(1)	28.6 (6)	C(28) -Eu(1) -C(1)	97.8 (6)
C(21) -Eu(1) -C(1)	113.8 (7)	C(3) -Eu(1) -C(5)	48.7 (6)
C(4) -Eu(1) -C(5)	29.3 (5)	C(27) -Eu(1) -C(5)	123.7 (6)
C(2) -Eu(1) -C(5)	48.2 (6)	C(28) -Eu(1) -C(5)	127.1 (6)
C(21) -Eu(1) -C(5)	137.2 (6)	C(1) -Eu(1) -C(5)	29.6 (6)
C(3) -Eu(1) -C(26)	149.1 (7)	C(4) -Eu(1) -C(26)	157.1 (6)
C(27) -Eu(1) -C(26)	29.4 (7)	C(2) -Eu(1) -C(26)	120.5 (6)
C(28) -Eu(1) -C(26)	55.6 (6)	C(21) -Eu(1) -C(26)	74.3 (7)
C(1) -Eu(1) -C(26)	111.2 (7)	C(5) -Eu(1) -C(26)	127.8 (6)
C(3) -Eu(1) -C(23)	121.3 (7)	C(4) -Eu(1) -C(23)	128.1 (7)
C(27) -Eu(1) -C(23)	82.4 (7)	C(2) -Eu(1) -C(23)	138.5 (6)
C(28) -Eu(1) -C(23)	75.2 (7)	C(21) -Eu(1) -C(23)	55.3 (7)
C(1) -Eu(1) -C(23)	167.0 (6)	C(5) -Eu(1) -C(23)	153.9 (7)
C(26) -Eu(1) -C(23)	74.2 (7)	C(3) -Eu(1) -C(24)	149.5 (7)
C(4) -Eu(1) -C(24)	142.8 (6)	C(27) -Eu(1) -C(24)	74.0 (6)
C(2) -Eu(1) -C(24)	163.5 (5)	C(28) -Eu(1) -C(24)	81.9 (6)
C(21) -Eu(1) -C(24)	74.2 (6)	C(1) -Eu(1) -C(24)	162.0 (6)
C(5) -Eu(1) -C(24)	148.3 (5)	C(26) -Eu(1) -C(24)	53.9 (6)
C(23) -Eu(1) -C(24)	29.4 (6)	C(3) -Eu(1) -C(22)	101.1 (6)
C(4) -Eu(1) -C(22)	120.9 (6)	C(27) -Eu(1) -C(22)	74.4 (6)
C(2) -Eu(1) -C(22)	110.6 (6)	C(28) -Eu(1) -C(22)	55.4 (7)
C(21) -Eu(1) -C(22)	29.0 (7)	C(1) -Eu(1) -C(22)	138.6 (6)
C(5) -Eu(1) -C(22)	149.0 (6)	C(26) -Eu(1) -C(22)	81.0 (6)
C(23) -Eu(1) -C(22)	28.9 (7)	C(24) -Eu(1) -C(22)	54.9 (6)
C(14) -Eu(2) -C(12)	48.2 (6)	C(14) -Eu(2) -C(21)	134.9 (6)
C(12) -Eu(2) -C(21)	88.8 (7)	C(14) -Eu(2) -C(28)	131.3 (6)
C(12) -Eu(2) -C(28)	84.8 (6)	C(21) -Eu(2) -C(28)	29.1 (7)
C(14) -Eu(2) -C(13)	29.8 (6)	C(12) -Eu(2) -C(13)	29.4 (6)
C(21) -Eu(2) -C(13)	105.9 (6)	C(28) -Eu(2) -C(13)	111.4 (6)
C(14) -Eu(2) -C(11)	47.9 (6)	C(12) -Eu(2) -C(11)	29.0 (6)
C(21) -Eu(2) -C(11)	102.6 (7)	C(28) -Eu(2) -C(11)	85.6 (6)
C(13) -Eu(2) -C(11)	48.4 (6)	C(14) -Eu(2) -C(27)	133.1 (7)
C(12) -Eu(2) -C(27)	99.4 (7)	C(21) -Eu(2) -C(27)	54.7 (7)
C(28) -Eu(2) -C(27)	28.9 (7)	C(13) -Eu(2) -C(27)	128.8 (6)
C(11) -Eu(2) -C(27)	86.8 (6)	C(14) -Eu(2) -C(15)	29.2 (6)

C(12) -Eu(2) -C(15)	48.8(6)	C(21) -Eu(2) -C(15)	132.2(7)
C(28) -Eu(2) -C(15)	112.9(6)	C(13) -Eu(2) -C(15)	49.3(6)
C(11) -Eu(2) -C(15)	29.6(6)	C(27) -Eu(2) -C(15)	105.1(7)
C(14) -Eu(2) -C(26)	137.2(6)	C(12) -Eu(2) -C(26)	124.6(7)
C(21) -Eu(2) -C(26)	74.3(6)	C(28) -Eu(2) -C(26)	55.5(6)
C(13) -Eu(2) -C(26)	151.9(6)	C(11) -Eu(2) -C(26)	103.7(6)
C(27) -Eu(2) -C(26)	29.1(6)	C(15) -Eu(2) -C(26)	109.3(6)
C(14) -Eu(2) -C(22)	140.5(6)	C(12) -Eu(2) -C(22)	108.1(6)
C(21) -Eu(2) -C(22)	29.1(7)	C(28) -Eu(2) -C(22)	55.4(7)
C(13) -Eu(2) -C(22)	112.8(6)	C(11) -Eu(2) -C(22)	129.2(6)
C(27) -Eu(2) -C(22)	73.8(7)	C(15) -Eu(2) -C(22)	156.9(6)
C(26) -Eu(2) -C(22)	81.4(5)	C(14) -Eu(2) -C(24)	147.7(5)
C(12) -Eu(2) -C(24)	162.1(6)	C(21) -Eu(2) -C(24)	73.4(6)
C(28) -Eu(2) -C(24)	80.8(6)	C(13) -Eu(2) -C(24)	154.4(6)
C(11) -Eu(2) -C(24)	157.1(6)	C(27) -Eu(2) -C(24)	72.5(6)
C(15) -Eu(2) -C(24)	148.1(6)	C(26) -Eu(2) -C(24)	53.4(6)
C(22) -Eu(2) -C(24)	54.6(6)	C(14) -Eu(2) -C(25)	143.1(6)
C(12) -Eu(2) -C(25)	152.9(7)	C(21) -Eu(2) -C(25)	81.2(7)
C(28) -Eu(2) -C(25)	74.2(6)	C(13) -Eu(2) -C(25)	172.9(6)
C(11) -Eu(2) -C(25)	129.8(6)	C(27) -Eu(2) -C(25)	54.4(7)
C(15) -Eu(2) -C(25)	125.0(6)	C(26) -Eu(2) -C(25)	28.3(7)
C(22) -Eu(2) -C(25)	73.9(6)	C(24) -Eu(2) -C(25)	28.1(6)
C(2) -C(1) -C(5)	109(2)	C(2) -C(1) -C(6)	127(2)
C(5) -C(1) -C(6)	124(2)	C(2) -C(1) -Eu(1)	74.8(13)
C(5) -C(1) -Eu(1)	75.5(13)	C(6) -C(1) -Eu(1)	119(2)
C(1) -C(2) -C(3)	109(2)	C(1) -C(2) -C(7)	126(2)
C(3) -C(2) -C(7)	126(2)	C(1) -C(2) -Eu(1)	76.6(13)
C(3) -C(2) -Eu(1)	73.2(13)	C(7) -C(2) -Eu(1)	117.8(14)
C(4) -C(3) -C(2)	108(2)	C(4) -C(3) -C(8)	124(2)
C(2) -C(3) -C(8)	129(2)	C(4) -C(3) -Eu(1)	76.1(12)
C(2) -C(3) -Eu(1)	77.0(13)	C(8) -C(3) -Eu(1)	115(2)
C(3) -C(4) -C(5)	109(2)	C(3) -C(4) -C(9)	126(2)
C(5) -C(4) -C(9)	126(2)	C(3) -C(4) -Eu(1)	74.3(13)
C(5) -C(4) -Eu(1)	77.5(14)	C(9) -C(4) -Eu(1)	116(2)
C(4) -C(5) -C(1)	107(2)	C(4) -C(5) -C(10)	128(2)
C(1) -C(5) -C(10)	125(2)	C(4) -C(5) -Eu(1)	73.1(14)
C(1) -C(5) -Eu(1)	74.9(13)	C(10) -C(5) -Eu(1)	124.1(14)
C(12) -C(11) -C(15)	109(2)	C(12) -C(11) -C(16)	125(2)
C(15) -C(11) -C(16)	126(2)	C(12) -C(11) -Eu(2)	75.0(13)

C(15)-C(11)-Eu(2)	75.3(12)	C(16)-C(11)-Eu(2)	118.1(13)
C(11)-C(12)-C(13)	109(2)	C(11)-C(12)-C(17)	127(2)
C(13)-C(12)-C(17)	124(2)	C(11)-C(12)-Eu(2)	75.9(13)
C(13)-C(12)-Eu(2)	75.7(12)	C(17)-C(12)-Eu(2)	117.6(14)
C(12)-C(13)-C(14)	106(2)	C(12)-C(13)-C(18)	128(2)
C(14)-C(13)-C(18)	126(2)	C(12)-C(13)-Eu(2)	74.9(11)
C(14)-C(13)-Eu(2)	74.5(11)	C(18)-C(13)-Eu(2)	119.6(14)
C(15)-C(14)-C(13)	110(2)	C(15)-C(14)-C(19)	125(2)
C(13)-C(14)-C(19)	125(2)	C(15)-C(14)-Eu(2)	76.2(11)
C(13)-C(14)-Eu(2)	75.7(11)	C(19)-C(14)-Eu(2)	121.7(13)
C(14)-C(15)-C(11)	106(2)	C(14)-C(15)-C(20)	128(2)
C(11)-C(15)-C(20)	126(2)	C(14)-C(15)-Eu(2)	74.6(11)
C(11)-C(15)-Eu(2)	75.0(11)	C(20)-C(15)-Eu(2)	121.2(14)
C(28)-C(21)-C(22)	136(2)	C(28)-C(21)-Eu(1)	75.1(13)
C(22)-C(21)-Eu(1)	77.4(14)	C(28)-C(21)-Eu(2)	75.6(13)
C(22)-C(21)-Eu(2)	76.4(14)	Eu(1)-C(21)-Eu(2)	100.1(7)
C(23)-C(22)-C(21)	135(2)	C(23)-C(22)-Eu(2)	79.1(14)
C(21)-C(22)-Eu(2)	74.5(14)	C(23)-C(22)-Eu(1)	74.6(12)
C(21)-C(22)-Eu(1)	73.6(14)	Eu(2)-C(22)-Eu(1)	98.3(6)
C(22)-C(23)-C(24)	134(2)	C(22)-C(23)-Eu(1)	76.5(13)
C(24)-C(23)-Eu(1)	76.0(11)	C(22)-C(23)-Eu(2)	72.4(14)
C(24)-C(23)-Eu(2)	74.5(12)	Eu(1)-C(23)-Eu(2)	96.9(7)
C(25)-C(24)-C(23)	137(2)	C(25)-C(24)-Eu(1)	76.2(12)
C(23)-C(24)-Eu(1)	74.6(12)	C(25)-C(24)-Eu(2)	76.1(11)
C(23)-C(24)-Eu(2)	76.8(12)	Eu(1)-C(24)-Eu(2)	97.2(6)
C(26)-C(25)-C(24)	133(2)	C(26)-C(25)-Eu(1)	74.5(12)
C(24)-C(25)-Eu(1)	75.3(11)	C(26)-C(25)-Eu(2)	73.0(12)
C(24)-C(25)-Eu(2)	75.7(11)	Eu(1)-C(25)-Eu(2)	96.8(6)
C(25)-C(26)-C(27)	136(2)	C(25)-C(26)-Eu(2)	78.7(13)
C(27)-C(26)-Eu(2)	75.3(12)	C(25)-C(26)-Eu(1)	77.0(13)
C(27)-C(26)-Eu(1)	72.8(13)	Eu(2)-C(26)-Eu(1)	99.2(6)
C(28)-C(27)-C(26)	137(2)	C(28)-C(27)-Eu(1)	76.7(14)
C(26)-C(27)-Eu(1)	77.8(13)	C(28)-C(27)-Eu(2)	75.4(12)
C(26)-C(27)-Eu(2)	75.6(13)	Eu(1)-C(27)-Eu(2)	100.8(7)
C(27)-C(28)-C(21)	133(2)	C(27)-C(28)-Eu(1)	74.0(14)
C(21)-C(28)-Eu(1)	75.7(13)	C(27)-C(28)-Eu(2)	75.7(12)
C(21)-C(28)-Eu(2)	75.3(13)	Eu(1)-C(28)-Eu(2)	100.1(7)
C(30)-C(29)-C(34)	117(2)	C(30)-C(29)-C(35)	124(3)
C(34)-C(29)-C(35)	119(2)	C(31)-C(30)-C(29)	124(2)

C(30)-C(31)-C(32)	119(3)	C(33)-C(32)-C(31)	121(3)
C(34)-C(33)-C(32)	116(2)	C(33)-C(34)-C(29)	124(2)

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 3.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(ha^*)^2 U_{11} + \dots + 2hka^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Eu(1)	25(1)	46(1)	19(1)	-2(1)	0(1)	5(1)
Eu(2)	24(1)	33(1)	18(1)	0(1)	0(1)	3(1)
C(1)	24(11)	40(13)	40(12)	-6(10)	0(10)	13(10)
C(2)	45(13)	33(12)	19(9)	9(8)	1(9)	-1(10)
C(3)	41(14)	26(11)	47(13)	-7(10)	-10(12)	16(10)
C(4)	43(13)	41(11)	17(9)	5(9)	-11(10)	-11(10)
C(5)	18(9)	29(10)	32(11)	0(9)	-1(9)	1(8)
C(6)	38(15)	65(18)	59(17)	6(15)	-8(13)	0(13)
C(7)	67(20)	81(19)	40(13)	-22(13)	0(14)	24(17)
C(8)	88(24)	46(16)	85(23)	-16(15)	-3(19)	40(17)
C(9)	67(19)	71(17)	32(12)	26(12)	-3(13)	-13(16)
C(10)	44(15)	41(13)	58(16)	-21(12)	-25(13)	23(12)
C(11)	31(11)	37(11)	13(9)	3(8)	-4(9)	-7(9)
C(12)	41(13)	27(10)	17(9)	-7(8)	-1(9)	11(10)
C(13)	24(10)	30(11)	22(10)	-1(8)	1(8)	-4(9)
C(14)	29(10)	32(10)	27(9)	6(8)	-1(8)	7(10)
C(15)	32(11)	32(11)	18(9)	13(8)	7(9)	3(10)
C(16)	12(9)	49(14)	41(13)	-3(11)	2(9)	-2(9)
C(17)	56(17)	47(12)	21(12)	-6(9)	11(11)	12(12)
C(18)	50(15)	45(13)	42(13)	-5(11)	6(13)	-9(12)
C(19)	54(13)	41(12)	21(9)	10(10)	-15(9)	2(12)
C(20)	21(11)	52(14)	27(11)	12(10)	3(9)	0(10)
C(21)	37(14)	41(13)	30(12)	-8(11)	-7(10)	12(11)
C(22)	36(12)	26(10)	40(12)	-6(9)	3(11)	0(10)
C(23)	52(15)	33(11)	27(12)	-8(10)	-8(11)	-13(10)
C(24)	22(9)	58(13)	14(8)	-9(9)	-2(7)	14(11)
C(25)	38(12)	31(11)	24(10)	-8(9)	6(10)	12(10)
C(26)	44(15)	25(10)	34(11)	9(8)	1(11)	9(10)
C(27)	27(12)	38(12)	29(11)	-19(10)	-10(9)	-17(10)
C(28)	33(11)	54(15)	30(10)	7(11)	-1(9)	5(13)
C(29)	25(10)	44(13)	38(12)	15(10)	2(9)	4(9)
C(30)	48(13)	54(14)	25(10)	0(11)	-9(9)	14(14)
C(31)	53(18)	68(18)	63(18)	32(15)	18(16)	-6(16)
C(32)	60(19)	50(16)	97(25)	16(16)	1(19)	7(16)
C(33)	50(16)	47(14)	61(16)	-11(13)	-13(14)	-7(13)
C(34)	30(11)	62(16)	35(11)	-2(11)	7(9)	19(12)
C(35)	46(17)	95(25)	115(30)	4(24)	-11(21)	-17(18)