Supporting Information for

Reductive Reactivity of the Organolanthanide Hydrides, $[(C_5Me_5)_2LnH]_x$ (Ln = La, Sm, and Y), including the Structure of the Ansa-Allyl Cyclopentadienyl Complex, $(C_5Me_5)Y(\eta^5\text{-}C_5Me_4CH_2\text{-}C_5Me_4CH_2\text{-}\eta^3)$

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Table 1. Crystal data and structure refinement for **[$(C_5Me_5)_2La(\mu$-SPh)]$_2$, 9**.

Empirical formula	$C_{52}\ H_{70}\ La_2\ S_2 \bullet 2(C_7H_8)$	
Formula weight	1221.29	
Temperature	163(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 10.3920(10) Å	α= 110.9480(10)°.
	b = 10.6563(11) Å	β= 98.645(2)°.
	c = 14.8522(15) Å	γ = 95.886(2)°.
Volume	1496.7(3) Å^3	
Z	1	
Density (calculated)	1.355 Mg/m^3	
Absorption coefficient	1.515 mm^{-1}	
F(000)	628	
Crystal color	colorless	
Crystal size	0.50 x 0.30 x 0.25 mm^3	
Theta range for data collection	2.01 to 28.29°	
Index ranges	$-13 \le h \le 13$, $-14 \le k \le 14$, $-19 \le l \le 19$	
Reflections collected	19221	
Independent reflections	7281 [R(int) = 0.0189]	
Completeness to theta = 28.29°	98.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7032 and 0.5179	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7281 / 0 / 280	
Goodness-of-fit on F^2	1.055	
Final R indices [I>2sigma(I) = 6812 data]	R1 = 0.0245, wR2 = 0.0627	
R indices (all data; 0.75Å)	R1 = 0.0270, wR2 = 0.0648	
Largest diff. peak and hole	1.259 and -0.655 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **9**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
La(1)	5539(1)	6228(1)	1881(1)	21(1)
S(1)	6144(1)	4163(1)	64(1)	28(1)
C(1)	3550(2)	4237(2)	1849(2)	32(1)
C(2)	3209(2)	5480(2)	2413(2)	34(1)
C(3)	4130(3)	6036(3)	3319(2)	41(1)
C(4)	5056(3)	5146(3)	3286(2)	44(1)
C(5)	4695(3)	4050(3)	2378(2)	40(1)
C(6)	2749(4)	3256(4)	876(2)	66(1)
C(7)	2024(3)	6081(4)	2167(3)	71(1)
C(8)	3967(5)	7199(4)	4214(3)	83(2)
C(9)	6154(4)	5209(5)	4103(3)	91(2)
C(10)	5328(4)	2785(4)	2021(4)	83(2)
C(11)	7925(2)	7970(2)	2118(2)	29(1)
C(12)	6904(2)	8738(2)	2019(2)	27(1)
C(13)	6349(2)	9048(2)	2879(2)	29(1)
C(14)	7053(2)	8519(2)	3519(2)	32(1)
C(15)	7998(2)	7823(2)	3037(2)	32(1)
C(16)	8901(2)	7554(3)	1454(2)	37(1)
C(17)	6574(3)	9301(2)	1233(2)	34(1)
C(18)	5299(3)	9918(3)	3118(2)	38(1)
C(19)	7046(3)	8917(3)	4598(2)	47(1)
C(20)	9056(3)	7240(3)	3499(2)	45(1)
C(21)	7302(2)	3130(2)	245(2)	23(1)
C(22)	7277(2)	1840(2)	-448(2)	35(1)
C(23)	8180(3)	1030(3)	-278(2)	44(1)
C(24)	9103(3)	1484(3)	580(2)	45(1)
C(25)	9147(3)	2759(3)	1266(2)	48(1)
C(26)	8266(1)	3590(1)	1105(1)	39(1)
C(27)	10057(1)	7787(1)	6303(1)	38(1)
C(28)	9710(1)	9064(1)	6725(1)	42(1)
C(29)	8520(1)	9175(1)	7043(1)	52(1)

C(30)	7677(1)	8009(1)	6939(1)	54(1)
C(31)	8024(1)	6733(1)	6516(1)	41(1)
C(32)	9214(1)	6622(1)	6198(1)	41(1)
C(33)	11422(1)	7656(1)	5951(1)	62(1)
C(27B)	8782(1)	7965(1)	6679(1)	50(2)
C(28B)	8587(1)	6554(1)	6384(1)	40(2)
C(29B)	9563(1)	5834(1)	6025(1)	73(3)
C(30B)	10734(1)	6524(1)	5960(1)	86(4)
C(31B)	10929(1)	7934(1)	6255(1)	73(3)
C(32B)	9953(1)	8655(1)	6614(1)	32(2)
C(33B)	7622(1)	8425(1)	6992(1)	70(3)

Table 3. Bond lengths [Å] and angles [°] for **9**.

La(1)-Cnt1	2.525	C(14)-C(15)	1.417(3)
La(1)-Cnt2	2.560	C(14)-C(19)	1.506(3)
La(1)-C(5)	2.776(2)	C(15)-C(20)	1.511(3)
La(1)-C(2)	2.785(2)	C(21)-C(22)	1.386(3)
La(1)-C(1)	2.789(2)	C(21)-C(26)	1.393(2)
La(1)-C(13)	2.803(2)	C(22)-C(23)	1.393(3)
La(1)-C(4)	2.803(2)	C(23)-C(24)	1.370(4)
La(1)-C(3)	2.818(2)	C(24)-C(25)	1.368(4)
La(1)-C(12)	2.819(2)	C(25)-C(26)	1.390(3)
La(1)-C(11)	2.836(2)	C(27)-C(28)	1.3899
La(1)-C(15)	2.841(2)	C(27)-C(32)	1.3900
La(1)-C(14)	2.858(2)	C(27)-C(33)	1.5860
La(1)-S(1)#1	3.0076(6)	C(28)-C(29)	1.3900
La(1)-S(1)	3.0102(6)	C(29)-C(30)	1.3900
S(1)-C(21)	1.766(2)	C(30)-C(31)	1.3900
S(1)-La(1)#1	3.0075(6)	C(31)-C(32)	1.3900
C(1)-C(5)	1.398(4)	C(27B)-C(28B)	1.3899
C(1)-C(2)	1.405(3)	C(27B)-C(32B)	1.3900
C(1)-C(6)	1.501(4)	C(27B)-C(33B)	1.4271
C(2)-C(3)	1.416(4)	C(28B)-C(29B)	1.3900
C(2)-C(7)	1.500(4)	C(29B)-C(30B)	1.3900
C(3)-C(4)	1.412(4)	C(30B)-C(31B)	1.3900
C(3)-C(8)	1.505(4)	C(31B)-C(32B)	1.3900
C(4)-C(5)	1.399(4)		
C(4)-C(9)	1.513(4)	Cnt1-La(1)-S(1)	108.6
C(5)-C(10)	1.518(4)	Cnt2-La(1)-S(1)	115.2
C(11)-C(15)	1.421(3)	Cnt1-La(1)-S(1)#1	105.4
C(11)-C(12)	1.425(3)	Cnt2-La(1)-S(1)#1	116.8
C(11)-C(16)	1.509(3)	Cnt1-La(1)-Cnt2	129.1
C(12)-C(13)	1.424(3)	C(5)-La(1)-C(2)	48.23(7)
C(12)-C(17)	1.504(3)	C(5)-La(1)-C(1)	29.09(8)
C(13)-C(14)	1.420(3)	C(2)-La(1)-C(1)	29.21(7)
C(13)-C(18)	1.506(3)	C(5)-La(1)-C(13)	136.13(8)

C(2)-La(1)-C(13)	108.18(7)	C(4)-La(1)-C(14)	85.28(8)
C(1)-La(1)-C(13)	137.09(7)	C(3)-La(1)-C(14)	81.87(7)
C(5)-La(1)-C(4)	29.04(9)	C(12)-La(1)-C(14)	47.91(6)
C(2)-La(1)-C(4)	48.24(8)	C(11)-La(1)-C(14)	47.69(7)
C(1)-La(1)-C(4)	47.90(8)	C(15)-La(1)-C(14)	28.79(7)
C(13)-La(1)-C(4)	107.19(8)	C(5)-La(1)-S(1)#1	107.85(6)
C(5)-La(1)-C(3)	47.93(7)	C(2)-La(1)-S(1)#1	86.68(5)
C(2)-La(1)-C(3)	29.27(8)	C(1)-La(1)-S(1)#1	82.75(5)
C(1)-La(1)-C(3)	47.90(7)	C(13)-La(1)-S(1)#1	106.21(5)
C(13)-La(1)-C(3)	92.50(7)	C(4)-La(1)-S(1)#1	130.27(6)
C(4)-La(1)-C(3)	29.10(9)	C(3)-La(1)-S(1)#1	115.09(6)
C(5)-La(1)-C(12)	160.72(8)	C(12)-La(1)-S(1)#1	91.28(5)
C(2)-La(1)-C(12)	133.61(7)	C(11)-La(1)-S(1)#1	107.39(5)
C(1)-La(1)-C(12)	161.74(7)	C(15)-La(1)-S(1)#1	136.06(5)
C(13)-La(1)-C(12)	29.35(6)	C(14)-La(1)-S(1)#1	135.08(5)
C(4)-La(1)-C(12)	133.11(8)	C(5)-La(1)-S(1)	87.02(6)
C(3)-La(1)-C(12)	121.84(7)	C(2)-La(1)-S(1)	115.42(5)
C(5)-La(1)-C(11)	138.46(8)	C(1)-La(1)-S(1)	88.29(5)
C(2)-La(1)-C(11)	154.56(7)	C(13)-La(1)-S(1)	133.61(5)
C(1)-La(1)-C(11)	167.52(7)	C(4)-La(1)-S(1)	113.16(7)
C(13)-La(1)-C(11)	48.13(6)	C(3)-La(1)-S(1)	133.70(5)
C(4)-La(1)-C(11)	122.33(7)	C(12)-La(1)-S(1)	104.36(5)
C(3)-La(1)-C(11)	129.07(7)	C(11)-La(1)-S(1)	89.99(5)
C(12)-La(1)-C(11)	29.20(6)	C(15)-La(1)-S(1)	106.55(5)
C(5)-La(1)-C(15)	114.22(8)	C(14)-La(1)-S(1)	134.89(5)
C(2)-La(1)-C(15)	131.30(7)	S(1)#1-La(1)-S(1)	62.841(17)
C(1)-La(1)-C(15)	141.13(7)	C(21)-S(1)-La(1)#1	125.30(7)
C(13)-La(1)-C(15)	47.91(7)	C(21)-S(1)-La(1)	116.96(7)
C(4)-La(1)-C(15)	93.58(8)	La(1)#1-S(1)-La(1)	117.159(17)
C(3)-La(1)-C(15)	102.44(8)	C(5)-C(1)-C(2)	108.3(2)
C(12)-La(1)-C(15)	47.97(7)	C(5)-C(1)-C(6)	126.9(3)
C(11)-La(1)-C(15)	29.00(7)	C(2)-C(1)-C(6)	124.7(3)
C(5)-La(1)-C(14)	113.26(8)	C(5)-C(1)-La(1)	74.96(14)
C(2)-La(1)-C(14)	107.50(7)	C(2)-C(1)-La(1)	75.24(13)
C(1)-La(1)-C(14)	129.15(7)	C(6)-C(1)-La(1)	119.12(16)
C(13)-La(1)-C(14)	29.03(7)	C(1)-C(2)-C(3)	107.6(2)

C(1)-C(2)-C(7)	127.6(3)	C(14)-C(13)-C(18)	125.5(2)
C(3)-C(2)-C(7)	124.7(3)	C(12)-C(13)-C(18)	125.9(2)
C(1)-C(2)-La(1)	75.55(13)	C(14)-C(13)-La(1)	77.66(13)
C(3)-C(2)-La(1)	76.67(14)	C(12)-C(13)-La(1)	75.95(12)
C(7)-C(2)-La(1)	118.11(17)	C(18)-C(13)-La(1)	117.93(15)
C(4)-C(3)-C(2)	107.7(2)	C(15)-C(14)-C(13)	107.8(2)
C(4)-C(3)-C(8)	126.5(3)	C(15)-C(14)-C(19)	124.7(2)
C(2)-C(3)-C(8)	124.7(3)	C(13)-C(14)-C(19)	125.8(2)
C(4)-C(3)-La(1)	74.86(14)	C(15)-C(14)-La(1)	74.94(13)
C(2)-C(3)-La(1)	74.06(13)	C(13)-C(14)-La(1)	73.31(12)
C(8)-C(3)-La(1)	126.33(19)	C(19)-C(14)-La(1)	129.10(17)
C(5)-C(4)-C(3)	107.9(2)	C(14)-C(15)-C(11)	108.4(2)
C(5)-C(4)-C(9)	123.4(3)	C(14)-C(15)-C(20)	125.2(2)
C(3)-C(4)-C(9)	128.3(3)	C(11)-C(15)-C(20)	125.6(2)
C(5)-C(4)-La(1)	74.42(14)	C(14)-C(15)-La(1)	76.27(13)
C(3)-C(4)-La(1)	76.04(14)	C(11)-C(15)-La(1)	75.29(12)
C(9)-C(4)-La(1)	121.4(2)	C(20)-C(15)-La(1)	122.71(17)
C(1)-C(5)-C(4)	108.5(2)	C(22)-C(21)-C(26)	117.91(18)
C(1)-C(5)-C(10)	123.5(3)	C(22)-C(21)-S(1)	121.69(16)
C(4)-C(5)-C(10)	127.8(3)	C(26)-C(21)-S(1)	120.40(14)
C(1)-C(5)-La(1)	75.95(13)	C(21)-C(22)-C(23)	120.7(2)
C(4)-C(5)-La(1)	76.54(14)	C(24)-C(23)-C(22)	120.8(3)
C(10)-C(5)-La(1)	117.83(17)	C(25)-C(24)-C(23)	119.2(2)
C(15)-C(11)-C(12)	107.8(2)	C(24)-C(25)-C(26)	120.9(2)
C(15)-C(11)-C(16)	124.5(2)	C(25)-C(26)-C(21)	120.58(18)
C(12)-C(11)-C(16)	127.1(2)	C(28)-C(27)-C(32)	120.0
C(15)-C(11)-La(1)	75.71(13)	C(28)-C(27)-C(33)	120.2
C(12)-C(11)-La(1)	74.73(12)	C(32)-C(27)-C(33)	119.8
C(16)-C(11)-La(1)	122.31(15)	C(27)-C(28)-C(29)	120.0
C(13)-C(12)-C(11)	107.62(19)	C(30)-C(29)-C(28)	120.0
C(13)-C(12)-C(17)	124.7(2)	C(29)-C(30)-C(31)	120.0
C(11)-C(12)-C(17)	127.2(2)	C(32)-C(31)-C(30)	120.0
C(13)-C(12)-La(1)	74.70(12)	C(31)-C(32)-C(27)	120.0
C(11)-C(12)-La(1)	76.07(12)	C(28B)-C(27B)-C(32B)	120.0
C(17)-C(12)-La(1)	121.50(15)	C(28B)-C(27B)-C(33B)	107.9
C(14)-C(13)-C(12)	108.3(2)	C(32B)-C(27B)-C(33B)	132.1

C(27B)-C(28B)-C(29B)	120.0	C(30B)-C(31B)-C(32B)	120.0
C(28B)-C(29B)-C(30B)	120.0	C(31B)-C(32B)-C(27B)	120.0
C(31B)-C(30B)-C(29B)	120.0		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **9**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
La(1)	25(1)	20(1)	18(1)	7(1)	5(1)	6(1)
S(1)	32(1)	30(1)	22(1)	8(1)	5(1)	17(1)
C(1)	41(1)	28(1)	28(1)	9(1)	14(1)	0(1)
C(2)	34(1)	37(1)	43(1)	22(1)	19(1)	13(1)
C(3)	60(2)	31(1)	30(1)	5(1)	24(1)	-1(1)
C(4)	43(1)	61(2)	37(1)	34(1)	4(1)	0(1)
C(5)	48(1)	36(1)	54(2)	30(1)	28(1)	19(1)
C(6)	81(2)	60(2)	35(1)	3(1)	16(2)	-33(2)
C(7)	44(2)	95(3)	119(3)	78(3)	41(2)	36(2)
C(8)	126(4)	46(2)	62(2)	-8(2)	66(2)	-12(2)
C(9)	72(2)	140(4)	81(3)	89(3)	-20(2)	-20(3)
C(10)	103(3)	69(2)	143(4)	81(3)	91(3)	60(2)
C(11)	26(1)	28(1)	28(1)	6(1)	3(1)	0(1)
C(12)	31(1)	23(1)	25(1)	6(1)	5(1)	1(1)
C(13)	34(1)	22(1)	27(1)	4(1)	8(1)	3(1)
C(14)	37(1)	30(1)	23(1)	5(1)	3(1)	0(1)
C(15)	31(1)	33(1)	28(1)	9(1)	-1(1)	2(1)
C(16)	29(1)	43(1)	37(1)	10(1)	8(1)	5(1)
C(17)	42(1)	31(1)	34(1)	15(1)	13(1)	8(1)
C(18)	45(1)	33(1)	36(1)	7(1)	15(1)	11(1)
C(19)	60(2)	46(2)	24(1)	6(1)	5(1)	-4(1)
C(20)	41(1)	52(2)	37(1)	16(1)	-4(1)	10(1)
C(21)	22(1)	27(1)	23(1)	12(1)	7(1)	9(1)
C(22)	32(1)	32(1)	36(1)	7(1)	3(1)	13(1)
C(23)	42(1)	34(1)	59(2)	15(1)	12(1)	19(1)
C(24)	35(1)	57(2)	63(2)	39(2)	15(1)	26(1)
C(25)	37(1)	69(2)	41(1)	27(1)	-3(1)	19(1)
C(26)	39(1)	42(1)	29(1)	8(1)	-2(1)	14(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **9**.

	x	y	z	U(eq)
H(6A)	2590	2343	894	98
H(6B)	3231	3233	354	98
H(6C)	1902	3551	746	98
H(7A)	1293	5769	2425	106
H(7B)	1764	5787	1451	106
H(7C)	2242	7078	2466	106
H(8A)	3211	6919	4462	124
H(8B)	3816	7982	4037	124
H(8C)	4769	7455	4725	124
H(9A)	6009	4378	4242	137
H(9B)	6161	6005	4697	137
H(9C)	7004	5283	3900	137
H(10A)	4753	2003	2031	124
H(10B)	6186	2931	2453	124
H(10C)	5452	2605	1347	124
H(16A)	9782	7696	1856	56
H(16B)	8917	8107	1051	56
H(16C)	8636	6589	1025	56
H(17A)	6418	10238	1535	51
H(17B)	5778	8737	760	51
H(17C)	7312	9293	892	51
H(18A)	5702	10812	3626	57
H(18B)	4634	9474	3360	57
H(18C)	4878	10036	2524	57
H(19A)	7781	9661	4984	71
H(19B)	7142	8131	4782	71
H(19C)	6210	9220	4731	71
H(20A)	9885	7892	3736	67
H(20B)	9185	6384	3008	67
H(20C)	8783	7064	4053	67

H(22A)	6637	1506	-1044	42
H(23A)	8155	152	-764	53
H(24A)	9706	920	697	54
H(25A)	9789	3082	1861	58
H(26A)	8321	4479	1584	46
H(28A)	10286	9860	6796	51
H(29A)	8282	10047	7331	62
H(30A)	6863	8085	7156	65
H(31A)	7448	5936	6445	49
H(32A)	9451	5750	5910	49
H(33A)	11894	8565	6076	92
H(33B)	11257	7100	5245	92
H(33C)	11958	7220	6315	92
H(28B)	7787	6083	6428	48
H(29B)	9430	4870	5823	88
H(30B)	11401	6031	5715	103
H(31B)	11729	8406	6211	87
H(32B)	10086	9619	6816	38
H(33D)	6986	7644	6938	105
H(33E)	7228	8877	6575	105
H(33F)	7856	9070	7678	105

Table 6. Crystal data and structure refinement for **[$(C_5Me_5)_2Y(\mu$-SPh)]$_2$**, **13**.

Empirical formula	$C_{52}H_{70}S_2Y_2 \bullet 2(C_7H_8)$	
Formula weight	1121.29	
Temperature	163(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 10.3399(11) Å	α= 69.574(2)°.
	b = 10.4821(11) Å	β= 76.507(2)°.
	c = 14.6925(16) Å	γ = 83.370(2)°.
Volume	1450.1(3) Å^3	
Z	1	
Density (calculated)	1.284 Mg/m^3	
Absorption coefficient	2.102 mm^{-1}	
F(000)	592	
Crystal color	pale yellow	
Crystal size	0.32 x 0.26 x 0.23 mm^3	
Theta range for data collection	2.03 to 28.31°	
Index ranges	$-13 \le h \le 13$, $-13 \le k \le 13$, $-19 \le l \le 19$	
Reflections collected	16112	
Independent reflections	7023 [R(int) = 0.0248]	
Completeness to theta = 28.31°	97.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6435 and 0.5528	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7023 / 0 / 327	
Goodness-of-fit on F^2	1.057	
Final R indices [I>2sigma(I) = 6248 data]	R1 = 0.0390, wR2 = 0.0949	
R indices (all data; 0.75Å)	R1 = 0.0459, wR2 = 0.0982	
Largest diff. peak and hole	1.021 and -0.707 e.Å^{-3}	

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **13**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Y(1)	5508(1)	652(1)	3158(1)	16(1)
S(1)	3948(1)	-899(1)	5068(1)	21(1)
C(1)	3258(3)	1811(3)	2654(2)	32(1)
C(2)	4201(3)	2189(3)	1743(2)	39(1)
C(3)	5099(3)	3059(3)	1799(2)	40(1)
C(4)	4700(3)	3232(3)	2728(2)	35(1)
C(5)	3566(3)	2497(3)	3239(2)	29(1)
C(6)	2075(4)	978(4)	2853(4)	74(2)
C(7)	4047(5)	1990(5)	805(3)	79(2)
C(8)	6167(5)	3897(4)	994(4)	81(2)
C(9)	5234(5)	4190(3)	3119(4)	71(1)
C(10)	2684(4)	2517(5)	4201(2)	64(1)
C(11)	6829(2)	-1654(2)	3044(2)	22(1)
C(12)	6267(3)	-1102(3)	2180(2)	25(1)
C(13)	6967(3)	72(3)	1540(2)	29(1)
C(14)	7895(3)	311(3)	2025(2)	28(1)
C(15)	7835(2)	-773(3)	2949(2)	23(1)
C(16)	6552(3)	-3051(3)	3801(2)	29(1)
C(17)	5262(3)	-1777(3)	1917(2)	34(1)
C(18)	7024(4)	700(4)	437(2)	47(1)
C(19)	8983(3)	1324(3)	1546(2)	40(1)
C(20)	8869(3)	-1024(3)	3572(2)	32(1)
C(21)	2761(2)	-2087(2)	5234(2)	19(1)
C(22)	2731(3)	-2631(3)	4504(2)	30(1)
C(23)	1809(3)	-3602(3)	4665(2)	36(1)
C(24)	914(3)	-4037(3)	5554(2)	34(1)
C(25)	926(3)	-3498(3)	6280(2)	40(1)
C(26)	1834(3)	-2529(3)	6121(2)	33(1)
C(27)	10110(3)	3519(3)	-1268(2)	44(1)
C(28)	9769(3)	2682(3)	-1688(2)	43(1)
C(29)	8579(4)	2864(5)	-2022(3)	61(1)

C(30)	7723(4)	3921(5)	-1937(3)	61(1)
C(31)	8060(4)	4804(4)	-1508(3)	57(1)
C(32)	9217(4)	4611(4)	-1177(3)	51(1)
C(33)	11388(4)	3301(5)	-928(4)	67(1)

Table 8. Bond lengths [Å] and angles [°] for **13**.

Y(1)-Cnt1	2.370	C(14)-C(15)	1.428(4)
Y(1)-Cnt2	2.402	C(14)-C(19)	1.508(4)
Y(1)-C(5)	2.635(2)	C(15)-C(20)	1.508(4)
Y(1)-C(4)	2.635(3)	C(21)-C(22)	1.387(3)
Y(1)-C(1)	2.638(3)	C(21)-C(26)	1.389(3)
Y(1)-C(12)	2.654(2)	C(22)-C(23)	1.397(4)
Y(1)-C(11)	2.673(2)	C(23)-C(24)	1.374(4)
Y(1)-C(3)	2.676(3)	C(24)-C(25)	1.373(4)
Y(1)-C(2)	2.685(3)	C(25)-C(26)	1.386(4)
Y(1)-C(15)	2.694(2)	C(27)-C(28)	1.352(5)
Y(1)-C(14)	2.699(2)	C(27)-C(32)	1.409(5)
Y(1)-C(13)	2.724(2)	C(27)-C(33)	1.486(5)
Y(1)-S(1)#1	2.8931(6)	C(28)-C(29)	1.397(5)
Y(1)-S(1)	2.9031(6)	C(29)-C(30)	1.359(6)
S(1)-C(21)	1.766(2)	C(30)-C(31)	1.399(6)
S(1)-Y(1)#1	2.8931(7)	C(31)-C(32)	1.362(6)
C(1)-C(5)	1.404(4)		
C(1)-C(2)	1.417(5)	Cnt1-Y(1)-S(1)	107.4
C(1)-C(6)	1.498(4)	Cnt2-Y(1)-S(1)	116.0
C(2)-C(3)	1.409(5)	Cnt1-Y(1)-S(1)#1	108.9
C(2)-C(7)	1.511(4)	Cnt2-Y(1)-S(1)#1	115.3
C(3)-C(4)	1.399(5)	Cnt1-Y(1)-Cnt2	128.5
C(3)-C(8)	1.510(4)	C(5)-Y(1)-C(4)	30.55(9)
C(4)-C(5)	1.388(4)	C(5)-Y(1)-C(1)	30.90(9)
C(4)-C(9)	1.523(4)	C(4)-Y(1)-C(1)	51.03(8)
C(5)-C(10)	1.498(4)	C(5)-Y(1)-C(12)	136.30(8)
C(11)-C(15)	1.420(3)	C(4)-Y(1)-C(12)	136.65(9)
C(11)-C(12)	1.428(3)	C(1)-Y(1)-C(12)	105.59(9)
C(11)-C(16)	1.508(3)	C(5)-Y(1)-C(11)	161.26(8)
C(12)-C(13)	1.416(4)	C(4)-Y(1)-C(11)	162.16(9)
C(12)-C(17)	1.509(4)	C(1)-Y(1)-C(11)	132.24(8)
C(13)-C(14)	1.411(4)	C(12)-Y(1)-C(11)	31.09(7)
C(13)-C(18)	1.511(4)	C(5)-Y(1)-C(3)	50.42(9)

C(4)-Y(1)-C(3)	30.54(10)	C(1)-Y(1)-S(1)#1	116.37(7)
C(1)-Y(1)-C(3)	50.95(9)	C(12)-Y(1)-S(1)#1	134.57(6)
C(12)-Y(1)-C(3)	106.30(9)	C(11)-Y(1)-S(1)#1	103.55(5)
C(11)-Y(1)-C(3)	133.33(9)	C(3)-Y(1)-S(1)#1	113.13(8)
C(5)-Y(1)-C(2)	50.44(8)	C(2)-Y(1)-S(1)#1	135.21(6)
C(4)-Y(1)-C(2)	50.43(9)	C(15)-Y(1)-S(1)#1	88.68(5)
C(1)-Y(1)-C(2)	30.85(10)	C(14)-Y(1)-S(1)#1	106.26(6)
C(12)-Y(1)-C(2)	90.06(8)	C(13)-Y(1)-S(1)#1	135.93(6)
C(11)-Y(1)-C(2)	121.14(8)	C(5)-Y(1)-S(1)	83.14(6)
C(3)-Y(1)-C(2)	30.47(10)	C(4)-Y(1)-S(1)	108.84(8)
C(5)-Y(1)-C(15)	167.57(8)	C(1)-Y(1)-S(1)	87.94(7)
C(4)-Y(1)-C(15)	137.25(9)	C(12)-Y(1)-S(1)	105.39(6)
C(1)-Y(1)-C(15)	154.95(9)	C(11)-Y(1)-S(1)	89.00(5)
C(12)-Y(1)-C(15)	50.88(8)	C(3)-Y(1)-S(1)	133.36(7)
C(11)-Y(1)-C(15)	30.69(7)	C(2)-Y(1)-S(1)	118.03(8)
C(3)-Y(1)-C(15)	121.05(8)	C(15)-Y(1)-S(1)	105.47(6)
C(2)-Y(1)-C(15)	128.45(8)	C(14)-Y(1)-S(1)	135.95(6)
C(5)-Y(1)-C(14)	140.69(8)	C(13)-Y(1)-S(1)	135.62(6)
C(4)-Y(1)-C(14)	112.33(9)	S(1)#1-Y(1)-S(1)	61.59(2)
C(1)-Y(1)-C(14)	130.63(9)	C(21)-S(1)-Y(1)#1	117.02(8)
C(12)-Y(1)-C(14)	50.62(8)	C(21)-S(1)-Y(1)	124.41(8)
C(11)-Y(1)-C(14)	50.75(8)	Y(1)#1-S(1)-Y(1)	118.41(2)
C(3)-Y(1)-C(14)	90.69(9)	C(5)-C(1)-C(2)	107.0(2)
C(2)-Y(1)-C(14)	100.21(9)	C(5)-C(1)-C(6)	128.6(4)
C(15)-Y(1)-C(14)	30.71(8)	C(2)-C(1)-C(6)	124.0(3)
C(5)-Y(1)-C(13)	128.69(8)	C(5)-C(1)-Y(1)	74.42(14)
C(4)-Y(1)-C(13)	112.46(9)	C(2)-C(1)-Y(1)	76.43(16)
C(1)-Y(1)-C(13)	105.61(9)	C(6)-C(1)-Y(1)	121.0(2)
C(12)-Y(1)-C(13)	30.49(8)	C(3)-C(2)-C(1)	108.0(2)
C(11)-Y(1)-C(13)	50.49(8)	C(3)-C(2)-C(7)	125.6(4)
C(3)-Y(1)-C(13)	82.86(9)	C(1)-C(2)-C(7)	124.7(4)
C(2)-Y(1)-C(13)	78.81(8)	C(3)-C(2)-Y(1)	74.39(15)
C(15)-Y(1)-C(13)	50.19(8)	C(1)-C(2)-Y(1)	72.72(14)
C(14)-Y(1)-C(13)	30.15(8)	C(7)-C(2)-Y(1)	130.5(2)
C(5)-Y(1)-S(1)#1	87.64(6)	C(4)-C(3)-C(2)	107.7(3)
C(4)-Y(1)-S(1)#1	85.87(7)	C(4)-C(3)-C(8)	122.0(4)

C(2)-C(3)-C(8)	129.5(4)	C(12)-C(13)-Y(1)	72.02(14)
C(4)-C(3)-Y(1)	73.12(15)	C(18)-C(13)-Y(1)	133.76(19)
C(2)-C(3)-Y(1)	75.15(15)	C(13)-C(14)-C(15)	108.1(2)
C(8)-C(3)-Y(1)	125.4(2)	C(13)-C(14)-C(19)	125.2(3)
C(5)-C(4)-C(3)	108.5(3)	C(15)-C(14)-C(19)	125.1(3)
C(5)-C(4)-C(9)	122.2(3)	C(13)-C(14)-Y(1)	75.91(15)
C(3)-C(4)-C(9)	128.9(3)	C(15)-C(14)-Y(1)	74.45(14)
C(5)-C(4)-Y(1)	74.70(15)	C(19)-C(14)-Y(1)	127.06(19)
C(3)-C(4)-Y(1)	76.33(16)	C(11)-C(15)-C(14)	107.9(2)
C(9)-C(4)-Y(1)	121.48(19)	C(11)-C(15)-C(20)	128.0(2)
C(4)-C(5)-C(1)	108.8(3)	C(14)-C(15)-C(20)	123.1(2)
C(4)-C(5)-C(10)	127.7(3)	C(11)-C(15)-Y(1)	73.85(13)
C(1)-C(5)-C(10)	123.1(3)	C(14)-C(15)-Y(1)	74.85(14)
C(4)-C(5)-Y(1)	74.75(15)	C(20)-C(15)-Y(1)	126.52(17)
C(1)-C(5)-Y(1)	74.68(15)	C(22)-C(21)-C(26)	117.6(2)
C(10)-C(5)-Y(1)	122.13(18)	C(22)-C(21)-S(1)	121.95(19)
C(15)-C(11)-C(12)	107.6(2)	C(26)-C(21)-S(1)	120.39(19)
C(15)-C(11)-C(16)	127.5(2)	C(21)-C(22)-C(23)	120.9(2)
C(12)-C(11)-C(16)	124.0(2)	C(24)-C(23)-C(22)	120.4(3)
C(15)-C(11)-Y(1)	75.46(14)	C(25)-C(24)-C(23)	119.3(2)
C(12)-C(11)-Y(1)	73.73(14)	C(24)-C(25)-C(26)	120.4(3)
C(16)-C(11)-Y(1)	125.24(17)	C(25)-C(26)-C(21)	121.3(3)
C(13)-C(12)-C(11)	108.1(2)	C(28)-C(27)-C(32)	117.5(3)
C(13)-C(12)-C(17)	125.4(2)	C(28)-C(27)-C(33)	121.0(3)
C(11)-C(12)-C(17)	125.8(2)	C(32)-C(27)-C(33)	121.5(4)
C(13)-C(12)-Y(1)	77.49(14)	C(27)-C(28)-C(29)	122.4(3)
C(11)-C(12)-Y(1)	75.19(14)	C(30)-C(29)-C(28)	120.0(4)
C(17)-C(12)-Y(1)	121.24(17)	C(29)-C(30)-C(31)	118.5(4)
C(14)-C(13)-C(12)	108.2(2)	C(32)-C(31)-C(30)	121.1(3)
C(14)-C(13)-C(18)	124.0(3)	C(31)-C(32)-C(27)	120.5(4)
C(12)-C(13)-C(18)	125.5(3)		
C(14)-C(13)-Y(1)	73.94(14)		

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+1

Table 9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **13**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Y(1)	18(1)	16(1)	15(1)	-5(1)	-4(1)	-1(1)
S(1)	23(1)	23(1)	18(1)	-6(1)	-5(1)	-9(1)
C(1)	27(1)	21(1)	49(2)	-4(1)	-23(1)	1(1)
C(2)	61(2)	37(2)	26(1)	-15(1)	-27(1)	25(1)
C(3)	33(2)	28(1)	36(2)	10(1)	0(1)	5(1)
C(4)	40(2)	17(1)	52(2)	-6(1)	-27(1)	2(1)
C(5)	33(1)	28(1)	24(1)	-8(1)	-11(1)	13(1)
C(6)	42(2)	41(2)	135(4)	0(2)	-50(2)	-9(2)
C(7)	122(4)	84(3)	62(3)	-52(2)	-66(3)	60(3)
C(8)	67(3)	45(2)	73(3)	24(2)	23(2)	7(2)
C(9)	87(3)	26(2)	123(4)	-22(2)	-77(3)	9(2)
C(10)	71(3)	76(3)	31(2)	-16(2)	-11(2)	46(2)
C(11)	23(1)	23(1)	22(1)	-11(1)	-5(1)	2(1)
C(12)	27(1)	28(1)	24(1)	-15(1)	-8(1)	6(1)
C(13)	33(1)	32(1)	19(1)	-10(1)	-2(1)	6(1)
C(14)	25(1)	29(1)	25(1)	-10(1)	4(1)	-1(1)
C(15)	20(1)	26(1)	25(1)	-12(1)	-3(1)	2(1)
C(16)	37(1)	23(1)	28(1)	-8(1)	-11(1)	1(1)
C(17)	38(2)	41(2)	32(1)	-20(1)	-13(1)	2(1)
C(18)	61(2)	52(2)	21(1)	-12(1)	-4(1)	16(2)
C(19)	37(2)	39(2)	37(2)	-10(1)	8(1)	-9(1)
C(20)	23(1)	40(2)	35(1)	-16(1)	-8(1)	2(1)
C(21)	17(1)	17(1)	24(1)	-5(1)	-7(1)	-2(1)
C(22)	31(1)	34(1)	27(1)	-13(1)	-2(1)	-12(1)
C(23)	39(2)	36(2)	42(2)	-19(1)	-13(1)	-12(1)
C(24)	26(1)	27(1)	49(2)	-8(1)	-11(1)	-10(1)
C(25)	32(2)	46(2)	36(2)	-9(1)	6(1)	-18(1)
C(26)	35(2)	39(2)	26(1)	-13(1)	1(1)	-14(1)
C(27)	39(2)	44(2)	34(2)	-5(1)	4(1)	1(1)
C(28)	43(2)	43(2)	35(2)	-12(1)	-1(1)	10(1)
C(29)	62(2)	73(3)	46(2)	-20(2)	-11(2)	1(2)

C(30)	53(2)	75(3)	40(2)	-4(2)	-13(2)	15(2)
C(31)	58(2)	48(2)	36(2)	5(2)	7(2)	22(2)
C(32)	63(2)	40(2)	36(2)	-9(1)	10(2)	1(2)
C(33)	45(2)	78(3)	79(3)	-30(2)	-7(2)	-6(2)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **13**.

	x	y	z	U(eq)
H(6A)	2340	227	2588	112
H(6B)	1383	1554	2531	112
H(6C)	1729	609	3570	112
H(7A)	4858	2261	294	118
H(7B)	3287	2551	570	118
H(7C)	3896	1028	942	118
H(8A)	6268	3656	394	122
H(8B)	7011	3713	1219	122
H(8C)	5913	4867	848	122
H(9A)	6103	4505	2704	106
H(9B)	5330	3706	3804	106
H(9C)	4612	4974	3100	106
H(10A)	1850	2081	4301	96
H(10B)	2492	3462	4184	96
H(10C)	3135	2022	4749	96
H(16A)	6358	-3660	3476	43
H(16B)	5784	-2990	4322	43
H(16C)	7333	-3413	4095	43
H(17A)	4987	-2620	2463	51
H(17B)	5664	-1991	1311	51
H(17C)	4484	-1160	1807	51
H(18A)	6227	472	280	70
H(18B)	7818	342	76	70
H(18C)	7063	1692	239	70
H(19A)	9165	1666	2043	60
H(19B)	8698	2086	1009	60
H(19C)	9791	879	1275	60
H(20A)	8917	-1995	3961	47
H(20B)	8626	-490	4021	47
H(20C)	9738	-750	3137	47

H(22A)	3345	-2341	3887	35
H(23A)	1800	-3964	4157	43
H(24A)	293	-4704	5665	41
H(25A)	308	-3791	6895	48
H(26A)	1824	-2161	6629	39
H(28A)	10360	1943	-1760	52
H(29A)	8369	2249	-2308	73
H(30A)	6912	4058	-2164	73
H(31A)	7472	5550	-1447	69
H(32A)	9423	5217	-883	61
H(33A)	11450	3982	-624	100
H(33B)	12131	3389	-1496	100
H(33C)	11426	2387	-438	100

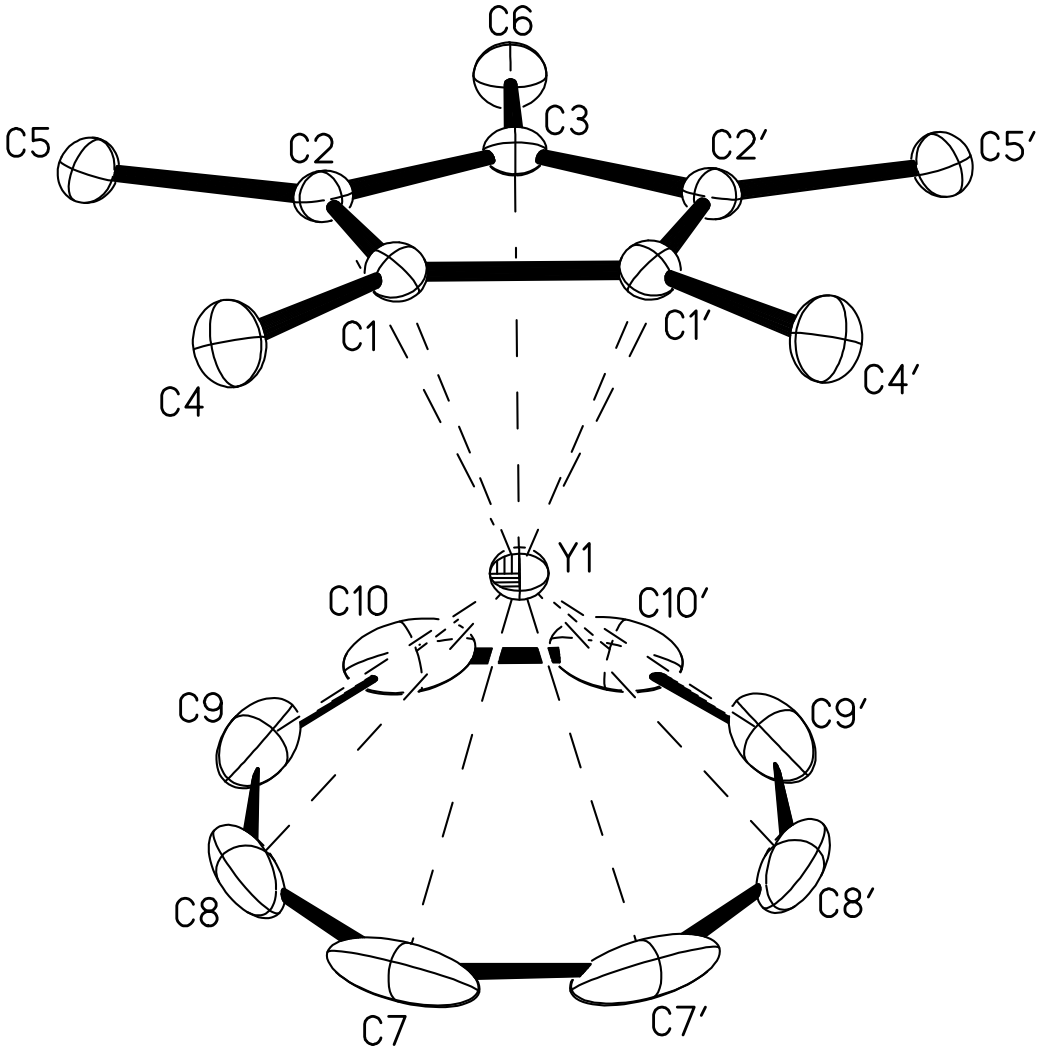

Figure 1. Molecular structure of **$(C_5Me_5)Y(C_8H_8)$, 14**, with thermal ellipsoids drawn at the 50% level. Hydrogen atoms have been omitted for clarity.

Table 11. Crystal data and structure refinement for **$(C_5Me_5)Y(C_8H_8)$, 14**.

Empirical formula	$C_{18}H_{23}Y$	
Formula weight	328.27	
Temperature	163(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	*Pnma*	
Unit cell dimensions	a = 10.3396(13) Å	α= 90°.
	b = 12.9085(16) Å	β= 90°.
	c = 11.7145(14) Å	γ = 90°.
Volume	1563.5(3) Å^3	
Z	4	
Density (calculated)	1.395 Mg/m^3	
Absorption coefficient	3.715 mm^{-1}	
F(000)	680	
Crystal color	yellow	
Crystal size	0.30 x 0.29 x 0.22 mm^3	
Theta range for data collection	2.35 to 28.31°.	
Index ranges	$-13 \le h \le 8$, $-16 \le k \le 16$, $-15 \le l \le 15$	
Reflections collected	9918	
Independent reflections	2000 [R(int) = 0.0251]	
Completeness to theta = 28.31°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.4954 and 0.4020	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2000 / 0 / 138	
Goodness-of-fit on F^2	1.085	
Final R indices [I>2sigma(I) = 1705 data]	R1 = 0.0298, wR2 = 0.0694	
R indices (all data; 0.75Å)	R1 = 0.0378, wR2 = 0.0730	
Largest diff. peak and hole	0.781 and -0.430 e.Å^{-3}	

Table 12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **14**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Y(1)	1333(1)	7500	90(1)	20(1)
C(1)	2286(2)	6949(2)	-1869(2)	20(1)
C(2)	3185(2)	6607(2)	-1033(2)	20(1)
C(3)	3745(3)	7500	-517(2)	21(1)
C(4)	1497(3)	6273(2)	-2649(2)	29(1)
C(5)	3515(2)	5501(2)	-747(2)	28(1)
C(6)	4770(3)	7500	397(3)	32(1)
C(7)	-972(3)	6944(4)	384(3)	78(2)
C(8)	-201(5)	6195(3)	922(4)	68(1)
C(9)	843(5)	6212(3)	1631(3)	67(1)
C(10)	1589(4)	6964(4)	2129(3)	73(1)

Table 13. Bond lengths [Å] and angles [°] for **14**.

Y(1)-Cnt1	2.295	C(10)-Y(1)-C(8)	60.72(16)
Y(1)-Cnt2	1.734	C(9)#1-Y(1)-C(8)	92.19(10)
Y(1)-C(10)	2.500(3)	C(9)-Y(1)-C(8)	31.51(15)
Y(1)-C(9)	2.506(3)	C(8)#1-Y(1)-C(8)	84.31(18)
Y(1)-C(8)	2.511(3)	C(10)#1-Y(1)-C(7)	92.81(11)
Y(1)-C(7)	2.513(3)	C(10)-Y(1)-C(7)	83.74(14)
Y(1)-C(2)	2.593(2)	C(9)#1-Y(1)-C(7)	84.23(13)
Y(1)-C(3)	2.594(3)	C(9)-Y(1)-C(7)	61.31(17)
Y(1)-C(1)	2.5967(18)	C(8)#1-Y(1)-C(7)	62.59(18)
C(1)-C(2)	1.421(3)	C(8)-Y(1)-C(7)	32.42(15)
C(1)-C(1)#1	1.422(4)	C(10)#1-Y(1)-C(7)#1	83.74(14)
C(1)-C(4)	1.504(3)	C(10)-Y(1)-C(7)#1	92.81(11)
C(2)-C(3)	1.425(3)	C(9)#1-Y(1)-C(7)#1	61.31(17)
C(2)-C(5)	1.505(3)	C(9)-Y(1)-C(7)#1	84.23(13)
C(3)-C(2)#1	1.425(3)	C(8)#1-Y(1)-C(7)#1	32.42(15)
C(3)-C(6)	1.506(4)	C(8)-Y(1)-C(7)#1	62.59(18)
C(7)-C(8)	1.403(6)	C(7)-Y(1)-C(7)#1	33.2(3)
C(7)-C(7)#1	1.437(11)	C(10)#1-Y(1)-C(2)#1	106.45(9)
C(8)-C(9)	1.362(6)	C(10)-Y(1)-C(2)#1	121.95(11)
C(9)-C(10)	1.371(6)	C(9)#1-Y(1)-C(2)#1	102.69(9)
C(10)-C(10)#1	1.383(10)	C(9)-Y(1)-C(2)#1	144.06(12)
		C(8)#1-Y(1)-C(2)#1	111.39(10)
Cnt1-Y(1)-Cnt2	171.1	C(8)-Y(1)-C(2)#1	164.06(9)
C(10)#1-Y(1)-C(10)	32.1(2)	C(7)-Y(1)-C(2)#1	153.72(12)
C(10)#1-Y(1)-C(9)#1	31.79(15)	C(7)#1-Y(1)-C(2)#1	129.98(11)
C(10)-Y(1)-C(9)#1	61.13(18)	C(10)#1-Y(1)-C(2)	121.95(11)
C(10)#1-Y(1)-C(9)	61.13(18)	C(10)-Y(1)-C(2)	106.45(9)
C(10)-Y(1)-C(9)	31.79(15)	C(9)#1-Y(1)-C(2)	144.06(12)
C(9)#1-Y(1)-C(9)	83.15(19)	C(9)-Y(1)-C(2)	102.68(9)
C(10)#1-Y(1)-C(8)#1	60.72(16)	C(8)#1-Y(1)-C(2)	164.06(9)
C(10)-Y(1)-C(8)#1	83.23(13)	C(8)-Y(1)-C(2)	111.39(10)
C(9)#1-Y(1)-C(8)#1	31.51(15)	C(7)-Y(1)-C(2)	129.98(11)
C(9)-Y(1)-C(8)#1	92.19(10)	C(7)#1-Y(1)-C(2)	153.72(12)
C(10)#1-Y(1)-C(8)	83.23(13)	C(2)#1-Y(1)-C(2)	52.79(9)

C(10)#1-Y(1)-C(3)	99.22(10)	C(1)-Y(1)-C(1)#1	31.78(9)
C(10)-Y(1)-C(3)	99.22(10)	C(2)-C(1)-C(1)#1	108.13(11)
C(9)#1-Y(1)-C(3)	113.09(11)	C(2)-C(1)-C(4)	126.38(19)
C(9)-Y(1)-C(3)	113.09(11)	C(1)#1-C(1)-C(4)	125.47(12)
C(8)#1-Y(1)-C(3)	135.56(12)	C(2)-C(1)-Y(1)	73.99(11)
C(8)-Y(1)-C(3)	135.56(12)	C(1)#1-C(1)-Y(1)	74.11(4)
C(7)-Y(1)-C(3)	161.72(11)	C(4)-C(1)-Y(1)	119.36(14)
C(7)#1-Y(1)-C(3)	161.72(11)	C(1)-C(2)-C(3)	107.84(18)
C(2)#1-Y(1)-C(3)	31.88(5)	C(1)-C(2)-C(5)	126.63(19)
C(2)-Y(1)-C(3)	31.88(5)	C(3)-C(2)-C(5)	125.52(19)
C(10)#1-Y(1)-C(1)	151.60(10)	C(1)-C(2)-Y(1)	74.24(11)
C(10)-Y(1)-C(1)	136.73(10)	C(3)-C(2)-Y(1)	74.08(13)
C(9)#1-Y(1)-C(1)	153.50(9)	C(5)-C(2)-Y(1)	118.43(14)
C(9)-Y(1)-C(1)	122.11(10)	C(2)#1-C(3)-C(2)	108.1(2)
C(8)#1-Y(1)-C(1)	140.02(11)	C(2)#1-C(3)-C(6)	125.96(12)
C(8)-Y(1)-C(1)	113.50(9)	C(2)-C(3)-C(6)	125.96(12)
C(7)-Y(1)-C(1)	113.73(9)	C(2)#1-C(3)-Y(1)	74.04(13)
C(7)#1-Y(1)-C(1)	123.98(11)	C(2)-C(3)-Y(1)	74.04(13)
C(2)#1-Y(1)-C(1)	52.65(6)	C(6)-C(3)-Y(1)	118.8(2)
C(2)-Y(1)-C(1)	31.77(6)	C(8)-C(7)-C(7)#1	133.6(2)
C(3)-Y(1)-C(1)	52.60(7)	C(8)-C(7)-Y(1)	73.73(19)
C(10)#1-Y(1)-C(1)#1	136.73(10)	C(7)#1-C(7)-Y(1)	73.39(13)
C(10)-Y(1)-C(1)#1	151.60(10)	C(9)-C(8)-C(7)	135.5(3)
C(9)#1-Y(1)-C(1)#1	122.11(10)	C(9)-C(8)-Y(1)	74.03(19)
C(9)-Y(1)-C(1)#1	153.50(9)	C(7)-C(8)-Y(1)	73.85(19)
C(8)#1-Y(1)-C(1)#1	113.50(9)	C(8)-C(9)-C(10)	135.8(3)
C(8)-Y(1)-C(1)#1	140.02(11)	C(8)-C(9)-Y(1)	74.46(19)
C(7)-Y(1)-C(1)#1	123.98(11)	C(10)-C(9)-Y(1)	73.89(18)
C(7)#1-Y(1)-C(1)#1	113.73(9)	C(9)-C(10)-C(10)#1	135.1(2)
C(2)#1-Y(1)-C(1)#1	31.77(6)	C(9)-C(10)-Y(1)	74.32(18)
C(2)-Y(1)-C(1)#1	52.65(6)	C(10)#1-C(10)-Y(1)	73.94(12)
C(3)-Y(1)-C(1)#1	52.60(7)		

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+3/2,z

Table 14. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **14**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Y(1)	20(1)	22(1)	18(1)	0	4(1)	0
C(1)	22(1)	22(1)	16(1)	-3(1)	2(1)	-1(1)
C(2)	18(1)	22(1)	20(1)	1(1)	3(1)	1(1)
C(3)	15(1)	27(1)	22(1)	0	1(1)	0
C(4)	36(1)	27(1)	25(1)	-4(1)	-5(1)	-3(1)
C(5)	27(1)	23(1)	32(1)	3(1)	1(1)	4(1)
C(6)	25(2)	39(2)	31(2)	0	-9(1)	0
C(7)	34(2)	145(4)	56(2)	-28(2)	11(2)	-40(2)
C(8)	86(3)	42(2)	76(2)	-22(2)	54(2)	-33(2)
C(9)	88(3)	48(2)	64(2)	31(2)	48(2)	28(2)
C(10)	54(2)	136(4)	30(1)	30(2)	11(1)	29(2)

Table 15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **14**.

	x	y	z	U(eq)
H(4A)	730(30)	6550(20)	-2820(20)	43(8)
H(4B)	1360(30)	5590(30)	-2350(30)	50(9)
H(4C)	1900(30)	6220(30)	-3340(30)	60(9)
H(5A)	2870(30)	5040(20)	-980(20)	43(8)
H(5B)	3680(30)	5380(30)	40(30)	52(10)
H(5C)	4280(30)	5260(20)	-1130(20)	41(7)
H(6A)	4730(30)	6910(20)	830(30)	60(10)
H(6B)	5700(60)	7500	20(40)	73(17)
H(7)	-1540(40)	6790(40)	-70(30)	95(17)
H(8)	-430(50)	5610(40)	640(40)	110(16)
H(9)	1230(40)	5560(40)	1780(40)	100(15)
H(10)	2280(40)	6780(30)	2560(40)	107(15)

Table 16. Crystal data and structure refinement for **$(C_5Me_5)Y(\eta^5\text{-}C_5Me_4CH_2\text{-}C_5Me_4CH_2\text{-}\eta^3)$ 16**.

Empirical formula	$C_{30}H_{43}Y$	
Formula weight	492.55	
Temperature	163(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 9.2799(10) Å	α= 83.277(2)°.
	b = 11.1103(12) Å	β= 78.810(2)°.
	c = 12.6823(14) Å	γ = 83.363(2)°.
Volume	1268.1(2) $Å^3$	
Z	2	
Density (calculated)	1.290 Mg/m^3	
Absorption coefficient	2.314 mm^{-1}	
F(000)	524	
Crystal color	red	
Crystal size	0.37 x 0.33 x 0.10 mm^3	
Theta range for data collection	1.85 to 28.32°	
Index ranges	$-12 \le h \le 12$, $-14 \le k \le 14$, $-16 \le l \le 16$	
Reflections collected	14056	
Independent reflections	6114 [R(int) = 0.0223]	
Completeness to theta = 28.32°	96.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8016 and 0.4814	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6114 / 0 / 452	
Goodness-of-fit on F^2	1.058	
Final R indices [I>2sigma(I) = 5575 data]	R1 = 0.0256, wR2 = 0.0635	
R indices (all data; 0.75Å)	R1 = 0.0304, wR2 = 0.0656	
Largest diff. peak and hole	0.441 and -0.255 $e.Å^{-3}$	

Table 17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for **16**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Y(1)	2367(1)	2607(1)	2386(1)	15(1)
C(1)	3413(2)	902(1)	1079(1)	15(1)
C(2)	2946(2)	279(1)	2115(1)	17(1)
C(3)	3911(2)	494(1)	2799(1)	19(1)
C(4)	4970(2)	1255(1)	2193(1)	19(1)
C(5)	4674(2)	1501(1)	1128(1)	17(1)
C(6)	2703(2)	846(1)	116(1)	18(1)
C(7)	1727(2)	-546(2)	2426(2)	25(1)
C(8)	4022(2)	-192(2)	3876(2)	28(1)
C(9)	6331(2)	1535(2)	2560(2)	28(1)
C(10)	5667(2)	2133(2)	199(2)	22(1)
C(11)	485(2)	4210(2)	3612(1)	22(1)
C(12)	309(2)	3024(2)	4148(1)	22(1)
C(13)	1625(2)	2590(1)	4538(1)	21(1)
C(14)	2648(2)	3476(2)	4196(1)	21(1)
C(15)	1935(2)	4485(1)	3630(1)	22(1)
C(16)	-760(2)	5089(2)	3314(2)	36(1)
C(17)	-1076(2)	2393(2)	4356(2)	36(1)
C(18)	1703(2)	1549(2)	5402(2)	34(1)
C(19)	4113(2)	3465(2)	4545(2)	32(1)
C(20)	2546(3)	5691(2)	3275(2)	35(1)
C(21)	1923(2)	2054(1)	-341(1)	17(1)
C(22)	1274(2)	2900(1)	541(1)	17(1)
C(23)	1944(2)	3968(1)	274(1)	18(1)
C(24)	2941(2)	3918(1)	-782(1)	19(1)
C(25)	2960(2)	2826(1)	-1140(1)	19(1)
C(26)	694(2)	1740(2)	-893(2)	24(1)
C(27)	265(2)	2523(2)	1498(1)	20(1)

C(28)	1481(2)	5160(2)	759(2)	24(1)
C(29)	3760(2)	4972(2)	-1328(2)	28(1)
C(30)	3816(2)	2371(2)	-2163(1)	27(1)

Table 18. Bond lengths [Å] and angles [°] for **16**.

Y(1)-Cnt1	2.365	C(14)-C(19)	1.508(2)
Y(1)-Cnt2	2.410	C(15)-C(20)	1.502(2)
Y(1)-C(27)	2.4502(16)	C(21)-C(25)	1.516(2)
Y(1)-C(2)	2.6292(14)	C(21)-C(22)	1.533(2)
Y(1)-C(1)	2.6391(14)	C(21)-C(26)	1.541(2)
Y(1)-C(3)	2.6576(15)	C(22)-C(23)	1.380(2)
Y(1)-C(14)	2.6603(15)	C(22)-C(27)	1.434(2)
Y(1)-C(5)	2.6770(14)	C(23)-C(24)	1.476(2)
Y(1)-C(4)	2.6774(15)	C(23)-C(28)	1.508(2)
Y(1)-C(13)	2.6803(16)	C(24)-C(25)	1.341(2)
Y(1)-C(12)	2.6898(16)	C(24)-C(29)	1.497(2)
Y(1)-C(22)	2.6985(15)	C(25)-C(30)	1.494(2)
Y(1)-C(15)	2.7082(15)		
Y(1)-C(11)	2.7410(15)	Cnt1-Y(1)-C(22)	93.2
Y(1)-C(23)	2.9897(16)	Cnt1-Y(1)-C(23)	103.1
C(1)-C(2)	1.424(2)	Cnt1-Y(1)-C(27)	104.0
C(1)-C(5)	1.426(2)	Cnt2-Y(1)-C(22)	127.7
C(1)-C(6)	1.506(2)	Cnt2-Y(1)-C(23)	118.9
C(2)-C(3)	1.418(2)	Cnt2-Y(1)-C(27)	106.5
C(2)-C(7)	1.503(2)	Cnt1-Y(1)-Cnt2	137.3
C(3)-C(4)	1.420(2)	C(27)-Y(1)-C(2)	85.42(5)
C(3)-C(8)	1.500(2)	C(27)-Y(1)-C(1)	78.85(5)
C(4)-C(5)	1.419(2)	C(2)-Y(1)-C(1)	31.36(5)
C(4)-C(9)	1.504(2)	C(27)-Y(1)-C(3)	116.06(5)
C(5)-C(10)	1.505(2)	C(2)-Y(1)-C(3)	31.11(5)
C(6)-C(21)	1.554(2)	C(1)-Y(1)-C(3)	51.45(5)
C(11)-C(15)	1.419(2)	C(27)-Y(1)-C(14)	133.47(5)
C(11)-C(12)	1.421(2)	C(2)-Y(1)-C(14)	121.72(5)
C(11)-C(16)	1.501(2)	C(1)-Y(1)-C(14)	143.96(5)
C(12)-C(13)	1.419(2)	C(3)-Y(1)-C(14)	94.13(5)
C(12)-C(17)	1.498(3)	C(27)-Y(1)-C(5)	104.95(5)
C(13)-C(14)	1.419(2)	C(2)-Y(1)-C(5)	51.45(5)
C(13)-C(18)	1.502(2)	C(1)-Y(1)-C(5)	31.11(4)
C(14)-C(15)	1.426(2)	C(3)-Y(1)-C(5)	51.08(5)

C(14)-Y(1)-C(5)	121.57(5)	C(5)-Y(1)-C(15)	135.86(5)
C(27)-Y(1)-C(4)	130.00(5)	C(4)-Y(1)-C(15)	118.10(5)
C(2)-Y(1)-C(4)	51.30(5)	C(13)-Y(1)-C(15)	50.51(5)
C(1)-Y(1)-C(4)	51.24(4)	C(12)-Y(1)-C(15)	50.36(5)
C(3)-Y(1)-C(4)	30.88(5)	C(22)-Y(1)-C(15)	118.68(5)
C(14)-Y(1)-C(4)	94.25(5)	C(27)-Y(1)-C(11)	84.48(5)
C(5)-Y(1)-C(4)	30.75(5)	C(2)-Y(1)-C(11)	142.42(5)
C(27)-Y(1)-C(13)	113.62(5)	C(1)-Y(1)-C(11)	162.52(5)
C(2)-Y(1)-C(13)	102.72(5)	C(3)-Y(1)-C(11)	135.14(5)
C(1)-Y(1)-C(13)	133.56(5)	C(14)-Y(1)-C(11)	50.42(5)
C(3)-Y(1)-C(13)	85.11(5)	C(5)-Y(1)-C(11)	165.05(5)
C(14)-Y(1)-C(13)	30.82(5)	C(4)-Y(1)-C(11)	144.67(5)
C(5)-Y(1)-C(13)	131.52(5)	C(13)-Y(1)-C(11)	50.16(5)
C(4)-Y(1)-C(13)	100.91(5)	C(12)-Y(1)-C(11)	30.32(5)
C(27)-Y(1)-C(12)	85.08(5)	C(22)-Y(1)-C(11)	101.74(5)
C(2)-Y(1)-C(12)	112.72(5)	C(15)-Y(1)-C(11)	30.18(5)
C(1)-Y(1)-C(12)	141.00(5)	C(27)-Y(1)-C(23)	54.66(5)
C(3)-Y(1)-C(12)	108.09(5)	C(2)-Y(1)-C(23)	108.48(4)
C(14)-Y(1)-C(12)	50.85(5)	C(1)-Y(1)-C(23)	79.99(4)
C(5)-Y(1)-C(12)	159.11(5)	C(3)-Y(1)-C(23)	130.05(4)
C(4)-Y(1)-C(12)	130.38(5)	C(14)-Y(1)-C(23)	128.90(5)
C(13)-Y(1)-C(12)	30.64(5)	C(5)-Y(1)-C(23)	81.96(4)
C(27)-Y(1)-C(22)	31.87(5)	C(4)-Y(1)-C(23)	111.09(5)
C(2)-Y(1)-C(22)	87.89(5)	C(13)-Y(1)-C(23)	144.81(4)
C(1)-Y(1)-C(22)	66.15(4)	C(12)-Y(1)-C(23)	118.32(5)
C(3)-Y(1)-C(22)	116.54(4)	C(22)-Y(1)-C(23)	27.47(4)
C(14)-Y(1)-C(22)	149.32(5)	C(15)-Y(1)-C(23)	99.69(5)
C(5)-Y(1)-C(22)	81.97(5)	C(11)-Y(1)-C(23)	94.66(5)
C(4)-Y(1)-C(22)	112.31(5)	C(2)-C(1)-C(5)	107.88(13)
C(13)-Y(1)-C(22)	143.80(5)	C(2)-C(1)-C(6)	123.89(13)
C(12)-Y(1)-C(22)	113.40(5)	C(5)-C(1)-C(6)	128.15(14)
C(27)-Y(1)-C(15)	111.75(5)	C(2)-C(1)-Y(1)	73.93(8)
C(2)-Y(1)-C(15)	151.82(5)	C(5)-C(1)-Y(1)	75.91(8)
C(1)-Y(1)-C(15)	166.97(5)	C(6)-C(1)-Y(1)	118.62(9)
C(3)-Y(1)-C(15)	124.73(5)	C(3)-C(2)-C(1)	108.01(13)
C(14)-Y(1)-C(15)	30.80(5)	C(3)-C(2)-C(7)	124.94(15)

C(1)-C(2)-C(7)	126.89(14)	C(12)-C(13)-C(18)	122.92(16)
C(3)-C(2)-Y(1)	75.55(8)	C(14)-C(13)-C(18)	127.03(16)
C(1)-C(2)-Y(1)	74.71(8)	C(12)-C(13)-Y(1)	75.05(9)
C(7)-C(2)-Y(1)	119.43(11)	C(14)-C(13)-Y(1)	73.81(9)
C(2)-C(3)-C(4)	108.09(14)	C(18)-C(13)-Y(1)	129.69(11)
C(2)-C(3)-C(8)	125.48(15)	C(13)-C(14)-C(15)	107.82(14)
C(4)-C(3)-C(8)	124.96(15)	C(13)-C(14)-C(19)	126.01(16)
C(2)-C(3)-Y(1)	73.34(8)	C(15)-C(14)-C(19)	125.24(16)
C(4)-C(3)-Y(1)	75.33(8)	C(13)-C(14)-Y(1)	75.37(9)
C(8)-C(3)-Y(1)	128.21(11)	C(15)-C(14)-Y(1)	76.46(9)
C(5)-C(4)-C(3)	108.19(13)	C(19)-C(14)-Y(1)	123.02(11)
C(5)-C(4)-C(9)	125.89(15)	C(11)-C(15)-C(14)	107.98(14)
C(3)-C(4)-C(9)	124.90(15)	C(11)-C(15)-C(20)	126.38(17)
C(5)-C(4)-Y(1)	74.61(8)	C(14)-C(15)-C(20)	125.01(17)
C(3)-C(4)-Y(1)	73.79(8)	C(11)-C(15)-Y(1)	76.19(9)
C(9)-C(4)-Y(1)	126.67(11)	C(14)-C(15)-Y(1)	72.75(8)
C(4)-C(5)-C(1)	107.82(13)	C(20)-C(15)-Y(1)	124.08(12)
C(4)-C(5)-C(10)	124.48(14)	C(25)-C(21)-C(22)	103.25(12)
C(1)-C(5)-C(10)	127.16(14)	C(25)-C(21)-C(26)	109.34(13)
C(4)-C(5)-Y(1)	74.64(8)	C(22)-C(21)-C(26)	110.08(13)
C(1)-C(5)-Y(1)	72.98(8)	C(25)-C(21)-C(6)	113.44(13)
C(10)-C(5)-Y(1)	124.77(10)	C(22)-C(21)-C(6)	112.22(12)
C(1)-C(6)-C(21)	116.98(12)	C(26)-C(21)-C(6)	108.42(12)
C(15)-C(11)-C(12)	107.93(14)	C(23)-C(22)-C(27)	129.32(14)
C(15)-C(11)-C(16)	126.52(17)	C(23)-C(22)-C(21)	107.66(13)
C(12)-C(11)-C(16)	124.27(17)	C(27)-C(22)-C(21)	122.74(14)
C(15)-C(11)-Y(1)	73.63(9)	C(23)-C(22)-Y(1)	88.09(9)
C(12)-C(11)-Y(1)	72.85(9)	C(27)-C(22)-Y(1)	64.48(8)
C(16)-C(11)-Y(1)	129.42(11)	C(21)-C(22)-Y(1)	118.80(9)
C(13)-C(12)-C(11)	108.09(14)	C(22)-C(23)-C(24)	109.43(13)
C(13)-C(12)-C(17)	125.82(17)	C(22)-C(23)-C(28)	127.60(15)
C(11)-C(12)-C(17)	125.86(17)	C(24)-C(23)-C(28)	120.82(14)
C(13)-C(12)-Y(1)	74.31(9)	C(22)-C(23)-Y(1)	64.43(8)
C(11)-C(12)-Y(1)	76.83(9)	C(24)-C(23)-Y(1)	127.82(10)
C(17)-C(12)-Y(1)	119.41(12)	C(28)-C(23)-Y(1)	93.29(10)
C(12)-C(13)-C(14)	108.10(14)	C(25)-C(24)-C(23)	109.78(14)

C(25)-C(24)-C(29)	127.78(15)
C(23)-C(24)-C(29)	122.44(14)
C(24)-C(25)-C(30)	128.27(15)
C(24)-C(25)-C(21)	109.75(13)
C(30)-C(25)-C(21)	121.98(14)
C(22)-C(27)-Y(1)	83.65(9)

Table 19. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **16**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Y(1)	15(1)	16(1)	13(1)	-4(1)	-3(1)	1(1)
C(1)	17(1)	12(1)	17(1)	-4(1)	-4(1)	3(1)
C(2)	20(1)	14(1)	17(1)	-2(1)	-3(1)	1(1)
C(3)	21(1)	20(1)	17(1)	-4(1)	-6(1)	4(1)
C(4)	17(1)	18(1)	22(1)	-7(1)	-6(1)	4(1)
C(5)	17(1)	13(1)	20(1)	-5(1)	-3(1)	2(1)
C(6)	23(1)	14(1)	17(1)	-3(1)	-6(1)	0(1)
C(7)	26(1)	25(1)	25(1)	3(1)	-5(1)	-8(1)
C(8)	34(1)	30(1)	19(1)	-3(1)	-8(1)	8(1)
C(9)	22(1)	32(1)	33(1)	-9(1)	-12(1)	0(1)
C(10)	20(1)	18(1)	26(1)	-3(1)	-2(1)	-2(1)
C(11)	24(1)	25(1)	16(1)	-8(1)	-2(1)	6(1)
C(12)	21(1)	28(1)	16(1)	-8(1)	2(1)	-3(1)
C(13)	25(1)	23(1)	15(1)	-5(1)	-2(1)	0(1)
C(14)	21(1)	26(1)	15(1)	-9(1)	-2(1)	-1(1)
C(15)	29(1)	21(1)	17(1)	-8(1)	1(1)	-2(1)
C(16)	34(1)	44(1)	24(1)	-9(1)	-3(1)	20(1)
C(17)	28(1)	53(1)	30(1)	-12(1)	4(1)	-14(1)
C(18)	44(1)	31(1)	20(1)	1(1)	2(1)	5(1)
C(19)	25(1)	48(1)	28(1)	-15(1)	-8(1)	-3(1)
C(20)	50(1)	23(1)	32(1)	-8(1)	1(1)	-9(1)
C(21)	21(1)	17(1)	15(1)	-2(1)	-6(1)	0(1)
C(22)	17(1)	19(1)	17(1)	-4(1)	-8(1)	3(1)
C(23)	20(1)	16(1)	18(1)	-3(1)	-6(1)	3(1)
C(24)	22(1)	17(1)	17(1)	0(1)	-5(1)	1(1)
C(25)	24(1)	18(1)	15(1)	-1(1)	-4(1)	1(1)
C(26)	28(1)	22(1)	25(1)	-6(1)	-13(1)	1(1)
C(27)	19(1)	21(1)	20(1)	-4(1)	-4(1)	0(1)
C(28)	31(1)	18(1)	22(1)	-6(1)	-5(1)	2(1)
C(29)	36(1)	20(1)	26(1)	0(1)	-2(1)	-4(1)
C(30)	38(1)	26(1)	17(1)	-4(1)	0(1)	-1(1)

Table 20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **16**.

	x	y	z	U(eq)
H(6A)	1970(20)	241(17)	350(16)	23(5)
H(6B)	3440(20)	510(16)	-462(16)	20(5)
H(7A)	1420(30)	-680(30)	3170(30)	69(9)
H(7B)	910(30)	-250(20)	2140(20)	61(8)
H(7C)	2000(30)	-1330(30)	2170(30)	72(9)
H(8A)	3140(30)	-443(19)	4271(18)	31(6)
H(8B)	4400(20)	320(20)	4327(19)	40(6)
H(8C)	4700(30)	-860(20)	3780(20)	53(7)
H(9A)	6210(30)	1470(30)	3350(30)	73(9)
H(9B)	7160(30)	980(30)	2300(20)	65(8)
H(9C)	6630(30)	2310(30)	2340(20)	62(8)
H(10A)	5720(20)	1780(20)	-411(19)	37(6)
H(10B)	5330(20)	2950(20)	71(17)	31(5)
H(10C)	6620(30)	2090(20)	332(19)	36(6)
H(16A)	-1420(30)	5310(20)	3930(20)	50(7)
H(16B)	-1280(30)	4750(20)	2900(20)	48(7)
H(16C)	-390(30)	5820(20)	2920(20)	51(7)
H(17A)	-1520(30)	2320(30)	5080(30)	70(9)
H(17B)	-1700(40)	2800(30)	4020(30)	97(13)
H(17C)	-970(30)	1670(30)	4080(30)	80(10)
H(18A)	1320(20)	820(20)	5238(19)	40(6)
H(18B)	2700(20)	1351(19)	5530(17)	30(5)
H(18C)	1100(30)	1780(20)	6140(20)	54(7)
H(19A)	4820(30)	3830(20)	3980(20)	49(7)
H(19B)	4050(30)	3970(20)	5160(20)	60(8)
H(19C)	4560(30)	2660(20)	4740(20)	45(7)
H(20A)	3120(30)	5770(30)	2550(20)	62(8)
H(20B)	1800(30)	6260(20)	3290(20)	57(8)
H(20C)	3180(30)	5910(30)	3720(30)	76(9)
H(26A)	-70(20)	1355(18)	-374(17)	25(5)

H(26B)	1080(20)	1187(18)	-1444(17)	29(5)
H(26C)	230(20)	2447(19)	-1248(17)	31(5)
H(27A)	-420(20)	3144(17)	1805(16)	21(5)
H(27B)	-150(20)	1785(19)	1481(17)	30(5)
H(28A)	2290(20)	5520(19)	919(17)	32(5)
H(28B)	1070(20)	5782(19)	233(17)	30(5)
H(28C)	820(30)	5060(20)	1380(20)	44(7)
H(29A)	4560(30)	5080(20)	-980(20)	45(7)
H(29B)	4200(20)	4850(20)	-2050(20)	39(6)
H(29C)	3160(30)	5700(20)	-1338(19)	43(6)
H(30A)	3180(30)	2140(20)	-2630(20)	68(8)
H(30B)	4400(30)	2920(20)	-2560(20)	47(7)
H(30C)	4400(30)	1650(30)	-2030(20)	61(8)

Table 21. Crystal data and structure refinement for, $(C_5Me_5)_2Y(\mu\text{-}\eta^8\text{:}\eta^1\text{-}C_8H_7)Y(C_5Me_5)$, **17**.

Empirical formula	C38 H52 Y2	
Formula weight	686.62	
Temperature	208(2) K	
Wavelength	0.71069 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 8.420(3) Å	α= 90°
	b = 16.807(5) Å	β= 93.001(5)°
	c = 24.239(8) Å	γ = 90°
Volume	3425.6(18) $Å^3$	
Z	4	
Density (calculated)	1.331 g/cm^3	
Absorption coefficient	3.394 mm^{-1}	
Absorption correction	Multi-scan	
F(000)	1432	
Crystal size	0.15 x 0.10 x 0.02 mm^3	
Theta range for data collection	2.07 to 25.03°	
Index ranges	-9<=h<=10, -9<=k<=20, -28<=l<=28	
Reflections collected	19053	
Independent reflections	6034 [R(int) = 0.0747]	
Completeness to theta = 25.00°	99.9 %	
Max. and min. transmission	0.9352 and 0.6300	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6034 / 0 / 376	
Goodness-of-fit on F^2	1.031	
Final R indices [I>2sigma(I)]	R1 = 0.0524, wR2 = 0.1109	
R indices (all data)	R1 = 0.1052, wR2 = 0.1285	
Largest diff. peak and hole	0.579 and -0.512 e $Å^{-3}$	

Table 22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for **17**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	13268(8)	2119(3)	6873(3)	42(2)
C(2)	11714(8)	1839(3)	6784(3)	45(2)
C(3)	11431(7)	1702(3)	6218(3)	50(2)
C(4)	12863(8)	1896(3)	5951(3)	44(2)
C(5)	13971(7)	2152(3)	6367(3)	41(2)
C(6)	14082(9)	2274(4)	7429(3)	74(2)
C(7)	10589(8)	1650(4)	7228(3)	75(2)
C(8)	9952(9)	1353(4)	5930(4)	94(3)
C(9)	13190(10)	1698(4)	5365(3)	86(3)
C(10)	15702(7)	2323(4)	6281(4)	78(3)
C(11)	11273(7)	3852(3)	5322(2)	41(2)
C(12)	10318(7)	4321(3)	5669(3)	42(2)
C(13)	11344(7)	4768(3)	6030(3)	39(2)
C(14)	12935(7)	4562(3)	5918(2)	38(1)
C(15)	12889(7)	4013(3)	5473(2)	38(1)
C(16)	10638(8)	3361(4)	4842(3)	68(2)
C(17)	8542(7)	4380(4)	5615(3)	66(2)
C(18)	10877(7)	5388(3)	6438(3)	52(2)
C(19)	14417(7)	4897(3)	6206(3)	55(2)
C(20)	14307(7)	3753(4)	5156(3)	58(2)
C(21)	7732(7)	3360(3)	8814(2)	42(2)
C(22)	8630(6)	2678(3)	8691(2)	35(1)
C(23)	10236(6)	2816(3)	8883(2)	36(1)
C(24)	10305(6)	3589(3)	9115(2)	35(1)
C(25)	8772(7)	3923(3)	9072(2)	39(1)
C(26)	5959(7)	3454(4)	8710(3)	66(2)
C(27)	8001(8)	1910(3)	8443(3)	57(2)
C(28)	11587(7)	2233(3)	8884(3)	49(2)
C(29)	11769(7)	3954(4)	9394(3)	61(2)
C(30)	8278(8)	4725(3)	9293(3)	60(2)

C(31)	11209(8)	3790(3)	7197(3)	45(2)
C(32)	9597(9)	3703(3)	7036(3)	52(2)
C(33)	8128(8)	4038(4)	7157(3)	61(2)
C(34)	7743(9)	4669(5)	7497(3)	65(2)
C(35)	8581(11)	5169(4)	7847(3)	73(2)
C(36)	10156(12)	5274(4)	8036(3)	71(2)
C(37)	11619(10)	4911(4)	7931(3)	67(2)
C(38)	12047(7)	4284(4)	7575(3)	54(2)
Y(1)	11758(1)	3257(1)	6320(1)	32(1)
Y(2)	9674(1)	3811(1)	8061(1)	35(1)

Table 23. Bond lengths [Å] and angles [°] for **17**.

C(1)-C(5)	1.390(8)	C(12)-C(13)	1.413(8)
C(1)-C(2)	1.397(8)	C(12)-C(17)	1.498(8)
C(1)-C(6)	1.502(8)	C(12)-Y(1)	2.638(5)
C(1)-Y(1)	2.624(5)	C(13)-C(14)	1.423(7)
C(2)-C(3)	1.399(9)	C(13)-C(18)	1.504(8)
C(2)-C(7)	1.505(8)	C(13)-Y(1)	2.654(5)
C(2)-Y(1)	2.636(5)	C(14)-C(15)	1.417(8)
C(3)-C(4)	1.435(8)	C(14)-C(19)	1.507(8)
C(3)-C(8)	1.513(9)	C(14)-Y(1)	2.616(5)
C(3)-Y(1)	2.639(6)	C(15)-C(20)	1.517(8)
C(4)-C(5)	1.405(8)	C(15)-Y(1)	2.635(5)
C(4)-C(9)	1.499(9)	C(16)-H(16A)	0.9700
C(4)-Y(1)	2.643(5)	C(16)-H(16B)	0.9700
C(5)-C(10)	1.511(8)	C(16)-H(16C)	0.9700
C(5)-Y(1)	2.628(5)	C(17)-H(17A)	0.9700
C(6)-H(6A)	0.9700	C(17)-H(17B)	0.9700
C(6)-H(6B)	0.9700	C(17)-H(17C)	0.9700
C(6)-H(6C)	0.9700	C(18)-H(18A)	0.9700
C(7)-H(7A)	0.9700	C(18)-H(18B)	0.9700
C(7)-H(7B)	0.9700	C(18)-H(18C)	0.9700
C(7)-H(7C)	0.9700	C(19)-H(19A)	0.9700
C(8)-H(8A)	0.9700	C(19)-H(19B)	0.9700
C(8)-H(8B)	0.9700	C(19)-H(19C)	0.9700
C(8)-H(8C)	0.9700	C(20)-H(20A)	0.9700
C(9)-H(9A)	0.9700	C(20)-H(20B)	0.9700
C(9)-H(9B)	0.9700	C(20)-H(20C)	0.9700
C(9)-H(9C)	0.9700	C(21)-C(25)	1.413(8)
C(10)-H(10A)	0.9700	C(21)-C(22)	1.413(7)
C(10)-H(10B)	0.9700	C(21)-C(26)	1.509(8)
C(10)-H(10C)	0.9700	C(21)-Y(2)	2.625(6)
C(11)-C(15)	1.417(8)	C(22)-C(23)	1.427(7)
C(11)-C(12)	1.430(8)	C(22)-C(27)	1.508(7)
C(11)-C(16)	1.501(8)	C(22)-Y(2)	2.620(5)
C(11)-Y(1)	2.630(6)	C(23)-C(24)	1.414(7)

C(23)-C(28)	1.502(7)	C(31)-C(38)	1.400(9)
C(23)-Y(2)	2.625(5)	C(31)-Y(2)	2.519(6)
C(24)-C(25)	1.407(7)	C(32)-C(33)	1.404(9)
C(24)-C(29)	1.506(8)	C(32)-Y(2)	2.489(6)
C(24)-Y(2)	2.608(6)	C(32)-H(32)	0.9400
C(25)-C(30)	1.517(7)	C(33)-C(34)	1.391(10)
C(25)-Y(2)	2.609(6)	C(33)-Y(2)	2.520(7)
C(26)-H(26A)	0.9700	C(33)-H(33)	0.9400
C(26)-H(26B)	0.9700	C(34)-C(35)	1.365(10)
C(26)-H(26C)	0.9700	C(34)-Y(2)	2.521(7)
C(27)-H(27A)	0.9700	C(34)-H(34)	0.9400
C(27)-H(27B)	0.9700	C(35)-C(36)	1.391(11)
C(27)-H(27C)	0.9700	C(35)-Y(2)	2.504(7)
C(28)-H(28A)	0.9700	C(35)-H(35)	0.9400
C(28)-H(28B)	0.9700	C(36)-C(37)	1.409(10)
C(28)-H(28C)	0.9700	C(36)-Y(2)	2.492(6)
C(29)-H(29A)	0.9700	C(36)-H(36)	0.9400
C(29)-H(29B)	0.9700	C(37)-C(38)	1.420(9)
C(29)-H(29C)	0.9700	C(37)-Y(2)	2.500(6)
C(30)-H(30A)	0.9700	C(37)-H(37)	0.9400
C(30)-H(30B)	0.9700	C(38)-Y(2)	2.502(6)
C(30)-H(30C)	0.9700	C(38)-H(38)	0.9400
C(31)-C(32)	1.399(9)		

C(5)-C(1)-C(2)	108.4(5)	C(2)-C(3)-C(4)	107.5(5)
C(5)-C(1)-C(6)	126.1(6)	C(2)-C(3)-C(8)	127.6(7)
C(2)-C(1)-C(6)	125.2(6)	C(4)-C(3)-C(8)	124.8(7)
C(5)-C(1)-Y(1)	74.8(3)	C(2)-C(3)-Y(1)	74.5(3)
C(2)-C(1)-Y(1)	75.1(3)	C(4)-C(3)-Y(1)	74.4(3)
C(6)-C(1)-Y(1)	121.2(4)	C(8)-C(3)-Y(1)	120.4(4)
C(1)-C(2)-C(3)	108.5(5)	C(5)-C(4)-C(3)	106.8(5)
C(1)-C(2)-C(7)	125.5(7)	C(5)-C(4)-C(9)	126.9(6)
C(3)-C(2)-C(7)	125.9(7)	C(3)-C(4)-C(9)	125.3(6)
C(1)-C(2)-Y(1)	74.1(3)	C(5)-C(4)-Y(1)	73.9(3)
C(3)-C(2)-Y(1)	74.7(3)	C(3)-C(4)-Y(1)	74.1(3)
C(7)-C(2)-Y(1)	121.3(4)	C(9)-C(4)-Y(1)	126.7(4)

C(1)-C(5)-C(4)	108.8(5)	C(15)-C(11)-C(12)	107.7(5)
C(1)-C(5)-C(10)	126.0(6)	C(15)-C(11)-C(16)	127.1(6)
C(4)-C(5)-C(10)	124.6(6)	C(12)-C(11)-C(16)	124.7(6)
C(1)-C(5)-Y(1)	74.5(3)	C(15)-C(11)-Y(1)	74.6(3)
C(4)-C(5)-Y(1)	75.1(3)	C(12)-C(11)-Y(1)	74.5(3)
C(10)-C(5)-Y(1)	123.2(4)	C(16)-C(11)-Y(1)	122.4(4)
C(1)-C(6)-H(6A)	109.5	C(13)-C(12)-C(11)	108.2(5)
C(1)-C(6)-H(6B)	109.5	C(13)-C(12)-C(17)	126.4(6)
H(6A)-C(6)-H(6B)	109.5	C(11)-C(12)-C(17)	125.1(6)
C(1)-C(6)-H(6C)	109.5	C(13)-C(12)-Y(1)	75.1(3)
H(6A)-C(6)-H(6C)	109.5	C(11)-C(12)-Y(1)	74.0(3)
H(6B)-C(6)-H(6C)	109.5	C(17)-C(12)-Y(1)	121.6(4)
C(2)-C(7)-H(7A)	109.5	C(12)-C(13)-C(14)	107.7(5)
C(2)-C(7)-H(7B)	109.5	C(12)-C(13)-C(18)	127.1(5)
H(7A)-C(7)-H(7B)	109.5	C(14)-C(13)-C(18)	125.1(5)
C(2)-C(7)-H(7C)	109.5	C(12)-C(13)-Y(1)	73.9(3)
H(7A)-C(7)-H(7C)	109.5	C(14)-C(13)-Y(1)	72.9(3)
H(7B)-C(7)-H(7C)	109.5	C(18)-C(13)-Y(1)	121.6(4)
C(3)-C(8)-H(8A)	109.5	C(15)-C(14)-C(13)	108.4(5)
C(3)-C(8)-H(8B)	109.5	C(15)-C(14)-C(19)	125.8(5)
H(8A)-C(8)-H(8B)	109.5	C(13)-C(14)-C(19)	125.8(5)
C(3)-C(8)-H(8C)	109.5	C(15)-C(14)-Y(1)	75.1(3)
H(8A)-C(8)-H(8C)	109.5	C(13)-C(14)-Y(1)	75.8(3)
H(8B)-C(8)-H(8C)	109.5	C(19)-C(14)-Y(1)	117.5(4)
C(4)-C(9)-H(9A)	109.5	C(14)-C(15)-C(11)	108.0(5)
C(4)-C(9)-H(9B)	109.5	C(14)-C(15)-C(20)	125.6(5)
H(9A)-C(9)-H(9B)	109.5	C(11)-C(15)-C(20)	125.8(6)
C(4)-C(9)-H(9C)	109.5	C(14)-C(15)-Y(1)	73.6(3)
H(9A)-C(9)-H(9C)	109.5	C(11)-C(15)-Y(1)	74.2(3)
H(9B)-C(9)-H(9C)	109.5	C(20)-C(15)-Y(1)	125.6(4)
C(5)-C(10)-H(10A)	109.5	C(11)-C(16)-H(16A)	109.5
C(5)-C(10)-H(10B)	109.5	C(11)-C(16)-H(16B)	109.5
H(10A)-C(10)-H(10B)	109.5	H(16A)-C(16)-H(16B)	109.5
C(5)-C(10)-H(10C)	109.5	C(11)-C(16)-H(16C)	109.5
H(10A)-C(10)-H(10C)	109.5	H(16A)-C(16)-H(16C)	109.5
H(10B)-C(10)-H(10C)	109.5	H(16B)-C(16)-H(16C)	109.5

C(12)-C(17)-H(17A)	109.5	C(24)-C(23)-C(22)	107.3(5)
C(12)-C(17)-H(17B)	109.5	C(24)-C(23)-C(28)	125.7(5)
H(17A)-C(17)-H(17B)	109.5	C(22)-C(23)-C(28)	126.8(5)
C(12)-C(17)-H(17C)	109.5	C(24)-C(23)-Y(2)	73.7(3)
H(17A)-C(17)-H(17C)	109.5	C(22)-C(23)-Y(2)	74.0(3)
H(17B)-C(17)-H(17C)	109.5	C(28)-C(23)-Y(2)	121.5(4)
C(13)-C(18)-H(18A)	109.5	C(25)-C(24)-C(23)	108.6(5)
C(13)-C(18)-H(18B)	109.5	C(25)-C(24)-C(29)	126.6(5)
H(18A)-C(18)-H(18B)	109.5	C(23)-C(24)-C(29)	124.7(5)
C(13)-C(18)-H(18C)	109.5	C(25)-C(24)-Y(2)	74.4(3)
H(18A)-C(18)-H(18C)	109.5	C(23)-C(24)-Y(2)	75.0(3)
H(18B)-C(18)-H(18C)	109.5	C(29)-C(24)-Y(2)	120.1(4)
C(14)-C(19)-H(19A)	109.5	C(24)-C(25)-C(21)	108.1(5)
C(14)-C(19)-H(19B)	109.5	C(24)-C(25)-C(30)	126.6(6)
H(19A)-C(19)-H(19B)	109.5	C(21)-C(25)-C(30)	125.2(5)
C(14)-C(19)-H(19C)	109.5	C(24)-C(25)-Y(2)	74.3(3)
H(19A)-C(19)-H(19C)	109.5	C(21)-C(25)-Y(2)	74.9(3)
H(19B)-C(19)-H(19C)	109.5	C(30)-C(25)-Y(2)	119.6(4)
C(15)-C(20)-H(20A)	109.5	C(21)-C(26)-H(26A)	109.5
C(15)-C(20)-H(20B)	109.5	C(21)-C(26)-H(26B)	109.5
H(20A)-C(20)-H(20B)	109.5	H(26A)-C(26)-H(26B)	109.5
C(15)-C(20)-H(20C)	109.5	C(21)-C(26)-H(26C)	109.5
H(20A)-C(20)-H(20C)	109.5	H(26A)-C(26)-H(26C)	109.5
H(20B)-C(20)-H(20C)	109.5	H(26B)-C(26)-H(26C)	109.5
C(25)-C(21)-C(22)	108.1(5)	C(22)-C(27)-H(27A)	109.5
C(25)-C(21)-C(26)	126.0(5)	C(22)-C(27)-H(27B)	109.5
C(22)-C(21)-C(26)	125.8(6)	H(27A)-C(27)-H(27B)	109.5
C(25)-C(21)-Y(2)	73.7(3)	C(22)-C(27)-H(27C)	109.5
C(22)-C(21)-Y(2)	74.2(3)	H(27A)-C(27)-H(27C)	109.5
C(26)-C(21)-Y(2)	120.1(4)	H(27B)-C(27)-H(27C)	109.5
C(21)-C(22)-C(23)	107.9(5)	C(23)-C(28)-H(28A)	109.5
C(21)-C(22)-C(27)	126.7(5)	C(23)-C(28)-H(28B)	109.5
C(23)-C(22)-C(27)	125.2(5)	H(28A)-C(28)-H(28B)	109.5
C(21)-C(22)-Y(2)	74.6(3)	C(23)-C(28)-H(28C)	109.5
C(23)-C(22)-Y(2)	74.4(3)	H(28A)-C(28)-H(28C)	109.5
C(27)-C(22)-Y(2)	120.8(4)	H(28B)-C(28)-H(28C)	109.5

C(24)-C(29)-H(29A)	109.5	C(34)-C(35)-H(35)	111.3
C(24)-C(29)-H(29B)	109.5	C(36)-C(35)-H(35)	111.3
H(29A)-C(29)-H(29B)	109.5	Y(2)-C(35)-H(35)	138.7
C(24)-C(29)-H(29C)	109.5	C(35)-C(36)-C(37)	135.5(7)
H(29A)-C(29)-H(29C)	109.5	C(35)-C(36)-Y(2)	74.3(4)
H(29B)-C(29)-H(29C)	109.5	C(37)-C(36)-Y(2)	73.9(3)
C(25)-C(30)-H(30A)	109.5	C(35)-C(36)-H(36)	112.2
C(25)-C(30)-H(30B)	109.5	C(37)-C(36)-H(36)	112.2
H(30A)-C(30)-H(30B)	109.5	Y(2)-C(36)-H(36)	136.3
C(25)-C(30)-H(30C)	109.5	C(36)-C(37)-C(38)	133.0(7)
H(30A)-C(30)-H(30C)	109.5	C(36)-C(37)-Y(2)	73.3(4)
H(30B)-C(30)-H(30C)	109.5	C(38)-C(37)-Y(2)	73.6(3)
C(32)-C(31)-C(38)	133.8(6)	C(36)-C(37)-H(37)	113.5
C(32)-C(31)-Y(2)	72.6(4)	C(38)-C(37)-H(37)	113.5
C(38)-C(31)-Y(2)	73.1(3)	Y(2)-C(37)-H(37)	135.7
C(31)-C(32)-C(33)	138.8(6)	C(31)-C(38)-C(37)	134.6(6)
C(31)-C(32)-Y(2)	75.0(4)	C(31)-C(38)-Y(2)	74.5(3)
C(33)-C(32)-Y(2)	74.9(4)	C(37)-C(38)-Y(2)	73.5(4)
C(31)-C(32)-H(32)	110.6	C(31)-C(38)-H(38)	112.7
C(33)-C(32)-H(32)	110.6	C(37)-C(38)-H(38)	112.7
Y(2)-C(32)-H(32)	137.5	Y(2)-C(38)-H(38)	135.7
C(34)-C(33)-C(32)	131.6(7)	C(14)-Y(1)-C(1)	128.21(19)
C(34)-C(33)-Y(2)	74.0(4)	C(14)-Y(1)-C(5)	109.08(18)
C(32)-C(33)-Y(2)	72.5(4)	C(1)-Y(1)-C(5)	30.70(18)
C(34)-C(33)-H(33)	114.2	C(14)-Y(1)-C(11)	51.81(18)
C(32)-C(33)-H(33)	114.2	C(1)-Y(1)-C(11)	142.59(19)
Y(2)-C(33)-H(33)	134.6	C(5)-Y(1)-C(11)	112.6(2)
C(35)-C(34)-C(33)	135.1(7)	C(14)-Y(1)-C(15)	31.30(17)
C(35)-C(34)-Y(2)	73.6(4)	C(1)-Y(1)-C(15)	124.34(19)
C(33)-C(34)-Y(2)	73.9(4)	C(5)-Y(1)-C(15)	95.17(18)
C(35)-C(34)-H(34)	112.4	C(11)-Y(1)-C(15)	31.23(17)
C(33)-C(34)-H(34)	112.4	C(14)-Y(1)-C(2)	158.60(19)
Y(2)-C(34)-H(34)	137.2	C(1)-Y(1)-C(2)	30.80(18)
C(34)-C(35)-C(36)	137.3(7)	C(5)-Y(1)-C(2)	50.87(18)
C(34)-C(35)-Y(2)	74.9(4)	C(11)-Y(1)-C(2)	137.0(2)
C(36)-C(35)-Y(2)	73.4(4)	C(15)-Y(1)-C(2)	141.47(18)

C(14)-Y(1)-C(12)	51.68(17)	C(32)-Y(2)-C(35)	82.5(2)
C(1)-Y(1)-C(12)	173.95(19)	C(36)-Y(2)-C(35)	32.3(3)
C(5)-Y(1)-C(12)	143.8(2)	C(37)-Y(2)-C(35)	62.4(3)
C(11)-Y(1)-C(12)	31.51(18)	C(38)-Y(2)-C(35)	84.7(2)
C(15)-Y(1)-C(12)	51.72(17)	C(32)-Y(2)-C(31)	32.4(2)
C(2)-Y(1)-C(12)	148.4(2)	C(36)-Y(2)-C(31)	84.4(2)
C(14)-Y(1)-C(3)	146.6(2)	C(37)-Y(2)-C(31)	62.4(2)
C(1)-Y(1)-C(3)	51.07(19)	C(38)-Y(2)-C(31)	32.4(2)
C(5)-Y(1)-C(3)	51.29(17)	C(35)-Y(2)-C(31)	92.3(2)
C(11)-Y(1)-C(3)	106.2(2)	C(32)-Y(2)-C(33)	32.5(2)
C(15)-Y(1)-C(3)	116.4(2)	C(36)-Y(2)-C(33)	84.6(3)
C(2)-Y(1)-C(3)	30.77(19)	C(37)-Y(2)-C(33)	95.2(2)
C(12)-Y(1)-C(3)	124.9(2)	C(38)-Y(2)-C(33)	86.0(2)
C(14)-Y(1)-C(4)	116.91(18)	C(35)-Y(2)-C(33)	60.9(3)
C(1)-Y(1)-C(4)	51.13(18)	C(31)-Y(2)-C(33)	62.8(2)
C(5)-Y(1)-C(4)	30.91(18)	C(32)-Y(2)-C(34)	61.2(2)
C(11)-Y(1)-C(4)	93.35(19)	C(36)-Y(2)-C(34)	61.6(3)
C(15)-Y(1)-C(4)	90.35(18)	C(37)-Y(2)-C(34)	85.2(3)
C(2)-Y(1)-C(4)	51.30(18)	C(38)-Y(2)-C(34)	94.1(2)
C(12)-Y(1)-C(4)	122.9(2)	C(35)-Y(2)-C(34)	31.5(2)
C(3)-Y(1)-C(4)	31.52(18)	C(31)-Y(2)-C(34)	84.3(2)
C(14)-Y(1)-C(13)	31.33(16)	C(33)-Y(2)-C(34)	32.0(2)
C(1)-Y(1)-C(13)	152.40(19)	C(32)-Y(2)-C(24)	163.83(19)
C(5)-Y(1)-C(13)	140.40(18)	C(36)-Y(2)-C(24)	98.1(2)
C(11)-Y(1)-C(13)	51.68(19)	C(37)-Y(2)-C(24)	97.4(2)
C(15)-Y(1)-C(13)	51.63(17)	C(38)-Y(2)-C(24)	112.3(2)
C(2)-Y(1)-C(13)	166.85(18)	C(35)-Y(2)-C(24)	112.8(2)
C(12)-Y(1)-C(13)	30.97(17)	C(31)-Y(2)-C(24)	136.5(2)
C(3)-Y(1)-C(13)	155.7(2)	C(33)-Y(2)-C(24)	160.6(2)
C(4)-Y(1)-C(13)	141.47(18)	C(34)-Y(2)-C(24)	134.9(2)
C(32)-Y(2)-C(36)	92.4(2)	C(32)-Y(2)-C(25)	161.6(2)
C(32)-Y(2)-C(37)	84.9(2)	C(36)-Y(2)-C(25)	90.5(2)
C(36)-Y(2)-C(37)	32.8(2)	C(37)-Y(2)-C(25)	106.9(2)
C(32)-Y(2)-C(38)	62.1(2)	C(38)-Y(2)-C(25)	134.3(2)
C(36)-Y(2)-C(38)	62.6(2)	C(35)-Y(2)-C(25)	90.4(2)
C(37)-Y(2)-C(38)	33.0(2)	C(31)-Y(2)-C(25)	165.7(2)

C(33)-Y(2)-C(25)	130.1(2)	C(25)-Y(2)-C(22)	51.89(17)
C(34)-Y(2)-C(25)	104.9(2)	C(32)-Y(2)-C(21)	133.5(2)
C(24)-Y(2)-C(25)	31.30(16)	C(36)-Y(2)-C(21)	114.2(2)
C(32)-Y(2)-C(22)	122.43(18)	C(37)-Y(2)-C(21)	137.5(2)
C(36)-Y(2)-C(22)	142.3(2)	C(38)-Y(2)-C(21)	164.0(2)
C(37)-Y(2)-C(22)	148.5(2)	C(35)-Y(2)-C(21)	99.9(2)
C(38)-Y(2)-C(22)	143.66(19)	C(31)-Y(2)-C(21)	160.0(2)
C(35)-Y(2)-C(22)	130.7(2)	C(33)-Y(2)-C(21)	109.7(2)
C(31)-Y(2)-C(22)	132.57(17)	C(34)-Y(2)-C(21)	97.7(2)
C(33)-Y(2)-C(22)	116.28(19)	C(24)-Y(2)-C(21)	51.71(18)
C(34)-Y(2)-C(22)	120.3(2)	C(25)-Y(2)-C(21)	31.32(17)
C(24)-Y(2)-C(22)	51.92(17)	C(22)-Y(2)-C(21)	31.26(16)

Table 24. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **17**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	62(4)	26(3)	36(4)	0(3)	-7(3)	8(3)
C(2)	58(4)	26(3)	54(5)	11(3)	22(3)	10(3)
C(3)	47(4)	32(3)	71(6)	0(3)	-6(4)	-2(3)
C(4)	66(4)	32(3)	33(4)	-4(3)	11(3)	6(3)
C(5)	41(4)	28(3)	55(5)	-5(3)	1(3)	3(3)
C(6)	107(6)	55(4)	57(5)	-1(4)	-25(4)	34(4)
C(7)	97(6)	49(4)	83(6)	19(4)	44(5)	14(4)
C(8)	86(6)	55(4)	136(9)	-22(5)	-26(6)	-15(4)
C(9)	145(8)	56(4)	57(6)	-10(4)	13(5)	21(5)
C(10)	44(4)	53(4)	139(8)	13(5)	19(5)	8(3)
C(11)	45(4)	45(3)	31(4)	13(3)	-7(3)	-7(3)
C(12)	36(4)	43(3)	46(4)	22(3)	-2(3)	1(3)
C(13)	46(4)	29(3)	43(4)	15(3)	0(3)	3(3)
C(14)	42(4)	31(3)	42(4)	11(3)	-1(3)	1(3)
C(15)	39(4)	47(3)	29(4)	17(3)	6(3)	5(3)
C(16)	83(5)	81(5)	39(5)	6(4)	-13(4)	-16(4)
C(17)	40(4)	82(5)	77(6)	36(4)	-1(4)	4(4)
C(18)	61(4)	37(3)	60(5)	16(3)	8(4)	10(3)
C(19)	46(4)	43(3)	75(5)	11(4)	-10(4)	-10(3)
C(20)	56(4)	62(4)	59(5)	15(4)	23(4)	-10(4)
C(21)	34(3)	56(4)	36(4)	6(3)	9(3)	7(3)
C(22)	43(4)	32(3)	29(3)	3(3)	4(3)	-5(3)
C(23)	35(3)	31(3)	42(4)	7(3)	4(3)	3(3)
C(24)	37(3)	38(3)	29(4)	-1(3)	-1(3)	0(3)
C(25)	47(4)	36(3)	33(4)	-4(3)	2(3)	8(3)
C(26)	46(4)	89(5)	64(5)	10(4)	5(4)	8(4)
C(27)	70(5)	50(4)	52(5)	-1(3)	4(4)	-24(3)
C(28)	46(4)	50(4)	52(4)	10(3)	11(3)	6(3)
C(29)	61(5)	61(4)	59(5)	-14(4)	-4(4)	-7(4)
C(30)	89(5)	53(4)	38(4)	0(3)	19(4)	21(4)
C(31)	68(5)	35(3)	33(4)	12(3)	20(3)	14(3)

C(32)	90(6)	35(3)	30(4)	-1(3)	5(4)	-7(4)
C(33)	57(5)	74(5)	51(5)	18(4)	-8(4)	-17(4)
C(34)	60(5)	72(5)	66(6)	30(4)	18(4)	31(4)
C(35)	115(8)	44(4)	63(6)	11(4)	27(5)	28(5)
C(36)	139(8)	23(3)	52(5)	-9(3)	22(6)	-9(4)
C(37)	103(6)	48(4)	50(5)	7(4)	-4(4)	-41(4)
C(38)	44(4)	63(4)	55(5)	23(4)	8(3)	-1(3)
Y(1)	37(1)	29(1)	29(1)	3(1)	3(1)	2(1)
Y(2)	48(1)	27(1)	32(1)	1(1)	7(1)	2(1)

Table 25. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **17**.

	x	y	z	U(eq)
H(6A)	14684	1807	7548	111
H(6B)	13292	2391	7694	111
H(6C)	14797	2723	7403	111
H(7A)	9514	1609	7066	112
H(7B)	10634	2071	7503	112
H(7C)	10892	1150	7403	112
H(8A)	10001	777	5949	140
H(8B)	9889	1520	5546	140
H(8C)	9020	1539	6110	140
H(9A)	14208	1921	5276	129
H(9B)	12358	1921	5120	129
H(9C)	13215	1125	5320	129
H(10A)	15821	2873	6169	118
H(10B)	16072	1975	5995	118
H(10C)	16325	2229	6622	118
H(16A)	9901	2967	4971	102
H(16B)	11511	3095	4673	102
H(16C)	10089	3704	4573	102
H(17A)	8087	3851	5582	99
H(17B)	8230	4688	5289	99
H(17C)	8157	4640	5940	99
H(18A)	10850	5907	6262	79
H(18B)	11646	5394	6750	79
H(18C)	9832	5264	6565	79
H(19A)	15239	4493	6227	83
H(19B)	14183	5064	6576	83
H(19C)	14782	5351	6000	83
H(20A)	14711	4204	4957	87
H(20B)	13982	3338	4897	87
H(20C)	15134	3552	5413	87
H(26A)	5611	3149	8387	99

H(26B)	5706	4011	8649	99
H(26C)	5419	3262	9028	99
H(27A)	6885	1973	8331	86
H(27B)	8119	1489	8716	86
H(27C)	8594	1774	8124	86
H(28A)	12578	2517	8846	74
H(28B)	11416	1865	8578	74
H(28C)	11639	1939	9229	74
H(29A)	11695	4529	9372	91
H(29B)	12703	3776	9212	91
H(29C)	11851	3793	9779	91
H(30A)	7773	4651	9640	90
H(30B)	7534	4977	9028	90
H(30C)	9209	5060	9352	90
H(32)	9457	3302	6768	62
H(33)	7245	3793	6975	73
H(34)	6646	4775	7483	78
H(35)	7912	5545	8004	88
H(36)	10273	5687	8296	85
H(37)	12488	5128	8139	81
H(38)	13143	4175	7599	64