Cyclisation of α,ω-Dienes Promoted by Bis(Indenyl)zirconium Sandwich and *ansa*-Titanocene Dinitrogen Complexes.

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Contribution to Special Issue on d^0 Metallocenes

-- Supporting Information --

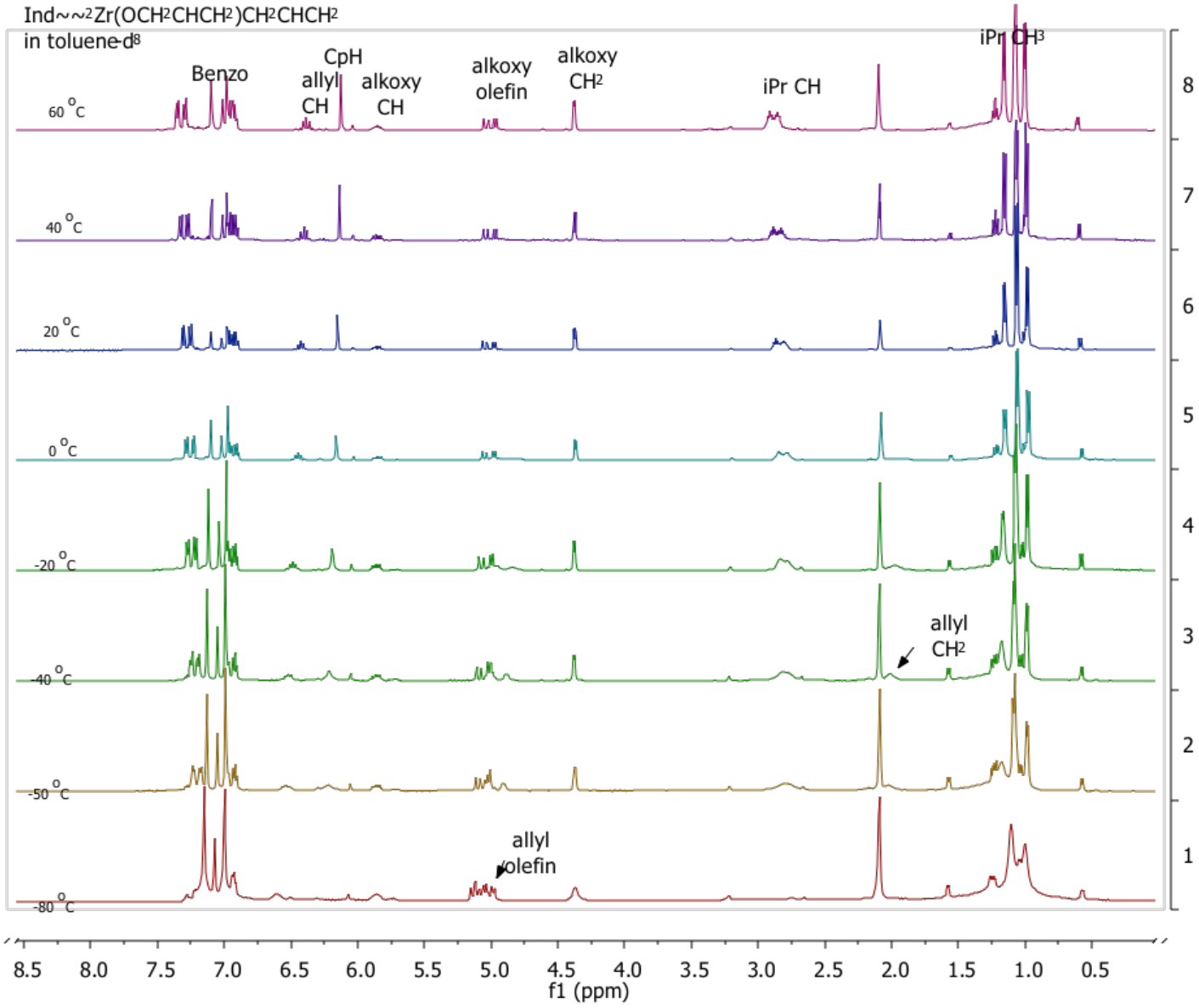

Figure S1. Variable temperature ^{1}H NMR spectra of **1-(CH_2CHCH_2)OCH_2CHCH_2** recorded in toluene-d_8.

Table S1. Crystal data and structure refinement for dp14 = *cis*-**1-(CH_2CHCH_2)$_2$N^{t}Bu**

Identification code	dp14 = *cis*-**1-(CH_2CHCH_2)$_2$N^{t}Bu**	
Empirical formula	C45 H69 N Zr	
Formula weight	715.23	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 13.2599(4) Å	α= 90°.
	b = 17.5475(6) Å	β= 92.942(2)°.
	c = 17.0737(6) Å	γ = 90°.
Volume	3967.4(2) Å^3	
Z	4	
Density (calculated)	1.197 Mg/m^3	
Absorption coefficient	0.308 mm^{-1}	
F(000)	1544	
Crystal size	0.45 x 0.40 x 0.35 mm^3	
Theta range for data collection	1.93 to 30.51°.	
Index ranges	-18<=h<=18, -23<=k<=25, -24<=l<=24	
Reflections collected	54861	
Independent reflections	12109 [R(int) = 0.0643]	
Completeness to theta = 30.51°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9000 and 0.8740	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12109 / 0 / 531	
Goodness-of-fit on F^2	1.073	
Final R indices [I>2sigma(I)]	R1 = 0.0414, wR2 = 0.0942	
R indices (all data)	R1 = 0.0612, wR2 = 0.1024	
Largest diff. peak and hole	0.797 and -0.472 e.Å^{-3}	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for *cis*-**1-(CH_2CHCH_2)$_2$N^{t}Bu**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zr(1)	1857(1)	4712(1)	2587(1)	16(1)
N(1)	3077(1)	6155(1)	247(1)	26(1)
C(1)	2169(1)	3373(1)	2085(1)	19(1)
C(2)	1900(1)	3312(1)	2869(1)	20(1)
C(3)	880(1)	3508(1)	2954(1)	19(1)
C(4)	475(1)	3688(1)	2185(1)	18(1)
C(5)	-507(1)	3886(1)	1875(1)	23(1)
C(6)	-673(1)	3983(1)	1089(1)	25(1)
C(7)	109(1)	3899(1)	569(1)	24(1)
C(8)	1059(1)	3716(1)	837(1)	20(1)
C(9)	1269(1)	3607(1)	1651(1)	18(1)
C(10)	2358(1)	4914(1)	4022(1)	21(1)
C(11)	1335(1)	5135(1)	3906(1)	20(1)
C(12)	1245(1)	5801(1)	3446(1)	19(1)
C(13)	2249(1)	6023(1)	3295(1)	19(1)
C(14)	2618(1)	6665(1)	2901(1)	23(1)
C(15)	3631(1)	6770(1)	2883(1)	28(1)
C(16)	4315(1)	6246(1)	3241(1)	29(1)
C(17)	3991(1)	5620(1)	3616(1)	25(1)
C(18)	2940(1)	5485(1)	3654(1)	20(1)
C(19)	3118(1)	3088(1)	1741(1)	22(1)
C(20)	3980(1)	2990(1)	2349(1)	29(1)
C(21)	2909(1)	2332(1)	1316(1)	34(1)
C(22)	349(1)	3345(1)	3698(1)	22(1)
C(23)	341(2)	2494(1)	3853(1)	44(1)
C(24)	-722(1)	3647(1)	3723(1)	41(1)
C(25)	2734(1)	4333(1)	4619(1)	25(1)
C(26)	2820(2)	4714(1)	5425(1)	41(1)
C(27)	3724(1)	3940(1)	4460(1)	36(1)
C(28)	326(1)	6278(1)	3273(1)	24(1)
C(29)	-617(1)	5824(1)	3072(1)	39(1)

C(30)	161(1)	6811(1)	3958(1)	38(1)
C(31)	1152(1)	5441(1)	1601(1)	20(1)
C(32)	1875(1)	5479(1)	923(1)	21(1)
C(33)	2249(1)	6274(1)	763(1)	24(1)
C(34)	3618(1)	5476(1)	541(1)	31(1)
C(35)	2880(1)	5025(1)	1034(1)	21(1)
C(36)	3229(1)	4953(1)	1896(1)	21(1)
C(37)	3704(1)	6826(1)	89(1)	32(1)
C(38)	4274(2)	7139(1)	816(1)	47(1)
C(39)	3006(2)	7453(1)	-246(1)	54(1)
C(40)	4444(2)	6608(1)	-515(1)	52(1)
C(1S)	7342(2)	6054(2)	1082(2)	101(1)
C(2S)	6624(2)	5693(2)	1618(1)	70(1)
C(3S)	6946(2)	4978(1)	2012(2)	57(1)
C(4S)	6203(2)	4614(1)	2521(1)	57(1)
C(5S)	6547(2)	3922(1)	2909(2)	74(1)

Table S3. Bond lengths [Å] and angles [°] for *cis*-**1-(CH_2CHCH_2)$_2$N^{t}Bu**.

Zr(1)-C(36)	2.2589(15)
Zr(1)-C(31)	2.2765(14)
Zr(1)-C(11)	2.5021(14)
Zr(1)-C(2)	2.5034(14)
Zr(1)-C(10)	2.5300(13)
Zr(1)-C(1)	2.5426(14)
Zr(1)-C(12)	2.5657(14)
Zr(1)-C(3)	2.5717(14)
Zr(1)-C(9)	2.6063(13)
Zr(1)-C(4)	2.6318(13)
Zr(1)-C(18)	2.6367(14)
Zr(1)-C(13)	2.6376(13)
N(1)-C(33)	1.457(2)
N(1)-C(34)	1.466(2)
N(1)-C(37)	1.474(2)
C(1)-C(2)	1.406(2)
C(1)-C(9)	1.4319(19)
C(1)-C(19)	1.503(2)
C(2)-C(3)	1.411(2)
C(3)-C(4)	1.4281(19)
C(3)-C(22)	1.511(2)
C(4)-C(5)	1.4233(19)
C(4)-C(9)	1.435(2)
C(5)-C(6)	1.360(2)
C(6)-C(7)	1.407(2)
C(7)-C(8)	1.356(2)
C(8)-C(9)	1.4156(19)
C(10)-C(11)	1.415(2)
C(10)-C(18)	1.429(2)
C(10)-C(25)	1.509(2)
C(11)-C(12)	1.409(2)
C(12)-C(13)	1.423(2)
C(12)-C(28)	1.495(2)
C(13)-C(14)	1.413(2)

C(13)-C(18)	1.4307(19)
C(14)-C(15)	1.359(2)
C(15)-C(16)	1.409(2)
C(16)-C(17)	1.352(2)
C(17)-C(18)	1.419(2)
C(19)-C(20)	1.514(2)
C(19)-C(21)	1.529(2)
C(22)-C(23)	1.518(2)
C(22)-C(24)	1.518(2)
C(25)-C(27)	1.521(2)
C(25)-C(26)	1.528(2)
C(28)-C(29)	1.508(2)
C(28)-C(30)	1.522(2)
C(31)-C(32)	1.542(2)
C(32)-C(33)	1.512(2)
C(32)-C(35)	1.555(2)
C(34)-C(35)	1.543(2)
C(35)-C(36)	1.525(2)
C(37)-C(40)	1.509(3)
C(37)-C(38)	1.523(2)
C(37)-C(39)	1.529(3)
C(1S)-C(2S)	1.495(4)
C(2S)-C(3S)	1.477(4)
C(3S)-C(4S)	1.491(3)
C(4S)-C(5S)	1.446(3)

C(36)-Zr(1)-C(31)	79.62(5)
C(36)-Zr(1)-C(11)	133.01(5)
C(31)-Zr(1)-C(11)	112.10(5)
C(36)-Zr(1)-C(2)	105.84(5)
C(31)-Zr(1)-C(2)	134.27(5)
C(11)-Zr(1)-C(2)	97.08(5)
C(36)-Zr(1)-C(10)	107.51(5)
C(31)-Zr(1)-C(10)	135.59(5)
C(11)-Zr(1)-C(10)	32.66(5)
C(2)-Zr(1)-C(10)	87.12(5)

C(36)-Zr(1)-C(1)	81.23(5)
C(31)-Zr(1)-C(1)	109.74(5)
C(11)-Zr(1)-C(1)	129.43(5)
C(2)-Zr(1)-C(1)	32.36(5)
C(10)-Zr(1)-C(1)	114.66(5)
C(36)-Zr(1)-C(12)	116.51(5)
C(31)-Zr(1)-C(12)	82.75(5)
C(11)-Zr(1)-C(12)	32.25(4)
C(2)-Zr(1)-C(12)	128.75(5)
C(10)-Zr(1)-C(12)	54.35(4)
C(1)-Zr(1)-C(12)	160.52(5)
C(36)-Zr(1)-C(3)	135.25(5)
C(31)-Zr(1)-C(3)	116.66(5)
C(11)-Zr(1)-C(3)	81.87(5)
C(2)-Zr(1)-C(3)	32.24(5)
C(10)-Zr(1)-C(3)	89.44(5)
C(1)-Zr(1)-C(3)	54.25(5)
C(12)-Zr(1)-C(3)	107.11(5)
C(36)-Zr(1)-C(9)	92.42(5)
C(31)-Zr(1)-C(9)	82.29(5)
C(11)-Zr(1)-C(9)	133.24(5)
C(2)-Zr(1)-C(9)	52.50(4)
C(10)-Zr(1)-C(9)	138.93(4)
C(1)-Zr(1)-C(9)	32.26(4)
C(12)-Zr(1)-C(9)	144.19(4)
C(3)-Zr(1)-C(9)	53.14(4)
C(36)-Zr(1)-C(4)	124.06(5)
C(31)-Zr(1)-C(4)	86.37(5)
C(11)-Zr(1)-C(4)	102.50(5)
C(2)-Zr(1)-C(4)	52.34(4)
C(10)-Zr(1)-C(4)	119.56(5)
C(1)-Zr(1)-C(4)	53.43(4)
C(12)-Zr(1)-C(4)	114.89(4)
C(3)-Zr(1)-C(4)	31.83(4)
C(9)-Zr(1)-C(4)	31.80(4)
C(36)-Zr(1)-C(18)	80.78(5)

C(31)-Zr(1)-C(18)	114.20(5)
C(11)-Zr(1)-C(18)	52.53(5)
C(2)-Zr(1)-C(18)	111.48(4)
C(10)-Zr(1)-C(18)	32.03(5)
C(1)-Zr(1)-C(18)	128.06(4)
C(12)-Zr(1)-C(18)	53.07(4)
C(3)-Zr(1)-C(18)	121.18(4)
C(9)-Zr(1)-C(18)	160.32(4)
C(4)-Zr(1)-C(18)	151.49(4)
C(36)-Zr(1)-C(13)	86.07(5)
C(31)-Zr(1)-C(13)	84.98(5)
C(11)-Zr(1)-C(13)	52.09(4)
C(2)-Zr(1)-C(13)	139.96(4)
C(10)-Zr(1)-C(13)	52.98(4)
C(1)-Zr(1)-C(13)	158.28(4)
C(12)-Zr(1)-C(13)	31.71(4)
C(3)-Zr(1)-C(13)	133.96(4)
C(9)-Zr(1)-C(13)	167.25(4)
C(4)-Zr(1)-C(13)	146.39(4)
C(18)-Zr(1)-C(13)	31.48(4)
C(33)-N(1)-C(34)	106.26(12)
C(33)-N(1)-C(37)	116.47(13)
C(34)-N(1)-C(37)	116.14(13)
C(2)-C(1)-C(9)	105.66(12)
C(2)-C(1)-C(19)	127.23(13)
C(9)-C(1)-C(19)	125.85(13)
C(2)-C(1)-Zr(1)	72.29(8)
C(9)-C(1)-Zr(1)	76.32(8)
C(19)-C(1)-Zr(1)	126.41(9)
C(1)-C(2)-C(3)	111.73(12)
C(1)-C(2)-Zr(1)	75.35(8)
C(3)-C(2)-Zr(1)	76.54(8)
C(2)-C(3)-C(4)	106.05(12)
C(2)-C(3)-C(22)	122.10(12)
C(4)-C(3)-C(22)	130.17(13)
C(2)-C(3)-Zr(1)	71.22(8)

C(4)-C(3)-Zr(1)	76.41(8)
C(22)-C(3)-Zr(1)	128.51(9)
C(5)-C(4)-C(3)	133.61(14)
C(5)-C(4)-C(9)	118.33(12)
C(3)-C(4)-C(9)	108.00(12)
C(5)-C(4)-Zr(1)	122.83(10)
C(3)-C(4)-Zr(1)	71.76(8)
C(9)-C(4)-Zr(1)	73.12(7)
C(6)-C(5)-C(4)	119.80(14)
C(5)-C(6)-C(7)	121.43(13)
C(8)-C(7)-C(6)	120.95(14)
C(7)-C(8)-C(9)	119.69(14)
C(8)-C(9)-C(1)	131.56(13)
C(8)-C(9)-C(4)	119.78(12)
C(1)-C(9)-C(4)	108.54(12)
C(8)-C(9)-Zr(1)	122.65(9)
C(1)-C(9)-Zr(1)	71.42(8)
C(4)-C(9)-Zr(1)	75.08(8)
C(11)-C(10)-C(18)	106.39(12)
C(11)-C(10)-C(25)	124.05(13)
C(18)-C(10)-C(25)	127.18(13)
C(11)-C(10)-Zr(1)	72.59(8)
C(18)-C(10)-Zr(1)	78.10(8)
C(25)-C(10)-Zr(1)	128.37(10)
C(12)-C(11)-C(10)	110.99(13)
C(12)-C(11)-Zr(1)	76.36(8)
C(10)-C(11)-Zr(1)	74.75(8)
C(11)-C(12)-C(13)	105.89(12)
C(11)-C(12)-C(28)	128.31(13)
C(13)-C(12)-C(28)	124.81(13)
C(11)-C(12)-Zr(1)	71.39(8)
C(13)-C(12)-Zr(1)	76.93(8)
C(28)-C(12)-Zr(1)	125.65(9)
C(14)-C(13)-C(12)	130.85(13)
C(14)-C(13)-C(18)	119.98(13)
C(12)-C(13)-C(18)	109.11(12)

C(14)-C(13)-Zr(1)	122.82(10)
C(12)-C(13)-Zr(1)	71.36(8)
C(18)-C(13)-Zr(1)	74.23(8)
C(15)-C(14)-C(13)	119.10(14)
C(14)-C(15)-C(16)	121.11(15)
C(17)-C(16)-C(15)	121.51(15)
C(16)-C(17)-C(18)	119.62(14)
C(17)-C(18)-C(10)	133.72(14)
C(17)-C(18)-C(13)	118.67(13)
C(10)-C(18)-C(13)	107.54(12)
C(17)-C(18)-Zr(1)	123.78(10)
C(10)-C(18)-Zr(1)	69.87(8)
C(13)-C(18)-Zr(1)	74.30(8)
C(1)-C(19)-C(20)	112.81(12)
C(1)-C(19)-C(21)	109.80(12)
C(20)-C(19)-C(21)	109.84(13)
C(3)-C(22)-C(23)	109.94(13)
C(3)-C(22)-C(24)	115.81(13)
C(23)-C(22)-C(24)	108.87(15)
C(10)-C(25)-C(27)	116.34(13)
C(10)-C(25)-C(26)	108.64(13)
C(27)-C(25)-C(26)	109.51(14)
C(12)-C(28)-C(29)	113.97(13)
C(12)-C(28)-C(30)	109.89(12)
C(29)-C(28)-C(30)	110.40(14)
C(32)-C(31)-Zr(1)	109.36(9)
C(33)-C(32)-C(31)	113.48(12)
C(33)-C(32)-C(35)	101.94(12)
C(31)-C(32)-C(35)	116.65(12)
N(1)-C(33)-C(32)	104.01(12)
N(1)-C(34)-C(35)	106.90(13)
C(36)-C(35)-C(34)	113.57(13)
C(36)-C(35)-C(32)	112.11(12)
C(34)-C(35)-C(32)	103.58(12)
C(35)-C(36)-Zr(1)	107.85(9)
N(1)-C(37)-C(40)	108.38(15)

N(1)-C(37)-C(38)	113.59(13)
C(40)-C(37)-C(38)	109.59(15)
N(1)-C(37)-C(39)	107.83(14)
C(40)-C(37)-C(39)	109.27(16)
C(38)-C(37)-C(39)	108.10(16)
C(3S)-C(2S)-C(1S)	117.5(2)
C(2S)-C(3S)-C(4S)	116.4(2)
C(5S)-C(4S)-C(3S)	115.1(2)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for dp14. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zr(1)	15(1)	15(1)	17(1)	0(1)	1(1)	0(1)
N(1)	26(1)	28(1)	23(1)	6(1)	4(1)	-5(1)
C(1)	18(1)	15(1)	24(1)	-1(1)	2(1)	0(1)
C(2)	20(1)	16(1)	22(1)	2(1)	-1(1)	1(1)
C(3)	18(1)	17(1)	22(1)	1(1)	3(1)	-2(1)
C(4)	16(1)	15(1)	23(1)	-1(1)	1(1)	-2(1)
C(5)	16(1)	24(1)	28(1)	-2(1)	3(1)	-2(1)
C(6)	18(1)	27(1)	29(1)	1(1)	-4(1)	0(1)
C(7)	26(1)	24(1)	22(1)	-1(1)	-3(1)	-3(1)
C(8)	21(1)	19(1)	21(1)	-3(1)	4(1)	-4(1)
C(9)	18(1)	14(1)	22(1)	-1(1)	2(1)	-1(1)
C(10)	22(1)	22(1)	18(1)	-1(1)	0(1)	1(1)
C(11)	21(1)	20(1)	19(1)	-1(1)	4(1)	-1(1)
C(12)	20(1)	18(1)	20(1)	-3(1)	1(1)	1(1)
C(13)	20(1)	17(1)	20(1)	-3(1)	1(1)	0(1)
C(14)	29(1)	18(1)	22(1)	-2(1)	-1(1)	-2(1)
C(15)	33(1)	24(1)	28(1)	-1(1)	3(1)	-12(1)
C(16)	20(1)	34(1)	31(1)	-7(1)	0(1)	-8(1)
C(17)	21(1)	27(1)	26(1)	-2(1)	-3(1)	-2(1)
C(18)	20(1)	21(1)	19(1)	-3(1)	0(1)	-1(1)
C(19)	19(1)	20(1)	28(1)	-2(1)	4(1)	2(1)
C(20)	19(1)	33(1)	36(1)	0(1)	1(1)	7(1)
C(21)	29(1)	27(1)	45(1)	-12(1)	7(1)	3(1)
C(22)	22(1)	23(1)	21(1)	1(1)	4(1)	-5(1)
C(23)	66(1)	27(1)	41(1)	6(1)	21(1)	-8(1)
C(24)	26(1)	63(1)	34(1)	12(1)	11(1)	4(1)
C(25)	27(1)	26(1)	23(1)	3(1)	-1(1)	1(1)
C(26)	57(1)	44(1)	21(1)	2(1)	-1(1)	12(1)
C(27)	36(1)	37(1)	34(1)	6(1)	-4(1)	12(1)
C(28)	23(1)	24(1)	25(1)	1(1)	3(1)	7(1)
C(29)	22(1)	40(1)	54(1)	-13(1)	-2(1)	7(1)

C(30)	40(1)	31(1)	43(1)	-11(1)	1(1)	14(1)
C(31)	19(1)	20(1)	22(1)	2(1)	2(1)	0(1)
C(32)	20(1)	23(1)	19(1)	3(1)	0(1)	-1(1)
C(33)	23(1)	24(1)	25(1)	5(1)	2(1)	-2(1)
C(34)	27(1)	32(1)	34(1)	6(1)	10(1)	0(1)
C(35)	20(1)	21(1)	24(1)	1(1)	6(1)	-1(1)
C(36)	18(1)	20(1)	25(1)	-1(1)	2(1)	-1(1)
C(37)	33(1)	35(1)	28(1)	8(1)	3(1)	-12(1)
C(38)	52(1)	47(1)	41(1)	1(1)	4(1)	-26(1)
C(39)	58(1)	43(1)	63(1)	29(1)	4(1)	-11(1)
C(40)	54(1)	59(1)	44(1)	1(1)	24(1)	-24(1)
C(1S)	93(2)	122(2)	88(2)	-2(2)	8(2)	-62(2)
C(2S)	68(2)	88(2)	54(1)	-6(1)	2(1)	10(2)
C(3S)	33(1)	58(1)	81(2)	-22(1)	4(1)	-9(1)
C(4S)	37(1)	74(2)	61(1)	-5(1)	1(1)	6(1)
C(5S)	58(2)	64(2)	97(2)	-8(2)	-14(1)	-7(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for *cis*-**1-$(CH_2CHCH_2)_2N^tBu$**.

	x	y	z	U(eq)
H(2)	2357(12)	3142(9)	3270(9)	19(4)
H(5)	-1019(13)	3954(9)	2190(9)	22(4)
H(6)	-1336(12)	4087(9)	894(9)	22(4)
H(7)	-23(12)	3974(9)	56(10)	27(4)
H(8)	1546(12)	3651(8)	505(9)	18(4)
H(11)	810(13)	4858(9)	4118(9)	19(4)
H(14)	2177(13)	7024(9)	2669(9)	24(4)
H(15)	3873(13)	7156(9)	2647(10)	26(4)
H(16)	5037(14)	6352(10)	3244(10)	38(5)
H(17)	4475(14)	5282(9)	3847(10)	30(5)
H(19)	3344(11)	3463(8)	1354(8)	9(3)
H(20A)	4100	3473	2628	43
H(20B)	4592	2841	2089	43
H(20C)	3807	2594	2723	43
H(21A)	2714	1947	1695	51
H(21B)	3520	2164	1066	51
H(21C)	2361	2401	916	51
H(22)	715(12)	3542(9)	4119(9)	19(4)
H(23A)	-44	2235	3426	66
H(23B)	27	2394	4350	66
H(23C)	1036	2301	3884	66
H(24A)	-738	4183	3564	61
H(24B)	-951	3601	4258	61
H(24C)	-1169	3350	3364	61
H(25)	2243(13)	3953(10)	4664(9)	29(5)
H(26A)	3320	5125	5420	61
H(26B)	3033	4336	5823	61
H(26C)	2162	4925	5549	61
H(27A)	3728	3801	3904	54
H(27B)	3796	3479	4783	54

H(27C)	4288	4286	4591	54
H(28)	473(12)	6587(9)	2836(9)	19(4)
H(29A)	-504	5492	2623	58
H(29B)	-1177	6172	2938	58
H(29C)	-783	5512	3524	58
H(30A)	-2	6511	4419	57
H(30B)	-399	7158	3819	57
H(30C)	776	7107	4077	57
H(31B)	543(13)	5234(9)	1437(10)	25(4)
H(31A)	975(13)	5947(10)	1779(10)	29(5)
H(32)	1503(13)	5295(8)	431(10)	26(4)
H(33B)	1724(11)	6591(8)	521(8)	11(4)
H(33A)	2469(13)	6513(9)	1293(10)	29(4)
H(34B)	4208(13)	5601(9)	848(10)	25(4)
H(34A)	3872(16)	5161(11)	92(12)	51(6)
H(35)	2800(11)	4520(8)	805(9)	13(4)
H(36B)	3797(14)	4630(9)	1973(10)	27(5)
H(36A)	3425(13)	5439(9)	2067(10)	28(5)
H(38A)	3791	7303	1197	70
H(38B)	4687	7575	669	70
H(38C)	4712	6741	1049	70
H(39A)	2584	7249	-685	82
H(39B)	3412	7877	-430	82
H(39C)	2573	7634	164	82
H(40A)	4919	6229	-291	77
H(40B)	4817	7061	-670	77
H(40C)	4077	6392	-976	77
H(1SA)	7041	6521	859	152
H(1SB)	7482	5699	658	152
H(1SC)	7973	6179	1378	152
H(2SA)	6474	6069	2028	84
H(2SB)	5984	5591	1311	84
H(3SA)	7571	5082	2337	69
H(3SB)	7120	4606	1605	69
H(4SA)	6020	4986	2926	69
H(4SB)	5582	4498	2196	69

H(5SA)	6014	3725	3232	110
H(5SB)	7153	4030	3243	110
H(5SC)	6706	3540	2514	110

Table S6. Crystal data and structure refinement for djk3 = *cis*-**3-(CH_2CHCH_2)$_2$N^{t}Bu**.

Identification code	djk3 = *cis*-**3-(CH_2CHCH_2)$_2$N^{t}Bu**	
Empirical formula	C30 H49 N Si Ti	
Formula weight	499.69	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 17.6335(8) Å	α= 90°.
	b = 9.8554(6) Å	β= 115.665(3)°.
	c = 17.9416(11) Å	γ = 90°.
Volume	2810.4(3) Å^3	
Z	4	
Density (calculated)	1.181 Mg/m^3	
Absorption coefficient	0.365 mm^{-1}	
F(000)	1088	
Crystal size	0.35 x 0.20 x 0.15 mm^3	
Theta range for data collection	2.28 to 28.28°.	
Index ranges	-23<=h<=22, -13<=k<=12, -23<=l<=23	
Reflections collected	26243	
Independent reflections	6956 [R(int) = 0.0559]	
Completeness to theta = 28.28°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9473 and 0.8828	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6956 / 0 / 494	
Goodness-of-fit on F^2	1.019	
Final R indices [I>2sigma(I)]	R1 = 0.0457, wR2 = 0.1033	
R indices (all data)	R1 = 0.0722, wR2 = 0.1170	
Largest diff. peak and hole	0.529 and -0.279 e.Å^{-3}	

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for *cis*-**3-(CH_2CHCH_2)$_2$N^{t}Bu**.U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ti(1)	3267(1)	2157(1)	4783(1)	16(1)
Si(1)	4712(1)	2934(1)	6569(1)	20(1)
N(1)	1288(1)	134(2)	2455(1)	28(1)
C(1)	4270(1)	3811(2)	5549(1)	18(1)
C(2)	3462(1)	4461(2)	5188(1)	20(1)
C(3)	3193(1)	4559(2)	4327(1)	21(1)
C(4)	3809(1)	3947(2)	4136(1)	20(1)
C(5)	4463(1)	3469(2)	4880(1)	18(1)
C(6)	3927(1)	1537(2)	6201(1)	20(1)
C(7)	3058(1)	1712(2)	6004(1)	22(1)
C(8)	2584(1)	652(2)	5482(1)	23(1)
C(9)	3147(1)	-130(2)	5304(1)	23(1)
C(10)	3961(1)	412(2)	5737(1)	22(1)
C(11)	3001(1)	5126(2)	5623(1)	29(1)
C(12)	2461(1)	5387(2)	3753(1)	28(1)
C(13)	3838(1)	3948(2)	3315(1)	26(1)
C(14)	5245(1)	2800(2)	4934(1)	24(1)
C(15)	5811(1)	2312(2)	6933(1)	30(1)
C(16)	4661(1)	3919(2)	7423(1)	29(1)
C(17)	1689(1)	276(2)	5320(1)	30(1)
C(18)	1751(1)	-342(3)	6126(1)	48(1)
C(19)	1115(1)	1510(2)	5116(1)	39(1)
C(20)	1310(1)	-775(2)	4632(1)	39(1)
C(21)	2013(1)	2216(2)	3807(1)	23(1)
C(22)	2099(1)	2077(2)	3003(1)	24(1)
C(23)	2717(1)	928(2)	3076(1)	25(1)
C(24)	3503(1)	897(2)	3899(1)	21(1)
C(25)	2168(1)	-333(2)	2898(1)	30(1)
C(26)	1298(1)	1570(2)	2288(1)	29(1)
C(27)	711(1)	-734(2)	1777(1)	33(1)
C(28)	-165(1)	-104(3)	1453(2)	50(1)

C(29)	702(1)	-2114(2)	2140(1)	43(1)
C(30)	959(1)	-865(2)	1060(1)	44(1)

Table S8. Bond lengths [Å] and angles [°] for *cis*-**3-(CH_2CHCH_2)$_2$N^{t}Bu**.

Ti(1)-C(21)	2.1470(15)
Ti(1)-C(24)	2.1920(17)
Ti(1)-C(1)	2.3595(14)
Ti(1)-C(10)	2.3597(16)
Ti(1)-C(2)	2.3632(16)
Ti(1)-C(6)	2.3732(15)
Ti(1)-C(7)	2.4124(17)
Ti(1)-C(5)	2.4148(15)
Ti(1)-C(9)	2.4837(17)
Ti(1)-C(3)	2.4898(16)
Ti(1)-C(4)	2.5177(16)
Ti(1)-C(8)	2.5557(17)
Si(1)-C(16)	1.8489(19)
Si(1)-C(6)	1.8587(16)
Si(1)-C(1)	1.8623(15)
Si(1)-C(15)	1.8609(18)
N(1)-C(26)	1.449(2)
N(1)-C(27)	1.474(2)
N(1)-C(25)	1.477(2)
C(1)-C(5)	1.422(2)
C(1)-C(2)	1.434(2)
C(2)-C(3)	1.408(2)
C(2)-C(11)	1.500(2)
C(3)-C(4)	1.410(2)
C(3)-C(12)	1.497(2)
C(4)-C(5)	1.414(2)
C(4)-C(13)	1.495(2)
C(5)-C(14)	1.494(2)
C(6)-C(10)	1.403(2)
C(6)-C(7)	1.425(2)
C(7)-C(8)	1.410(2)
C(8)-C(9)	1.398(2)
C(8)-C(17)	1.522(2)
C(9)-C(10)	1.409(2)

C(17)-C(19)	1.522(3)
C(17)-C(20)	1.525(3)
C(17)-C(18)	1.528(3)
C(21)-C(22)	1.520(3)
C(22)-C(26)	1.524(2)
C(22)-C(23)	1.537(2)
C(23)-C(25)	1.522(3)
C(23)-C(24)	1.525(2)
C(27)-C(29)	1.511(3)
C(27)-C(30)	1.531(3)
C(27)-C(28)	1.528(3)

C(21)-Ti(1)-C(24)	82.86(6)
C(21)-Ti(1)-C(1)	134.72(6)
C(24)-Ti(1)-C(1)	118.93(6)
C(21)-Ti(1)-C(10)	129.73(6)
C(24)-Ti(1)-C(10)	84.89(6)
C(1)-Ti(1)-C(10)	93.38(5)
C(21)-Ti(1)-C(2)	100.72(6)
C(24)-Ti(1)-C(2)	135.93(6)
C(1)-Ti(1)-C(2)	35.36(5)
C(10)-Ti(1)-C(2)	121.11(5)
C(21)-Ti(1)-C(6)	137.34(6)
C(24)-Ti(1)-C(6)	118.13(6)
C(1)-Ti(1)-C(6)	70.01(5)
C(10)-Ti(1)-C(6)	34.48(6)
C(2)-Ti(1)-C(6)	88.84(6)
C(21)-Ti(1)-C(7)	103.74(6)
C(24)-Ti(1)-C(7)	134.88(6)
C(1)-Ti(1)-C(7)	88.14(5)
C(10)-Ti(1)-C(7)	56.26(6)
C(2)-Ti(1)-C(7)	87.42(6)
C(6)-Ti(1)-C(7)	34.65(5)
C(21)-Ti(1)-C(5)	127.08(6)
C(24)-Ti(1)-C(5)	85.54(6)
C(1)-Ti(1)-C(5)	34.63(5)

C(10)-Ti(1)-C(5)	100.12(5)
C(2)-Ti(1)-C(5)	57.09(5)
C(6)-Ti(1)-C(5)	93.05(5)
C(7)-Ti(1)-C(5)	120.24(5)
C(21)-Ti(1)-C(9)	96.08(6)
C(24)-Ti(1)-C(9)	80.34(6)
C(1)-Ti(1)-C(9)	124.94(5)
C(10)-Ti(1)-C(9)	33.71(5)
C(2)-Ti(1)-C(9)	141.38(6)
C(6)-Ti(1)-C(9)	56.32(5)
C(7)-Ti(1)-C(9)	54.72(6)
C(5)-Ti(1)-C(9)	132.32(5)
C(21)-Ti(1)-C(3)	79.45(6)
C(24)-Ti(1)-C(3)	107.48(6)
C(1)-Ti(1)-C(3)	56.89(5)
C(10)-Ti(1)-C(3)	150.24(5)
C(2)-Ti(1)-C(3)	33.60(5)
C(6)-Ti(1)-C(3)	121.91(5)
C(7)-Ti(1)-C(3)	117.63(6)
C(5)-Ti(1)-C(3)	55.55(5)
C(9)-Ti(1)-C(3)	170.24(6)
C(21)-Ti(1)-C(4)	93.85(6)
C(24)-Ti(1)-C(4)	80.43(6)
C(1)-Ti(1)-C(4)	56.35(5)
C(10)-Ti(1)-C(4)	131.60(5)
C(2)-Ti(1)-C(4)	55.56(6)
C(6)-Ti(1)-C(4)	124.55(5)
C(7)-Ti(1)-C(4)	141.62(6)
C(5)-Ti(1)-C(4)	33.24(5)
C(9)-Ti(1)-C(4)	157.04(6)
C(3)-Ti(1)-C(4)	32.71(5)
C(21)-Ti(1)-C(8)	83.03(6)
C(24)-Ti(1)-C(8)	107.70(6)
C(1)-Ti(1)-C(8)	120.59(5)
C(10)-Ti(1)-C(8)	55.10(5)
C(2)-Ti(1)-C(8)	116.35(6)

C(6)-Ti(1)-C(8)	56.02(5)
C(7)-Ti(1)-C(8)	32.82(5)
C(5)-Ti(1)-C(8)	149.08(5)
C(9)-Ti(1)-C(8)	32.18(6)
C(3)-Ti(1)-C(8)	138.09(6)
C(4)-Ti(1)-C(8)	170.75(6)
C(16)-Si(1)-C(6)	112.80(8)
C(16)-Si(1)-C(1)	114.89(8)
C(6)-Si(1)-C(1)	93.71(7)
C(16)-Si(1)-C(15)	107.36(8)
C(6)-Si(1)-C(15)	112.51(8)
C(1)-Si(1)-C(15)	115.29(8)
C(26)-N(1)-C(27)	117.52(13)
C(26)-N(1)-C(25)	108.15(13)
C(27)-N(1)-C(25)	116.90(15)
C(5)-C(1)-C(2)	106.15(13)
C(5)-C(1)-Si(1)	124.58(11)
C(2)-C(1)-Si(1)	124.21(12)
C(5)-C(1)-Ti(1)	74.81(8)
C(2)-C(1)-Ti(1)	72.46(8)
Si(1)-C(1)-Ti(1)	98.06(7)
C(3)-C(2)-C(1)	108.89(14)
C(3)-C(2)-C(11)	122.62(14)
C(1)-C(2)-C(11)	127.98(14)
C(3)-C(2)-Ti(1)	78.14(9)
C(1)-C(2)-Ti(1)	72.18(9)
C(11)-C(2)-Ti(1)	122.70(12)
C(2)-C(3)-C(4)	107.94(13)
C(2)-C(3)-C(12)	124.96(16)
C(4)-C(3)-C(12)	126.25(15)
C(2)-C(3)-Ti(1)	68.26(9)
C(4)-C(3)-Ti(1)	74.74(9)
C(12)-C(3)-Ti(1)	130.68(11)
C(3)-C(4)-C(5)	108.11(14)
C(3)-C(4)-C(13)	126.75(14)
C(5)-C(4)-C(13)	124.71(15)

C(3)-C(4)-Ti(1)	72.56(9)
C(5)-C(4)-Ti(1)	69.38(9)
C(13)-C(4)-Ti(1)	129.54(11)
C(4)-C(5)-C(1)	108.85(13)
C(4)-C(5)-C(14)	124.04(15)
C(1)-C(5)-C(14)	126.99(13)
C(4)-C(5)-Ti(1)	77.38(9)
C(1)-C(5)-Ti(1)	70.56(9)
C(14)-C(5)-Ti(1)	121.41(11)
C(10)-C(6)-C(7)	105.44(13)
C(10)-C(6)-Si(1)	125.39(13)
C(7)-C(6)-Si(1)	123.58(13)
C(10)-C(6)-Ti(1)	72.23(9)
C(7)-C(6)-Ti(1)	74.18(9)
Si(1)-C(6)-Ti(1)	97.69(7)
C(8)-C(7)-C(6)	109.83(15)
C(8)-C(7)-Ti(1)	79.18(10)
C(6)-C(7)-Ti(1)	71.17(9)
C(9)-C(8)-C(7)	106.55(14)
C(9)-C(8)-C(17)	126.99(16)
C(7)-C(8)-C(17)	125.13(16)
C(9)-C(8)-Ti(1)	71.08(10)
C(7)-C(8)-Ti(1)	68.00(9)
C(17)-C(8)-Ti(1)	135.84(11)
C(8)-C(9)-C(10)	108.62(15)
C(8)-C(9)-Ti(1)	76.75(10)
C(10)-C(9)-Ti(1)	68.32(9)
C(6)-C(10)-C(9)	109.35(15)
C(6)-C(10)-Ti(1)	73.28(9)
C(9)-C(10)-Ti(1)	77.98(9)
C(19)-C(17)-C(8)	112.24(16)
C(19)-C(17)-C(20)	109.58(15)
C(8)-C(17)-C(20)	112.05(16)
C(19)-C(17)-C(18)	108.20(17)
C(8)-C(17)-C(18)	105.82(13)
C(20)-C(17)-C(18)	108.76(17)

C(22)-C(21)-Ti(1)	106.29(11)
C(21)-C(22)-C(26)	113.01(15)
C(21)-C(22)-C(23)	110.15(13)
C(26)-C(22)-C(23)	101.23(14)
C(25)-C(23)-C(24)	114.53(14)
C(25)-C(23)-C(22)	102.73(13)
C(24)-C(23)-C(22)	114.23(14)
C(23)-C(24)-Ti(1)	108.15(11)
N(1)-C(25)-C(23)	106.46(15)
N(1)-C(26)-C(22)	103.66(13)
N(1)-C(27)-C(29)	107.38(15)
N(1)-C(27)-C(30)	113.35(16)
C(29)-C(27)-C(30)	110.23(18)
N(1)-C(27)-C(28)	107.53(16)
C(29)-C(27)-C(28)	109.33(18)
C(30)-C(27)-C(28)	108.94(17)

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters ($Å^2$x 10^3) for *cis*-**3-$(CH_2CHCH_2)_2N^tBu$**. 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}
Ti(1)	16(1)	16(1)	15(1)	0(1)	6(1)	-1(1)
Si(1)	20(1)	21(1)	16(1)	-2(1)	6(1)	-3(1)
N(1)	24(1)	27(1)	26(1)	-4(1)	6(1)	-4(1)
C(1)	17(1)	15(1)	20(1)	-3(1)	8(1)	-4(1)
C(2)	19(1)	17(1)	23(1)	-4(1)	10(1)	-2(1)
C(3)	21(1)	15(1)	24(1)	0(1)	8(1)	-2(1)
C(4)	22(1)	18(1)	20(1)	1(1)	9(1)	-5(1)
C(5)	17(1)	16(1)	20(1)	-1(1)	8(1)	-4(1)
C(6)	23(1)	20(1)	15(1)	2(1)	6(1)	-2(1)
C(7)	25(1)	24(1)	22(1)	0(1)	14(1)	-4(1)
C(8)	25(1)	23(1)	18(1)	3(1)	8(1)	-5(1)
C(9)	30(1)	16(1)	20(1)	1(1)	8(1)	-5(1)
C(10)	22(1)	21(1)	20(1)	5(1)	6(1)	2(1)
C(11)	31(1)	28(1)	33(1)	-4(1)	18(1)	3(1)
C(12)	27(1)	21(1)	32(1)	5(1)	8(1)	3(1)
C(13)	31(1)	28(1)	20(1)	1(1)	12(1)	-5(1)
C(14)	23(1)	24(1)	28(1)	-3(1)	13(1)	-1(1)
C(15)	24(1)	32(1)	28(1)	1(1)	7(1)	0(1)
C(16)	33(1)	38(1)	20(1)	-7(1)	14(1)	-10(1)
C(17)	28(1)	38(1)	26(1)	1(1)	14(1)	-11(1)
C(18)	43(1)	68(2)	36(1)	9(1)	19(1)	-20(1)
C(19)	28(1)	54(1)	37(1)	-6(1)	18(1)	-6(1)
C(20)	33(1)	41(1)	38(1)	-4(1)	12(1)	-18(1)
C(21)	19(1)	22(1)	26(1)	1(1)	7(1)	-3(1)
C(22)	22(1)	23(1)	22(1)	0(1)	6(1)	-2(1)
C(23)	25(1)	28(1)	21(1)	-5(1)	8(1)	-2(1)
C(24)	21(1)	20(1)	22(1)	-2(1)	10(1)	1(1)
C(25)	24(1)	31(1)	31(1)	-5(1)	7(1)	-2(1)
C(26)	26(1)	30(1)	23(1)	2(1)	4(1)	-1(1)
C(27)	24(1)	34(1)	34(1)	-10(1)	6(1)	-7(1)
C(28)	24(1)	49(1)	60(1)	-13(1)	4(1)	-7(1)

C(29)	40(1)	40(1)	45(1)	-10(1)	14(1)	-13(1)
C(30)	47(1)	47(1)	32(1)	-11(1)	11(1)	-9(1)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for *cis*-**3-$(CH_2CHCH_2)_2N^tBu$**.

	x	y	z	U(eq)
H(7)	2843(10)	2395(19)	6212(11)	25(5)
H(9)	3009(9)	-876(17)	4961(10)	16(4)
H(10)	4438(10)	101(18)	5705(10)	19(4)
H(11C)	3069(13)	6080(20)	5629(13)	54(7)
H(11B)	2406(12)	4990(20)	5331(13)	51(6)
H(11A)	3175(12)	4870(20)	6156(13)	46(6)
H(12C)	2055(14)	5410(30)	3926(14)	63(8)
H(12B)	2259(14)	5180(30)	3214(16)	76(8)
H(12A)	2619(12)	6300(20)	3777(13)	51(7)
H(13C)	3418(11)	4540(20)	2940(12)	41(6)
H(13B)	4379(12)	4340(20)	3368(12)	41(6)
H(13A)	3771(13)	3070(20)	3086(13)	52(7)
H(14C)	5314(11)	1940(20)	5145(11)	30(5)
H(14B)	5245(11)	2710(20)	4430(12)	37(6)
H(14A)	5728(13)	3260(20)	5267(13)	50(6)
H(15C)	5866(11)	1600(20)	6653(12)	37(6)
H(15B)	6211(12)	3020(20)	6934(13)	46(6)
H(15A)	5963(13)	2040(20)	7474(14)	53(7)
H(16C)	4079(12)	4070(20)	7371(12)	45(6)
H(16B)	4939(13)	3420(20)	7917(13)	53(7)
H(16A)	4930(12)	4720(20)	7476(12)	47(6)
H(18C)	2100(11)	-1110(20)	6248(11)	33(5)
H(18B)	1172(13)	-630(20)	6074(13)	57(7)
H(18A)	1966(13)	400(20)	6592(14)	57(7)
H(19C)	1314(13)	2060(20)	5533(14)	48(6)
H(19B)	992(13)	1910(20)	4539(14)	57(7)
H(19A)	584(14)	1200(30)	5043(14)	64(7)
H(20C)	1272(10)	-418(19)	4106(11)	28(5)
H(20B)	1607(12)	-1610(20)	4789(13)	42(6)
H(20A)	736(13)	-990(20)	4548(13)	52(6)

H(21B)	1679(11)	2977(19)	3804(11)	27(5)
H(21A)	1707(11)	1480(20)	3851(11)	35(5)
H(22)	2272(10)	2940(18)	2848(11)	23(5)
H(23)	2868(11)	990(20)	2562(12)	39(6)
H(24B)	3633(10)	18(19)	4068(11)	26(5)
H(24A)	3997(11)	1200(20)	3830(11)	36(5)
H(25)	2331(11)	-940(20)	2561(12)	37(6)
H(25B)	2283(11)	-830(20)	3446(12)	36(5)
H(26)	777(10)	2028(16)	2263(10)	15(4)
H(26B)	1320(11)	1700(20)	1763(12)	39(6)
H(28C)	-184(12)	730(20)	1114(13)	46(6)
H(28B)	-587(12)	-740(20)	1020(13)	48(6)
H(28A)	-305(14)	30(30)	1915(15)	66(8)
H(29C)	309(13)	-2680(20)	1767(13)	49(6)
H(29B)	559(12)	-2010(20)	2613(13)	42(6)
H(29A)	1262(15)	-2570(30)	2328(16)	70(8)
H(30C)	1516(13)	-1250(20)	1249(13)	52(7)
H(30B)	941(14)	20(30)	832(15)	64(8)
H(30A)	602(13)	-1420(20)	648(14)	56(7)