Supporting Information for:

Stereoselective Ring-Opening Polymerization of *meso*-Lactide: Synthesis of Syndiotactic Poly(lactic acid)

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General Considerations.

All reactions with air-and/or water-sensitive compounds were carried out under dry nitrogen using a Braun Labmaster drybox or standard Schlenk line techniques. NMR spectra were recorded on a Bruker AF300 (^{1}H, 300 MHz; ^{13}C, 75 MHz) spectrometer, and referenced versus residual solvent shifts. Gel permeation chromatography (GPC) analyses were carried out using a Waters instrument (M510 pump, U6K injector) equipped with Waters UV486 and Milton Roy differential refractive index detectors, and four 5 μm PL Gel columns (Polymer Laboratories; 100 Å, 500 Å, 1000 Å, and Mixed C porosities) in series. The GPC columns were eluted with tetrahydrofuran at 45°C at 1ml/min and were calibrated using 23 monodisperse polystyrene standards. Crystallographic data were collected using a SMART CCD Area Detector System (Mo K_α, λ = 0.71073Å), and frames were integrated with the Siemens SAINT program. DSC analyses were performed on a Seiko DSC 220C instrument using EXSTAR 6000 processing software. The measurements were made in aluminum crimped pans under nitrogen with a heating rate of 10 °C per minute. The reported values originate from the second heating scan. Elemental analysis was performed by Galbraith Laboratories.

Materials.

Toluene was distilled from sodium benzophenone ketyl, hexaned from $LiAlH_4$, and CH_2Cl_2 from CaH_2; residual gases were removed using a freeze-pump-thaw technique. *Meso*-lactide was

synthesized as described in the literature (Entenmann, G.; Bendix, D. (Boehringer Ingelheim), Ger. Offen. DE 3,820,299 (1988)) and was determined to be greater that 99% pure by ^{1}H NMR. Aluminum isopropoxide was distilled under vacuum immediately before use. (-)-(**2**) was synthesized according to a published procedure (Bernardo, K. D.; Robert, A.; Dahan, F.; Meunier, B. *New J. Chem.* **1995**, *19*, 129-131). Yttrium tris(dimethylaminoethanol) (Y(DMAE)$_3$) was synthesized according to a literature preparation (McLain, S. L.; Ford, T. M.; Drysdale, N. E. *Polym. Prepr.* **1992**, *33(2)*, 463-464). All other chemicals were commercially available and used as received.

Complex Synthesis.

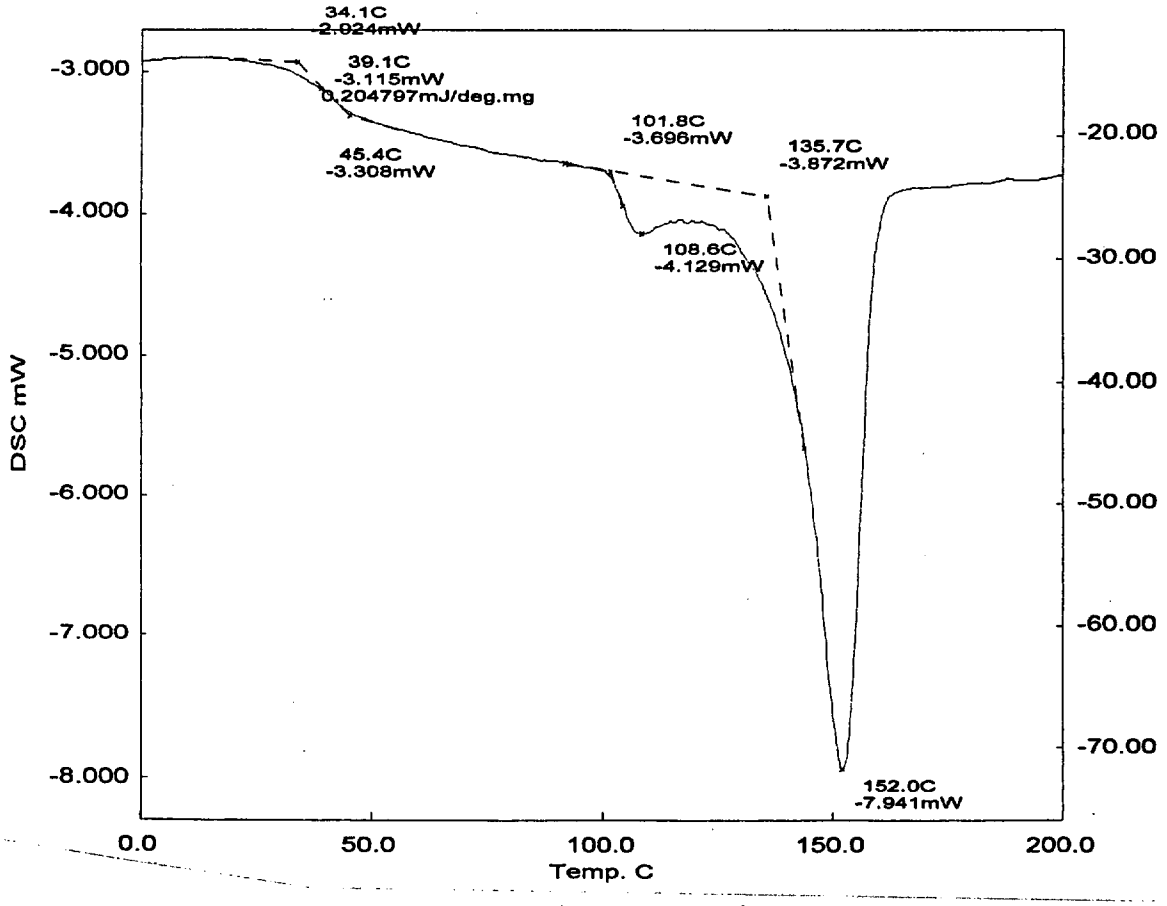
[(*R*)-(Salbinap)AlO^iPr] (**3**). In a glovebox, a dry Schlenk tube was loaded with freshly distilled aluminum isopropoxide (0.137 g, 0.671 mmol), (-)-(*R*)-(**2**) (0.329 g, 0.668 mmol), and toluene (10 mL). The mixture was heated to 70°C and stirred for two days. The solvent was removed *in vacuo*, yielding a yellow solid. ^{1}H NMR (Tol-d$_8$, 300 MHz) δ 7.92 (1H, s), 7.76 (2H, d, *J* =4.3 Mhz), 7.68 (2H, t), 7.43 (4H, d, *J* =8.6), 7.31 (4H, t), 7.18 (2H, t), 6.90-7.14 (18H, m), 6.53 (1H, d, *J* =8.6), 6.42 (1H, d, *J* =7.5), 6.28-6.36 (2H, m), 6.23 (2H, t), 4.08 (1H, m), 1.34 (3H, d, *J* =6.4), 0.71 (3H, d, *J* =5.9). Anal. calc. for $C_{37}H_{29}AlN_2O_3$: C, 77.07; H, 5.07; N, 4.86. Found: C, 76.37; H, 5.34; N, 4.50.

[(*R*)-(Salbinap)YOCH$_2$CH$_2$NMe$_2$]$_2$ (**4**). In a glovebox, a dry Schlenk tube was loaded with Y(DMAE)$_3$ (0.293 g, 0.829 mmol), (-)-(*R*)-(**2**) (0.412 g, 0.836 mmol), and toluene (50 mL). The mixture was heated to 70°C and stirred for one day. The solvent was removed *in vacuo*, yielding a yellow solid. The product was recrystallized by dissolving in a minimum amount of methylene chloride, then layering with hexanes, and allowing to sit for 24 hours. Cannulation of solvent and drying of the residual crystals *in vacuo* yielded **4** (0.365g, 66% yield). ^{1}H NMR (Tol-d$_8$, 300 MHz) δ 8.15 (1H, s), 7.67 (2H, m), 7.54 (1H, d, *J*=7.5), 7.2-7.4 (5H), 6.7-7.1 (13H), 3.27 (2H, m), 2.97 (2H, m), 2.55 (6H, br s), 1.59 (2H, m), 1.02 (2H, m).

Polymer Synthesis.

Representative procedure. In the drybox, [(*R*)-(Salbinap)AlO^{i}Pr] (**3**) (8.0 mg, 1.4 x 10^{-5} mol), *meso*-lactide (0.2013 g, 1.4 x 10^{-3} mol), toluene (7.00 ml) and a magnetic stir bar were placed in a Schlenk tube. The flask was heated to the desired temperature (50°C or 70°C), and stirred for 40 h. An aliquot was taken for percent conversion analysis by ^{1}H NMR. The solvent was removed *in vacuo* and the polymer dissolved in CH_2Cl_2 and precipitated from cold MeOH. The white crystalline solid was filtered and dried *in vacuo* to constant weight. Yield = 0.165 g. The product was then dried in vacuo to constant weight.

DSC Scan for Syndiotactic PLA Formed at 50°C



Crystallographic Data for 4.

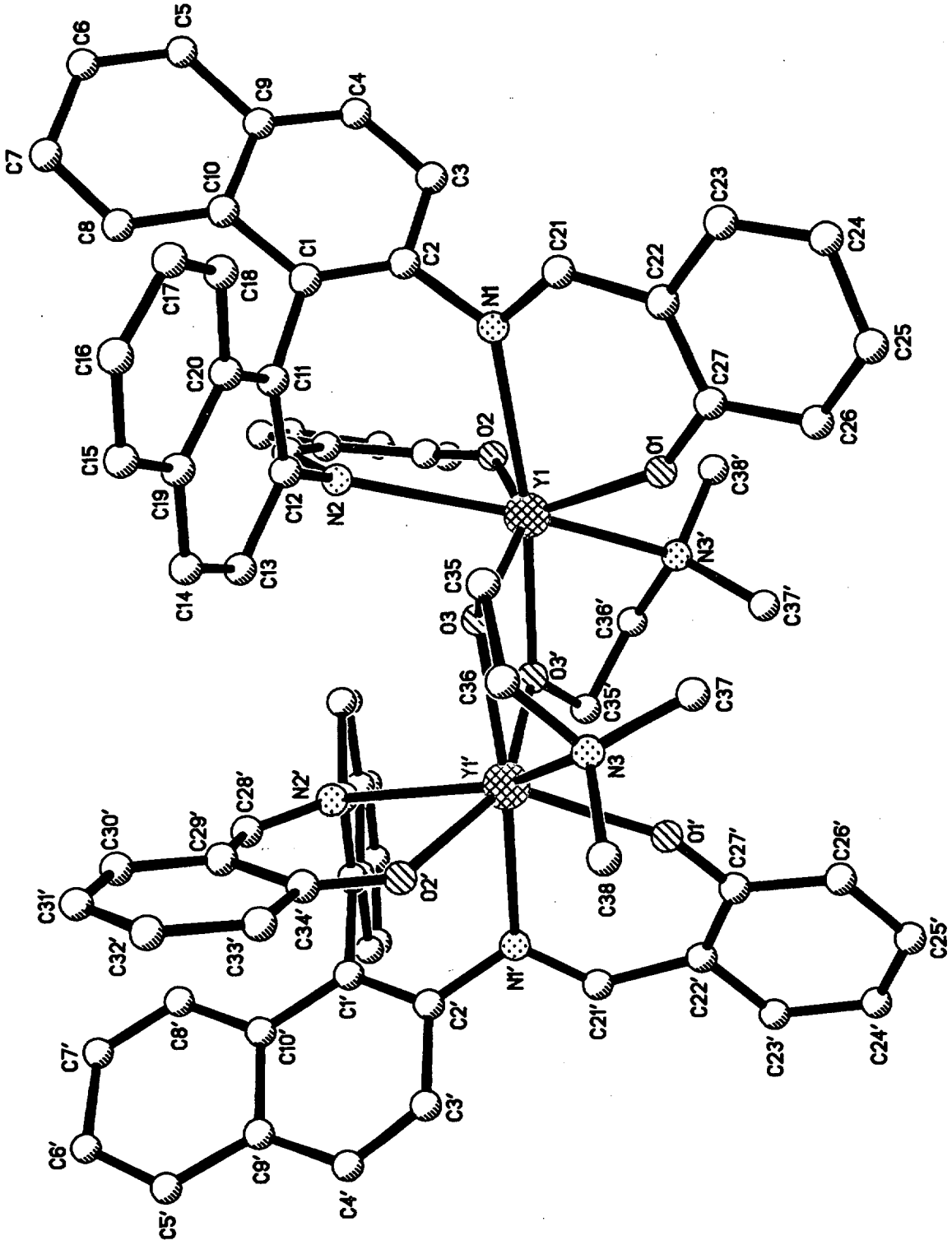


Table 1. Crystal data and structure refinement for jsb1.

Identification code	jsb1
Empirical formula	$C_{38}H_{32}N_3O_3Y$
Formula weight	667.58
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 16.0196(4) Å alpha = 90.000(1)°
	b = 18.3577(4) Å beta = 90.000(1)°
	c = 24.6578(5) Å gamma = 90.000(1)°
Volume, Z	7251.4(3) $Å^3$, 8
Density (calculated)	1.223 Mg/m^3
Absorption coefficient	1.645 mm^{-1}
F(000)	2752
Crystal size	.1 x .1 x .1 mm
θ range for data collection	1.38 to 20.86°
Limiting indices	$-16 \le h \le 14$, $-18 \le k \le 18$, $-24 \le l \le 22$
Reflections collected	24079
Independent reflections	7597 (R_{int} = 0.1002)
Absorption correction	SADABS
Max. and min. transmission	0.942261 and 0.608958
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6542 / 0 / 811
Goodness-of-fit on F^2	1.005
Final R indices [I>2σ(I)]	R1 = 0.0639, wR2 = 0.1450
R indices (all data)	R1 = 0.1173, wR2 = 0.1808
Absolute structure parameter	-0.027(11)
Largest diff. peak and hole	0.439 and -1.095 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for jsb1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Y(1)	3749(1)	4102(1)	7767(1)	51(1)
O(1)	5022(6)	3784(5)	7634(4)	75(3)
O(2)	3320(6)	4795(5)	8423(3)	68(3)
O(3)	3426(5)	3359(4)	7050(3)	48(2)
N(1)	4171(7)	3084(5)	8487(4)	50(3)
N(2)	2405(6)	3574(6)	8163(4)	48(3)
N(3)	4182(8)	3049(6)	6085(5)	67(3)
C(1)	2937(8)	2477(6)	8890(5)	47(3)
C(2)	3622(8)	2883(7)	8939(5)	47(3)
C(3)	3917(8)	3122(7)	9465(7)	62(4)
C(4)	3469(9)	2908(8)	9911(6)	63(4)
C(5)	2374(11)	2212(8)	10349(6)	75(4)
C(6)	1691(12)	1802(8)	10307(6)	85(5)
C(7)	1321(10)	1637(7)	9787(6)	77(4)
C(8)	1730(10)	1858(7)	9328(6)	67(4)
C(9)	2811(9)	2466(7)	9869(5)	54(3)
C(10)	2460(8)	2246(7)	9349(5)	49(3)
C(11)	2592(7)	2280(8)	8336(5)	49(3)
C(12)	2303(8)	2834(9)	8031(5)	54(4)
C(13)	1854(9)	2664(8)	7534(6)	68(4)
C(14)	1745(9)	1975(11)	7393(6)	80(5)
C(15)	2065(10)	628(12)	7545(6)	95(6)
C(16)	2439(12)	96(9)	7845(10)	104(6)
C(17)	2889(10)	274(9)	8286(7)	81(5)
C(18)	2932(7)	980(9)	8441(5)	63(4)
C(19)	2113(8)	1383(9)	7691(6)	64(4)
C(20)	2558(8)	1548(9)	8165(5)	58(4)
C(21)	4887(9)	2783(6)	8523(5)	50(3)
C(22)	5615(7)	2867(7)	8189(5)	43(3)
C(23)	6311(10)	2448(7)	8319(5)	56(4)
C(24)	7043(10)	2486(7)	8048(6)	64(4)
C(25)	7065(9)	2950(9)	7601(7)	85(5)
C(26)	6424(10)	3372(8)	7459(6)	76(4)
C(27)	5652(9)	3370(7)	7759(6)	58(4)
C(28)	1900(8)	3839(8)	8526(5)	62(4)
C(29)	1945(11)	4551(9)	8751(5)	62(4)
C(30)	1265(11)	4776(10)	9060(6)	79(5)
C(31)	1245(14)	5454(14)	9274(6)	101(6)
C(32)	1871(16)	5918(11)	9162(8)	102(6)
C(33)	2574(11)	5710(11)	8855(6)	86(5)
C(34)	2650(12)	4995(9)	8654(6)	62(4)
C(35)	3788(9)	2669(7)	7000(5)	63(4)

C(36)	3856(9)	2459(7)	6405(6)	79(4)
C(37)	5016(9)	3233(8)	6251(7)	99(5)
C(38)	4183(12)	2875(9)	5503(6)	118(6)
Y(1')	3104(1)	4069(1)	6334(1)	52(1)
O(1')	4118(6)	4638(5)	5949(4)	70(3)
O(2')	2392(7)	3326(6)	5844(4)	76(3)
O(3')	3249(6)	4781(4)	7076(3)	57(2)
N(1')	2476(7)	5151(6)	5751(4)	52(3)
N(2')	1571(6)	4162(7)	6598(4)	52(3)
N(3')	4538(7)	5323(6)	7657(4)	60(3)
C(1')	944(9)	5205(7)	5883(5)	56(4)
C(2')	1644(9)	5105(7)	5562(5)	49(4)
C(3')	1531(11)	4911(9)	4991(6)	82(5)
C(4')	808(12)	4808(9)	4777(6)	91(5)
C(5')	-740(12)	4644(9)	4913(7)	104(6)
C(6')	-1412(11)	4639(12)	5259(12)	146(9)
C(7')	-1297(15)	4873(11)	5811(8)	113(7)
C(8')	-559(11)	5043(8)	5995(6)	80(5)
C(9')	70(12)	4828(8)	5090(6)	84(5)
C(10')	140(10)	5036(7)	5681(6)	63(4)
C(11')	1048(8)	5411(9)	6472(5)	57(4)
C(12')	1349(7)	4863(9)	6792(5)	55(4)
C(13')	1419(9)	5039(9)	7386(6)	77(5)
C(14')	1192(10)	5675(10)	7576(6)	86(5)
C(15')	689(11)	6912(13)	7404(7)	102(6)
C(16')	391(11)	7441(10)	7080(10)	111(6)
C(17')	322(10)	7281(12)	6526(8)	98(6)
C(18')	524(9)	6631(9)	6336(6)	77(5)
C(19')	814(9)	6092(9)	6655(6)	67(4)
C(20')	909(9)	6233(9)	7215(7)	73(4)
C(21')	2927(10)	5624(7)	5506(5)	55(4)
C(22')	3822(11)	5725(7)	5504(5)	53(4)
C(23')	4131(11)	6322(8)	5203(6)	74(4)
C(24')	4963(13)	6458(9)	5131(6)	81(5)
C(25')	5492(11)	5981(12)	5327(6)	96(5)
C(26')	5221(12)	5341(9)	5609(6)	87(5)
C(27')	4388(9)	5215(8)	5706(5)	47(3)
C(28')	982(10)	3750(10)	6465(6)	74(5)
C(29')	1048(11)	3105(10)	6183(8)	73(6)
C(30')	376(16)	2682(13)	6196(8)	129(7)
C(31')	363(18)	2036(17)	5898(12)	155(10)
C(32')	996(23)	1859(16)	5594(11)	166(11)
C(33')	1678(14)	2290(14)	5573(10)	135(8)
C(34')	1760(14)	2940(10)	5860(7)	77(5)
C(35')	3376(9)	5548(7)	7023(6)	65(4)
C(36')	3866(9)	5802(7)	7513(5)	66(4)
C(37')	5165(9)	5301(8)	7200(7)	94(5)
C(38')	4958(11)	5561(9)	8152(7)	114(6)

Table 3. Bond lengths [Å] and angles [°] for jsb1.

Y(1)-O(1)	2.145(10)	Y(1)-O(2)	2.171(9)
Y(1)-O(3')	2.258(8)	Y(1)-O(3)	2.292(8)
Y(1)-N(2)	2.556(10)	Y(1)-N(3')	2.587(10)
Y(1)-N(1)	2.666(10)	Y(1)-Y(1')	3.682(2)
O(1)-C(27)	1.30(2)	O(2)-C(34)	1.27(2)
O(3)-C(35)	1.399(13)	O(3)-Y(1')	2.254(7)
N(1)-C(21)	1.277(14)	N(1)-C(2)	1.466(14)
N(2)-C(28)	1.30(2)	N(2)-C(12)	1.41(2)
N(3)-C(36)	1.44(2)	N(3)-C(37)	1.44(2)
N(3)-C(38)	1.47(2)	N(3)-Y(1')	2.621(11)
C(1)-C(2)	1.33(2)	C(1)-C(10)	1.43(2)
C(1)-C(11)	1.52(2)	C(2)-C(3)	1.45(2)
C(3)-C(4)	1.37(2)	C(4)-C(9)	1.33(2)
C(5)-C(6)	1.33(2)	C(5)-C(9)	1.45(2)
C(6)-C(7)	1.45(2)	C(7)-C(8)	1.37(2)
C(8)-C(10)	1.37(2)	C(9)-C(10)	1.46(2)
C(11)-C(12)	1.35(2)	C(11)-C(20)	1.41(2)
C(12)-C(13)	1.45(2)	C(13)-C(14)	1.32(2)
C(14)-C(19)	1.44(2)	C(15)-C(16)	1.36(2)
C(15)-C(19)	1.44(2)	C(16)-C(17)	1.35(2)
C(17)-C(18)	1.35(2)	C(18)-C(20)	1.38(2)
C(19)-C(20)	1.40(2)	C(21)-C(22)	1.44(2)
C(22)-C(23)	1.39(2)	C(22)-C(27)	1.41(2)
C(23)-C(24)	1.35(2)	C(24)-C(25)	1.39(2)
C(25)-C(26)	1.33(2)	C(26)-C(27)	1.44(2)
C(28)-C(29)	1.42(2)	C(29)-C(30)	1.39(2)
C(29)-C(34)	1.41(2)	C(30)-C(31)	1.35(2)
C(31)-C(32)	1.34(2)	C(32)-C(33)	1.41(2)
C(33)-C(34)	1.41(2)	C(35)-C(36)	1.52(2)
Y(1')-O(2')	2.149(11)	Y(1')-O(1')	2.152(10)
Y(1')-O(3')	2.261(8)	Y(1')-N(2')	2.546(10)
Y(1')-N(1')	2.650(10)	O(1')-C(27')	1.291(14)
O(2')-C(34')	1.24(2)	O(3')-C(35')	1.428(14)
N(1')-C(21')	1.28(2)	N(1')-C(2')	1.41(2)
N(2')-C(28')	1.25(2)	N(2')-C(12')	1.42(2)
N(3')-C(36')	1.43(2)	N(3')-C(38')	1.46(2)
N(3')-C(37')	1.51(2)	C(1')-C(2')	1.39(2)
C(1')-C(10')	1.42(2)	C(1')-C(11')	1.51(2)
C(2')-C(3')	1.46(2)	C(3')-C(4')	1.29(2)
C(4')-C(9')	1.41(2)	C(5')-C(6')	1.37(2)
C(5')-C(9')	1.41(2)	C(6')-C(7')	1.44(3)
C(7')-C(8')	1.30(2)	C(8')-C(10')	1.36(2)
C(9')-C(10')	1.51(2)	C(11')-C(12')	1.36(2)
C(11')-C(19')	1.38(2)	C(12')-C(13')	1.50(2)
C(13')-C(14')	1.31(2)	C(14')-C(20')	1.43(2)
C(15')-C(16')	1.34(2)	C(15')-C(20')	1.38(2)
C(16')-C(17')	1.40(2)	C(17')-C(18')	1.32(2)
C(18')-C(19')	1.35(2)	C(19')-C(20')	1.41(2)
C(21')-C(22')	1.45(2)	C(22')-C(27')	1.40(2)

C(22')-C(23')	1.41(2)	C(23')-C(24')	1.37(2)
C(24')-C(25')	1.31(2)	C(25')-C(26')	1.43(2)
C(26')-C(27')	1.38(2)	C(28')-C(29')	1.38(2)
C(29')-C(30')	1.33(2)	C(29')-C(34')	1.42(2)
C(30')-C(31')	1.39(3)	C(31')-C(32')	1.30(3)
C(32')-C(33')	1.35(3)	C(33')-C(34')	1.39(3)
C(35')-C(36')	1.51(2)		

O(1)-Y(1)-O(2)	125.0(4)	O(1)-Y(1)-O(3')	111.9(3)
O(2)-Y(1)-O(3')	97.3(3)	O(1)-Y(1)-O(3)	86.3(3)
O(2)-Y(1)-O(3)	148.5(3)	O(3')-Y(1)-O(3)	70.5(2)
O(1)-Y(1)-N(2)	139.1(3)	O(2)-Y(1)-N(2)	70.7(4)
O(3')-Y(1)-N(2)	101.4(3)	O(3)-Y(1)-N(2)	83.0(3)
O(1)-Y(1)-N(3')	75.9(3)	O(2)-Y(1)-N(3')	74.1(3)
O(3')-Y(1)-N(3')	67.4(3)	O(3)-Y(1)-N(3')	123.0(3)
N(2)-Y(1)-N(3')	141.3(4)	O(1)-Y(1)-N(1)	70.7(3)
O(2)-Y(1)-N(1)	89.7(3)	O(3')-Y(1)-N(1)	168.5(3)
O(3)-Y(1)-N(1)	98.9(3)	N(2)-Y(1)-N(1)	72.1(3)
N(3')-Y(1)-N(1)	123.6(3)	O(1)-Y(1)-Y(1')	96.7(2)
O(2)-Y(1)-Y(1')	129.5(2)	O(3')-Y(1)-Y(1')	35.5(2)
O(3)-Y(1)-Y(1')	35.6(2)	N(2)-Y(1)-Y(1')	97.1(2)
N(3')-Y(1)-Y(1')	92.9(2)	N(1)-Y(1)-Y(1')	134.4(2)
C(27)-O(1)-Y(1)	149.4(8)	C(34)-O(2)-Y(1)	140.6(9)
C(35)-O(3)-Y(1')	123.3(7)	C(35)-O(3)-Y(1)	120.9(7)
Y(1')-O(3)-Y(1)	108.2(3)	C(21)-N(1)-C(2)	112.2(10)
C(21)-N(1)-Y(1)	125.2(8)	C(2)-N(1)-Y(1)	122.1(7)
C(28)-N(2)-C(12)	116.6(11)	C(28)-N(2)-Y(1)	130.1(9)
C(12)-N(2)-Y(1)	112.1(8)	C(36)-N(3)-C(37)	110.9(11)
C(36)-N(3)-C(38)	111.9(12)	C(37)-N(3)-C(38)	109.1(13)
C(36)-N(3)-Y(1')	99.8(8)	C(37)-N(3)-Y(1')	112.2(9)
C(38)-N(3)-Y(1')	112.6(9)	C(2)-C(1)-C(10)	122.2(12)
C(2)-C(1)-C(11)	121.0(12)	C(10)-C(1)-C(11)	116.7(11)
C(1)-C(2)-C(3)	121.3(12)	C(1)-C(2)-N(1)	124.4(12)
C(3)-C(2)-N(1)	114.2(12)	C(4)-C(3)-C(2)	117.5(12)
C(9)-C(4)-C(3)	121.6(13)	C(6)-C(5)-C(9)	121(2)
C(5)-C(6)-C(7)	121.5(14)	C(8)-C(7)-C(6)	118.4(14)
C(7)-C(8)-C(10)	122.0(14)	C(4)-C(9)-C(5)	120.8(14)
C(4)-C(9)-C(10)	122.9(13)	C(5)-C(9)-C(10)	116.2(13)
C(8)-C(10)-C(1)	125.3(12)	C(8)-C(10)-C(9)	120.5(12)
C(1)-C(10)-C(9)	114.1(12)	C(12)-C(11)-C(20)	122.7(13)
C(12)-C(11)-C(1)	116.6(12)	C(20)-C(11)-C(1)	120.7(12)
C(11)-C(12)-N(2)	124.1(12)	C(11)-C(12)-C(13)	118.6(14)
N(2)-C(12)-C(13)	117.3(13)	C(14)-C(13)-C(12)	119.4(14)
C(13)-C(14)-C(19)	122.3(14)	C(16)-C(15)-C(19)	122(2)
C(17)-C(16)-C(15)	120(2)	C(16)-C(17)-C(18)	119(2)
C(17)-C(18)-C(20)	124.2(14)	C(20)-C(19)-C(15)	116(2)
C(20)-C(19)-C(14)	118(2)	C(15)-C(19)-C(14)	125(2)
C(18)-C(20)-C(19)	118(2)	C(18)-C(20)-C(11)	123.7(13)
C(19)-C(20)-C(11)	118.3(14)	N(1)-C(21)-C(22)	130.1(12)
C(23)-C(22)-C(27)	120.1(12)	C(23)-C(22)-C(21)	117.3(13)
C(27)-C(22)-C(21)	122.5(12)	C(24)-C(23)-C(22)	123.6(12)
C(23)-C(24)-C(25)	116.4(13)	C(26)-C(25)-C(24)	122.9(14)
C(25)-C(26)-C(27)	121.7(14)	O(1)-C(27)-C(22)	121.9(13)

O(1)-C(27)-C(26)	123.0(13)	C(22)-C(27)-C(26)	115.2(13)
N(2)-C(28)-C(29)	125.6(14)	C(30)-C(29)-C(34)	123(2)
C(30)-C(29)-C(28)	117(2)	C(34)-C(29)-C(28)	120(2)
C(31)-C(30)-C(29)	120(2)	C(32)-C(31)-C(30)	119(2)
C(31)-C(32)-C(33)	122(2)	C(34)-C(33)-C(32)	121(2)
O(2)-C(34)-C(33)	120(2)	O(2)-C(34)-C(29)	125.8(14)
C(33)-C(34)-C(29)	114(2)	O(3)-C(35)-C(36)	110.2(10)
N(3)-C(36)-C(35)	111.4(11)	O(2')-Y(1')-O(1')	117.5(4)
O(2')-Y(1')-O(3)	101.2(3)	O(1')-Y(1')-O(3)	116.9(3)
O(2')-Y(1')-O(3')	151.2(4)	O(1')-Y(1')-O(3')	89.9(3)
O(3)-Y(1')-O(3')	71.1(3)	O(2')-Y(1')-N(2')	71.0(4)
O(1')-Y(1')-N(2')	144.0(4)	O(3)-Y(1')-N(2')	93.4(3)
O(3')-Y(1')-N(2')	81.6(4)	O(2')-Y(1')-N(3)	76.4(4)
O(1')-Y(1')-N(3)	75.3(4)	O(3)-Y(1')-N(3)	67.6(3)
O(3')-Y(1')-N(3)	122.3(3)	N(2')-Y(1')-N(3)	138.0(4)
O(2')-Y(1')-N(1')	88.2(3)	O(1')-Y(1')-N(1')	71.6(3)
O(3)-Y(1')-N(1')	160.9(3)	O(3')-Y(1')-N(1')	92.6(3)
N(2')-Y(1')-N(1')	73.9(3)	N(3)-Y(1')-N(1')	131.2(3)
O(2')-Y(1')-Y(1)	134.3(3)	O(1')-Y(1')-Y(1)	101.7(2)
O(3)-Y(1')-Y(1)	36.3(2)	O(3')-Y(1')-Y(1)	35.4(2)
N(2')-Y(1')-Y(1)	91.4(2)	N(3)-Y(1')-Y(1)	92.9(3)
N(1')-Y(1')-Y(1)	128.0(2)	C(27')-O(1')-Y(1')	148.8(9)
C(34')-O(2')-Y(1')	141.4(10)	C(35')-O(3')-Y(1)	124.3(7)
C(35')-O(3')-Y(1')	120.6(7)	Y(1)-O(3')-Y(1')	109.1(3)
C(21')-N(1')-C(2')	114.7(11)	C(21')-N(1')-Y(1')	123.3(9)
C(2')-N(1')-Y(1')	119.4(8)	C(28')-N(2')-C(12')	116.6(12)
C(28')-N(2')-Y(1')	128.2(10)	C(12')-N(2')-Y(1')	112.9(8)
C(36')-N(3')-C(38')	111.7(12)	C(36')-N(3')-C(37')	109.3(10)
C(38')-N(3')-C(37')	108.9(11)	C(36')-N(3')-Y(1)	101.0(7)
C(38')-N(3')-Y(1)	113.3(8)	C(37')-N(3')-Y(1)	112.3(8)
C(2')-C(1')-C(10')	120.4(12)	C(2')-C(1')-C(11')	119.6(12)
C(10')-C(1')-C(11')	119.7(13)	C(1')-C(2')-N(1')	124.5(11)
C(1')-C(2')-C(3')	118.8(13)	N(1')-C(2')-C(3')	116.6(12)
C(4')-C(3')-C(2')	123(2)	C(3')-C(4')-C(9')	122(2)
C(6')-C(5')-C(9')	122(2)	C(5')-C(6')-C(7')	119(2)
C(8')-C(7')-C(6')	121(2)	C(7')-C(8')-C(10')	123(2)
C(5')-C(9')-C(4')	126(2)	C(5')-C(9')-C(10')	115(2)
C(4')-C(9')-C(10')	118(2)	C(8')-C(10')-C(1')	123.0(14)
C(8')-C(10')-C(9')	119(2)	C(1')-C(10')-C(9')	117.6(14)
C(12')-C(11')-C(19')	125.0(13)	C(12')-C(11')-C(1')	114.2(13)
C(19')-C(11')-C(1')	120.7(12)	C(11')-C(12')-N(2')	124.2(12)
C(11')-C(12')-C(13')	115.5(13)	N(2')-C(12')-C(13')	120.3(13)
C(14')-C(13')-C(12')	121.2(14)	C(13')-C(14')-C(20')	120.3(14)
C(16')-C(15')-C(20')	123(2)	C(15')-C(16')-C(17')	117(2)
C(18')-C(17')-C(16')	121(2)	C(17')-C(18')-C(19')	123(2)
C(18')-C(19')-C(11')	124.7(14)	C(18')-C(19')-C(20')	118.3(14)
C(11')-C(19')-C(20')	117.1(14)	C(15')-C(20')-C(19')	118(2)
C(15')-C(20')-C(14')	121(2)	C(19')-C(20')-C(14')	120.7(14)
N(1')-C(21')-C(22')	130.4(12)	C(27')-C(22')-C(23')	119(2)
C(27')-C(22')-C(21')	123.9(12)	C(23')-C(22')-C(21')	116.7(14)
C(24')-C(23')-C(22')	123(2)	C(25')-C(24')-C(23')	118(2)
C(24')-C(25')-C(26')	122(2)	C(27')-C(26')-C(25')	121(2)
O(1')-C(27')-C(26')	122.9(14)	O(1')-C(27')-C(22')	119.9(13)

C(26')-C(27')-C(22')	117(2)	N(2')-C(28')-C(29')	126(2)
C(30')-C(29')-C(28')	115(2)	C(30')-C(29')-C(34')	123(2)
C(28')-C(29')-C(34')	121.9(14)	C(29')-C(30')-C(31')	120(2)
C(32')-C(31')-C(30')	120(3)	C(31')-C(32')-C(33')	120(3)
C(32')-C(33')-C(34')	124(2)	O(2')-C(34')-C(33')	124(2)
O(2')-C(34')-C(29')	123(2)	C(33')-C(34')-C(29')	113(2)
O(3')-C(35')-C(36')	107.6(10)	N(3')-C(36')-C(35')	113.5(11)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for jsb1.

The anisotropic displacement factor exponent takes the form:

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

	U11	U22	U33	U23	U13	U12
Y(1)	62(1)	65(1)	27(1)	13(1)	2(1)	8(1)
O(1)	78(6)	94(7)	53(7)	38(5)	10(5)	12(6)
O(2)	84(7)	102(7)	19(5)	-10(5)	23(5)	14(6)
O(3)	64(6)	51(5)	30(5)	2(4)	13(4)	10(4)
N(1)	37(7)	75(7)	37(7)	-1(6)	-7(6)	5(6)
N(2)	53(7)	65(8)	26(7)	14(6)	-14(6)	-5(6)
N(3)	83(10)	80(8)	38(8)	5(7)	5(7)	18(7)
C(1)	50(9)	52(8)	40(10)	4(7)	-3(8)	-6(7)
C(2)	44(9)	60(8)	37(9)	6(7)	0(8)	7(7)
C(3)	44(9)	72(9)	71(12)	-16(9)	-13(9)	5(7)
C(4)	58(11)	98(12)	32(10)	-12(8)	12(8)	12(9)
C(5)	107(13)	67(10)	51(11)	4(8)	30(10)	-3(10)
C(6)	130(16)	76(11)	48(13)	14(9)	39(11)	-2(10)
C(7)	94(11)	85(10)	52(11)	-12(9)	36(11)	-16(9)
C(8)	70(11)	89(10)	42(10)	9(8)	13(9)	-12(9)
C(9)	63(10)	64(9)	34(10)	-3(8)	7(8)	2(8)
C(10)	52(9)	72(9)	22(9)	0(7)	13(8)	13(7)
C(11)	61(9)	56(10)	31(9)	12(8)	5(7)	7(7)
C(12)	49(9)	88(13)	25(9)	6(9)	4(7)	-7(8)
C(13)	78(10)	59(10)	68(12)	18(8)	-14(9)	-27(8)
C(14)	69(10)	130(15)	42(10)	23(11)	-12(8)	-12(11)
C(15)	86(13)	149(18)	51(11)	-37(12)	5(9)	-28(12)
C(16)	115(15)	78(12)	119(19)	34(14)	7(14)	30(11)
C(17)	97(14)	103(15)	42(11)	-3(10)	-11(10)	2(10)
C(18)	80(10)	66(10)	42(9)	-31(9)	6(7)	7(9)
C(19)	68(10)	93(13)	33(10)	-11(9)	-17(8)	-10(9)
C(20)	59(10)	82(12)	32(10)	16(10)	5(8)	1(9)
C(21)	58(10)	67(9)	26(9)	-2(7)	-12(8)	5(8)
C(22)	29(8)	54(8)	48(9)	-10(8)	-4(8)	7(7)
C(23)	68(10)	64(9)	38(9)	-1(7)	3(9)	-4(9)
C(24)	75(12)	56(9)	61(11)	9(8)	-1(9)	11(8)
C(25)	45(10)	93(12)	116(16)	-3(12)	13(10)	18(9)
C(26)	62(11)	86(11)	79(12)	21(9)	12(10)	5(9)
C(27)	66(11)	61(9)	47(10)	12(9)	-17(10)	-18(8)
C(28)	52(9)	107(13)	26(9)	24(8)	-3(8)	19(9)
C(29)	96(13)	73(11)	16(9)	11(8)	-6(9)	19(12)
C(30)	105(13)	95(13)	39(10)	25(9)	33(10)	25(11)
C(31)	125(17)	137(18)	41(11)	20(13)	32(11)	74(15)
C(32)	143(18)	104(14)	60(13)	27(13)	-29(14)	29(17)
C(33)	96(14)	131(19)	31(10)	15(10)	-11(9)	15(12)
C(34)	109(15)	56(10)	22(9)	2(9)	-23(10)	-6(11)
C(35)	95(11)	56(9)	38(9)	0(7)	5(8)	9(9)

C(36)	102(11)	80(10)	54(11)	0(9)	-3(10)	21(9)
C(37)	70(12)	126(13)	101(14)	42(12)	22(11)	28(10)
C(38)	156(18)	138(15)	61(14)	5(11)	23(12)	25(12)
Y(1')	64(1)	64(1)	28(1)	9(1)	3(1)	5(1)
O(1')	76(7)	86(7)	49(6)	27(6)	-4(5)	3(5)
O(2')	74(8)	99(8)	54(7)	0(6)	-5(6)	-13(6)
O(3')	88(7)	50(6)	34(6)	0(4)	-2(5)	2(5)
N(1')	51(8)	83(8)	21(7)	8(6)	12(7)	7(6)
N(2')	72(8)	65(8)	19(6)	18(6)	3(5)	13(8)
N(3')	49(7)	88(8)	42(8)	14(6)	-9(7)	-6(6)
C(1')	64(11)	88(10)	14(9)	6(7)	-27(8)	25(8)
C(2')	54(11)	82(10)	10(8)	6(7)	-4(8)	18(7)
C(3')	73(13)	136(14)	37(11)	-16(9)	5(9)	7(9)
C(4')	74(13)	161(16)	36(11)	-32(10)	-16(11)	23(11)
C(5')	67(13)	178(17)	69(13)	-26(12)	-43(12)	7(11)
C(6')	47(13)	185(19)	205(30)	31(21)	4(16)	-10(12)
C(7')	107(20)	169(18)	63(14)	-20(12)	17(13)	-7(14)
C(8')	53(11)	130(13)	56(11)	10(9)	4(11)	-4(10)
C(9')	104(15)	98(12)	51(12)	-5(9)	-27(12)	25(10)
C(10')	67(11)	87(10)	36(10)	6(8)	7(10)	14(8)
C(11')	59(9)	94(12)	19(9)	24(9)	1(7)	3(8)
C(12')	44(8)	100(13)	21(9)	13(9)	8(7)	5(8)
C(13')	87(12)	103(13)	41(12)	13(9)	-2(8)	28(9)
C(14')	106(12)	124(15)	29(10)	-9(10)	-4(9)	35(11)
C(15')	97(13)	135(17)	75(14)	-26(14)	9(11)	24(12)
C(16')	113(15)	95(14)	125(21)	-13(14)	39(14)	39(12)
C(17')	97(13)	141(19)	56(14)	18(12)	12(10)	22(12)
C(18')	106(12)	82(11)	43(10)	7(11)	38(10)	47(10)
C(19')	95(11)	81(13)	24(10)	-2(9)	9(8)	36(9)
C(20')	74(10)	75(11)	69(14)	-13(11)	21(10)	23(8)
C(21')	74(12)	67(10)	23(8)	2(7)	14(8)	19(8)
C(22')	89(13)	57(10)	14(7)	2(7)	16(8)	-9(10)
C(23')	91(13)	95(12)	34(10)	-20(9)	-1(9)	-10(10)
C(24')	112(16)	79(12)	52(11)	11(9)	-15(11)	-32(11)
C(25')	97(14)	129(15)	61(11)	19(12)	8(10)	-53(14)
C(26')	86(15)	117(15)	59(12)	-3(11)	-15(10)	-4(10)
C(27')	47(10)	66(10)	27(9)	1(8)	2(8)	4(9)
C(28')	88(12)	69(11)	65(12)	32(9)	-39(9)	-35(10)
C(29')	68(12)	77(12)	75(14)	38(11)	-55(12)	-63(11)
C(30')	198(26)	124(17)	64(14)	-8(13)	-16(14)	-19(17)
C(31')	157(26)	178(28)	130(25)	6(20)	-20(19)	-74(21)
C(32')	193(32)	180(26)	127(25)	-68(20)	-36(22)	-8(26)
C(33')	98(17)	153(20)	153(22)	-31(19)	-10(15)	-29(14)
C(34')	88(17)	99(16)	42(10)	-9(10)	-7(12)	-7(12)
C(35')	94(12)	46(9)	55(10)	3(7)	4(9)	-3(7)
C(36')	82(10)	71(10)	46(9)	-12(8)	8(8)	-25(10)
C(37')	81(11)	109(13)	93(14)	38(11)	24(11)	1(9)
C(38')	136(15)	136(15)	71(13)	6(11)	-39(12)	-54(12)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for jsb1.

	x	y	z	U(eq)
H(3A)	4392(8)	3410(7)	9499(7)	74
H(4A)	3627(9)	3076(8)	10252(6)	75
H(5A)	2574(11)	2338(8)	10690(6)	90
H(6A)	1447(12)	1617(8)	10621(6)	102
H(7A)	817(10)	1388(7)	9764(6)	92
H(8A)	1506(10)	1741(7)	8991(6)	80
H(13A)	1646(9)	3037(8)	7317(6)	82
H(14B)	1419(9)	1870(11)	7091(6)	96
H(15A)	1769(10)	497(12)	7235(6)	114
H(16B)	2384(12)	-390(9)	7744(10)	125
H(17A)	3167(10)	-84(9)	8483(7)	97
H(18A)	3233(7)	1090(9)	8753(5)	75
H(21B)	4947(9)	2459(6)	8811(5)	60
H(23A)	6270(10)	2124(7)	8608(5)	68
H(24A)	7508(10)	2218(7)	8155(6)	77
H(25A)	7548(9)	2966(9)	7392(7)	102
H(26B)	6477(10)	3675(8)	7159(6)	91
H(28A)	1474(8)	3537(8)	8648(5)	74
H(30A)	822(11)	4458(10)	9119(6)	95
H(31A)	804(14)	5598(14)	9495(6)	121
H(32A)	1840(16)	6393(11)	9293(8)	123
H(33A)	2992(11)	6049(11)	8784(6)	103
H(35A)	3449(9)	2313(7)	7190(5)	76
H(35B)	4338(9)	2671(7)	7163(5)	76
H(36C)	4220(9)	2039(7)	6370(6)	94
H(36D)	3309(9)	2323(7)	6270(6)	94
H(37A)	5220(9)	3627(8)	6032(7)	149
H(37B)	5373(9)	2816(8)	6207(7)	149
H(37C)	5013(9)	3377(8)	6625(7)	149
H(38D)	4403(12)	3280(9)	5303(6)	177
H(38E)	3623(12)	2777(9)	5386(6)	177
H(38F)	4525(12)	2453(9)	5440(6)	177
H(3'A)	2001(11)	4860(9)	4773(6)	98
H(4'A)	770(12)	4719(9)	4406(6)	109
H(5'A)	-821(12)	4521(9)	4551(7)	125
H(6'A)	-1934(11)	4488(12)	5138(12)	175
H(7'A)	-1757(15)	4904(11)	6040(8)	136
H(8'A)	-508(11)	5175(8)	6357(6)	96
H(13B)	1629(9)	4690(9)	7623(6)	92
H(14A)	1214(10)	5764(10)	7947(6)	103
H(15B)	748(11)	7009(13)	7772(7)	123
H(16A)	238(11)	7893(10)	7218(10)	133
H(17B)	131(10)	7638(12)	6289(8)	118

H(18B)	462(9)	6542(9)	5967(6)	93
H(21A)	2631(10)	5955(7)	5295(5)	66
H(23B)	3749(11)	6639(8)	5046(6)	88
H(24B)	5147(13)	6872(9)	4950(6)	97
H(25B)	6061(11)	6061(12)	5281(6)	115
H(26A)	5615(12)	5006(9)	5729(6)	105
H(28B)	448(10)	3894(10)	6567(6)	89
H(30B)	-84(16)	2815(13)	6403(8)	154
H(31B)	-100(18)	1731(17)	5917(12)	186
H(32B)	978(23)	1432(16)	5390(11)	200
H(33B)	2120(14)	2144(14)	5354(10)	162
H(35C)	2843(9)	5798(7)	7006(6)	78
H(35D)	3683(9)	5653(7)	6693(6)	78
H(36A)	4091(9)	6282(7)	7439(5)	79
H(36B)	3489(9)	5844(7)	7819(5)	79
H(37D)	5615(9)	4981(8)	7295(7)	142
H(37E)	5380(9)	5782(8)	7138(7)	142
H(37F)	4899(9)	5127(8)	6876(7)	142
H(38A)	5402(11)	5229(9)	8236(7)	172
H(38B)	4565(11)	5569(9)	8445(7)	172
H(38C)	5182(11)	6040(9)	8099(7)	172