© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 1

Supporting Information

for

Effect of Cyclopentadienyl and Amide Fragment in Olefin Polymerization by *Nonbridged* (Amide)(cyclopentadienyl)titanium(IV) Complexes of the Type, $Cp'TiCl_2[N(R^1)R^2]$, -Methylaluminoxane (MAO) Catalyst Systems

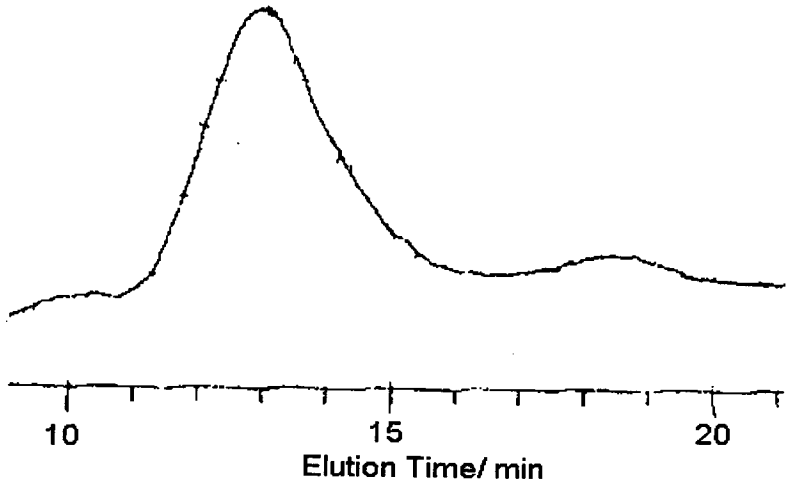
by

Kotohiro Nomura*, and Kensaku Fujii
Graduate School of Materials Science, Nara Institute of Science and Technology (NAIST), 8916-5 Takayama, Ikoma, Nara 630-0101, Japan

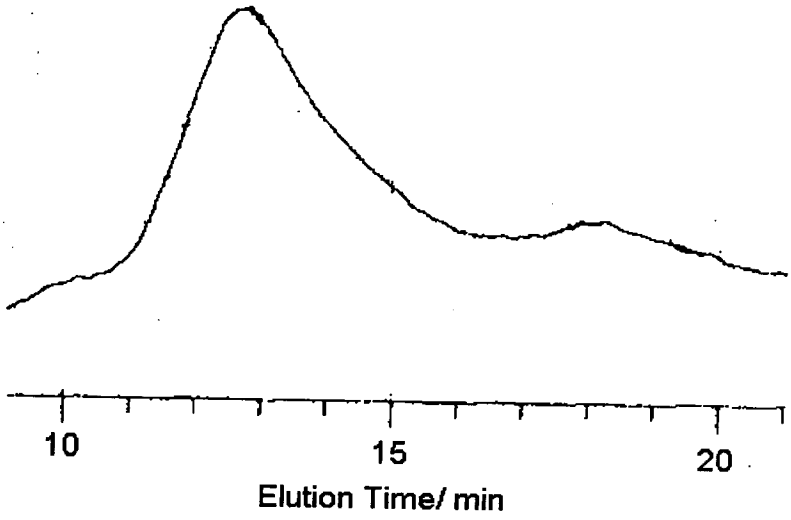
Contents

1. GPC traces and ^{13}C NMR spectra for poly(ethylene-*co*-1-hexene)s prepared by **1-6** - d-MAO catalyst system.
2. Detailed crystallographic analysis data for $Cp^*TiCl_2[N(Me)Cy]$ (**3**), $(1,3\text{-}Me_2C_5H_3)TiCl_2[N(Me)Cy]$ (**4**) and $(1,3\text{-}Me_2C_5H_3)TiCl_2(NCy_2)$ **5**.

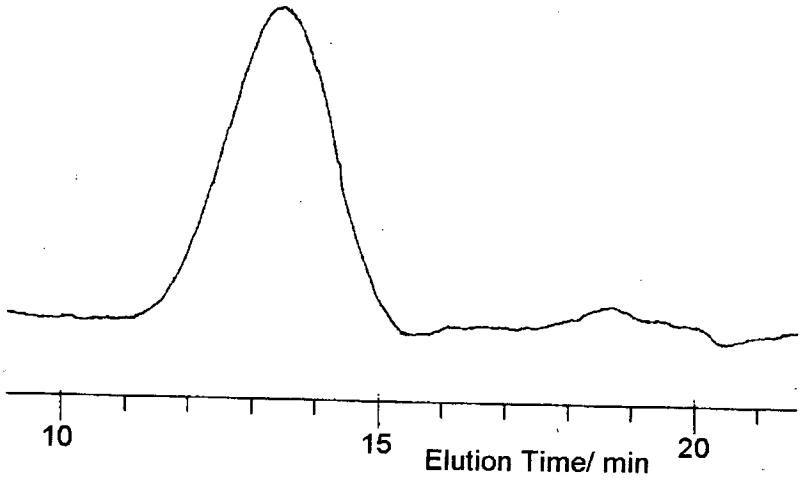
GPC trace for poly(ethylene-*co*-1-hexene) prepared by **4** - MAO catalyst system (ethylene 6 atm, 1-hexene 3 mL, run 35, **4** 3.0 μmol, Al/Ti = 1000)



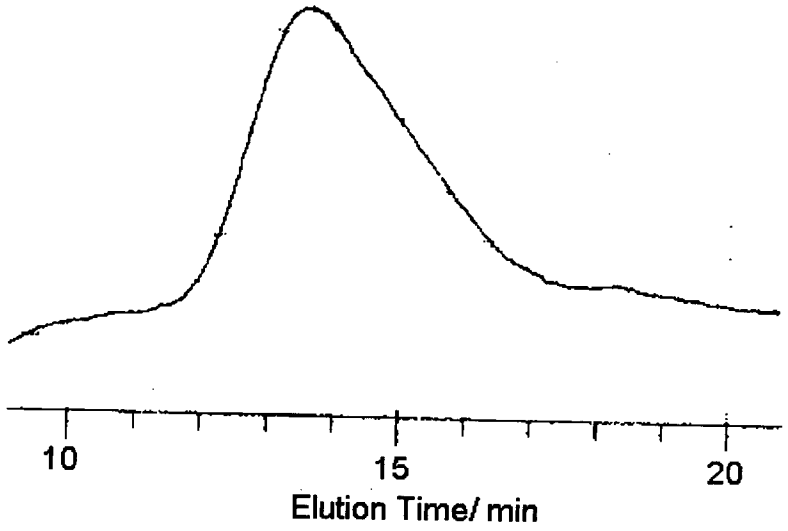
GPC trace for poly(ethylene-*co*-1-hexene) prepared by **4** - MAO catalyst system (ethylene 6 atm, 1-hexene 10 mL, run 37, **4** 3.0 μmol, Al/Ti = 1000)



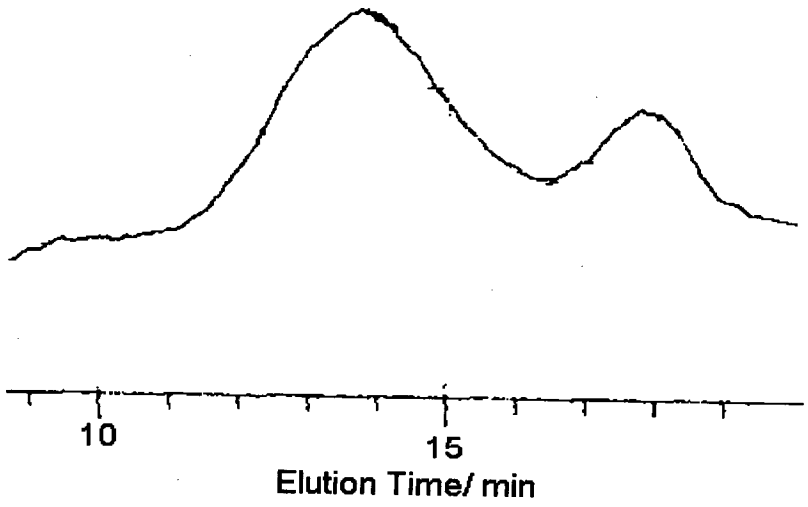
GPC trace for poly(ethylene-*co*-1-hexene) prepared by **4** - MAO catalyst system (ethylene 4 atm, 1-hexene 10 mL, run 38, **4** 1.0 μmol, Al/Ti = 3000)



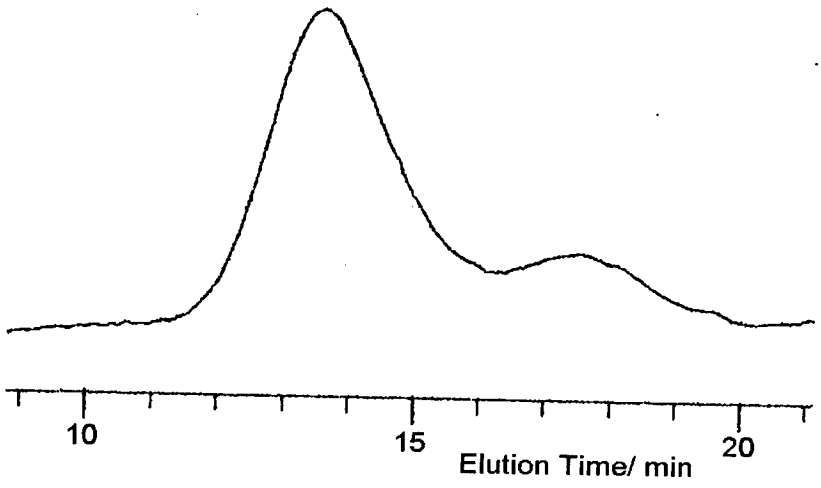
GPC trace for poly(ethylene-*co*-1-hexene) prepared by **5** - MAO catalyst system (ethylene 6 atm, 1-hexene 10 mL, run 39, **5** 3.0 μmol, Al/Ti = 1000)



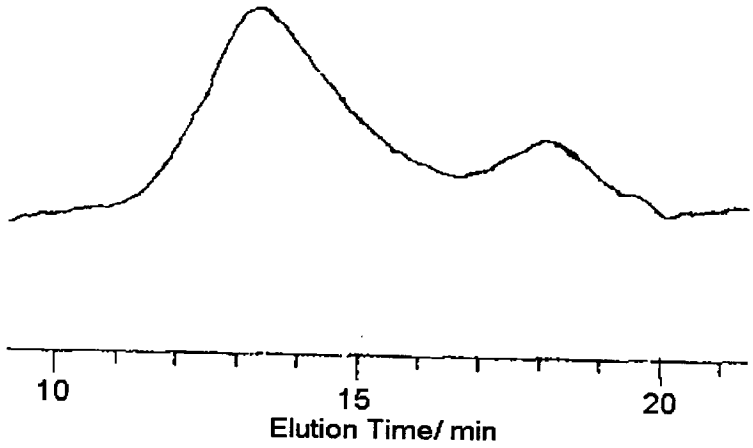
GPC trace for poly(ethylene-*co*-1-hexene) prepared by **1** - MAO catalyst system (ethylene 6 atm, 1-hexene 10 mL, run 29, **1** 3.0 μmol, Al/Ti = 1000)



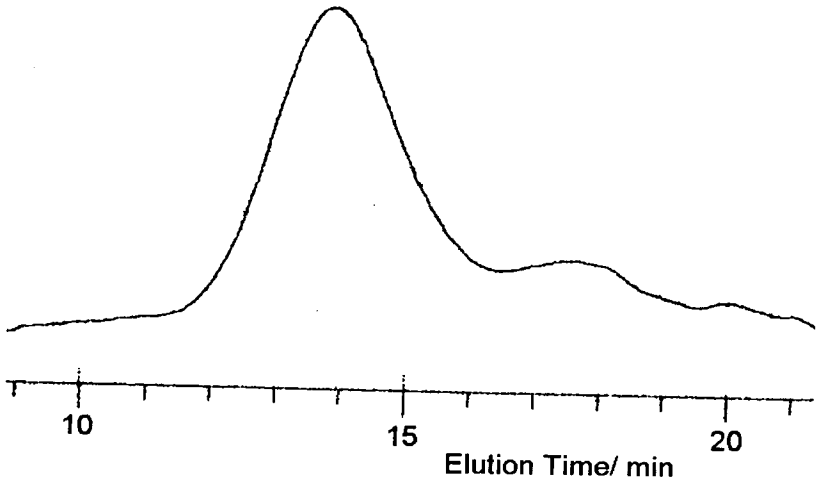
GPC trace for poly(ethylene-*co*-1-hexene) prepared by **1** - MAO catalyst system (ethylene 8 atm, 1-hexene 10 mL, run 30, **1** 1.0 μmol, Al/Ti = 4000).



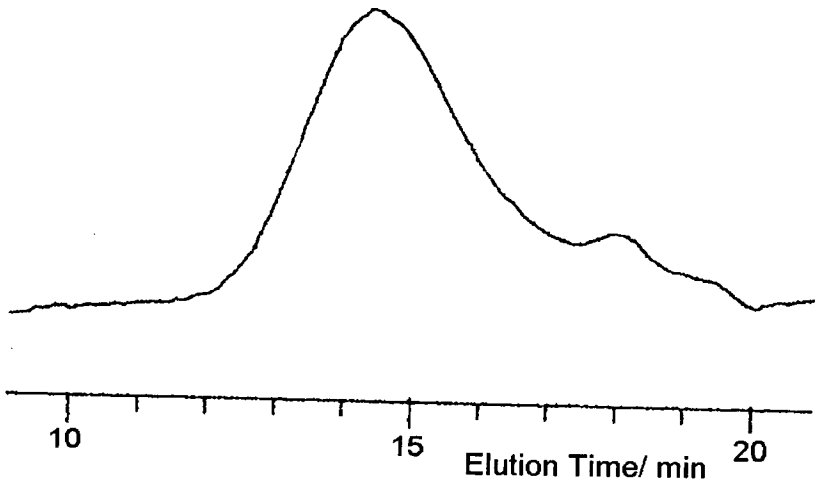
GPC trace for poly(ethylene-*co*-1-hexene) prepared by **3** - MAO catalyst system (ethylene 6 atm, 1-hexene 10 mL, run 31, **3** 3.0 μmol, Al/Ti = 1000).



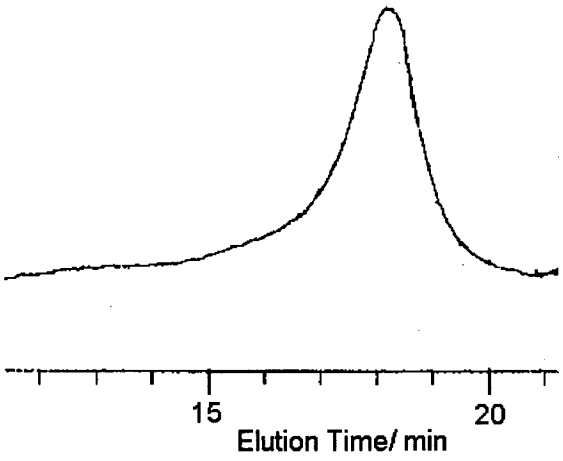
GPC trace for poly(ethylene-*co*-1-hexene) prepared by **3** - MAO catalyst system (ethylene 8 atm, 1-hexene 10 mL, run 33, **3** 1.0 μmol, Al/Ti = 3000).



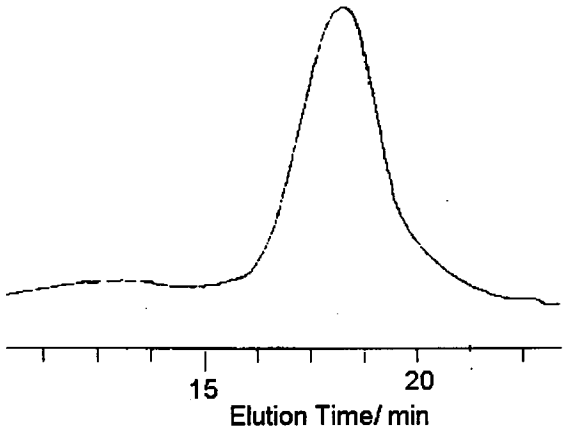
GPC trace for poly(ethylene-*co*-1-hexene) prepared by **3** - MAO catalyst system (ethylene 4 atm, 1-hexene 10 mL, run 34, **3** 1.0 μmol, Al/Ti = 3000).



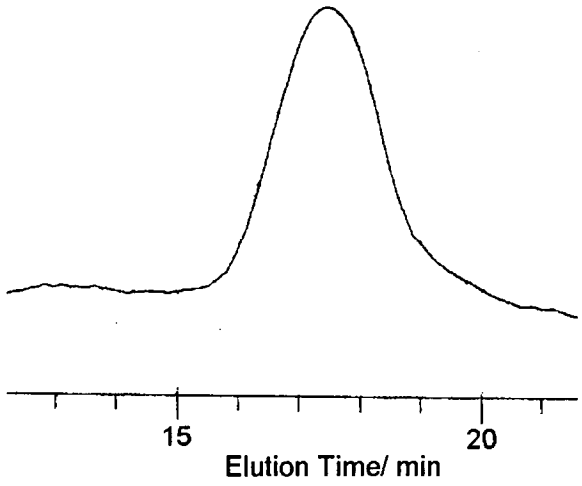
GPC trace for poly(ethylene-*co*-1-hexene) prepared by **6** - MAO catalyst system (ethylene 6 atm, 1-hexene 10 mL, run 41, **6** 10.0 μmol, Al/Ti = 500).



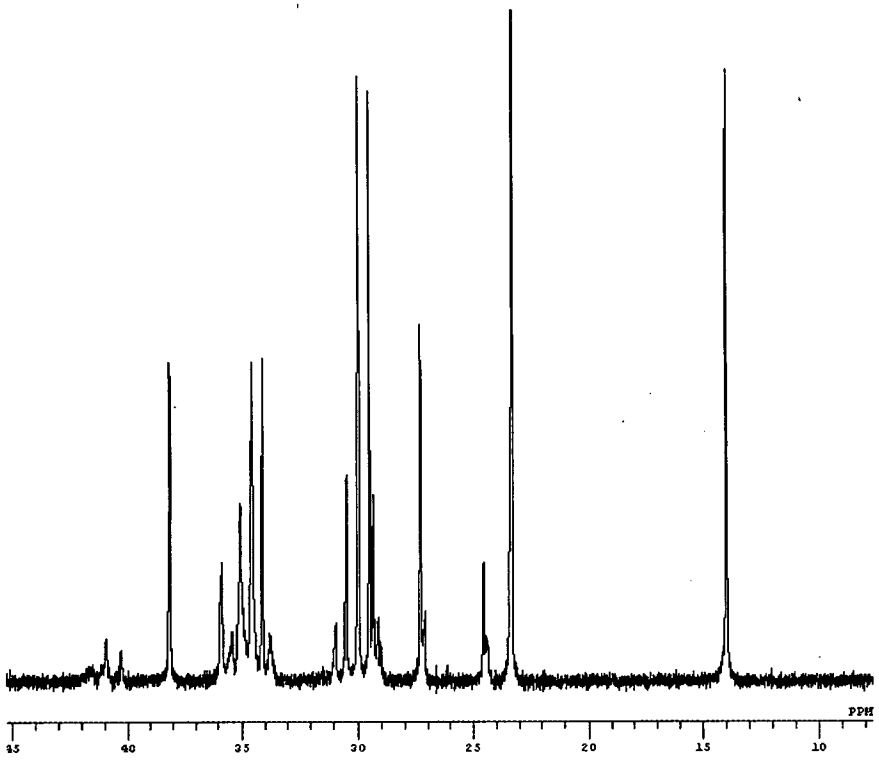
GPC trace for poly(ethylene-*co*-1-hexene) prepared by **6** - MAO catalyst system (ethylene 6 atm, 1-hexene 5 mL, run 42, **6** 10.0 μmol, Al/Ti = 500).



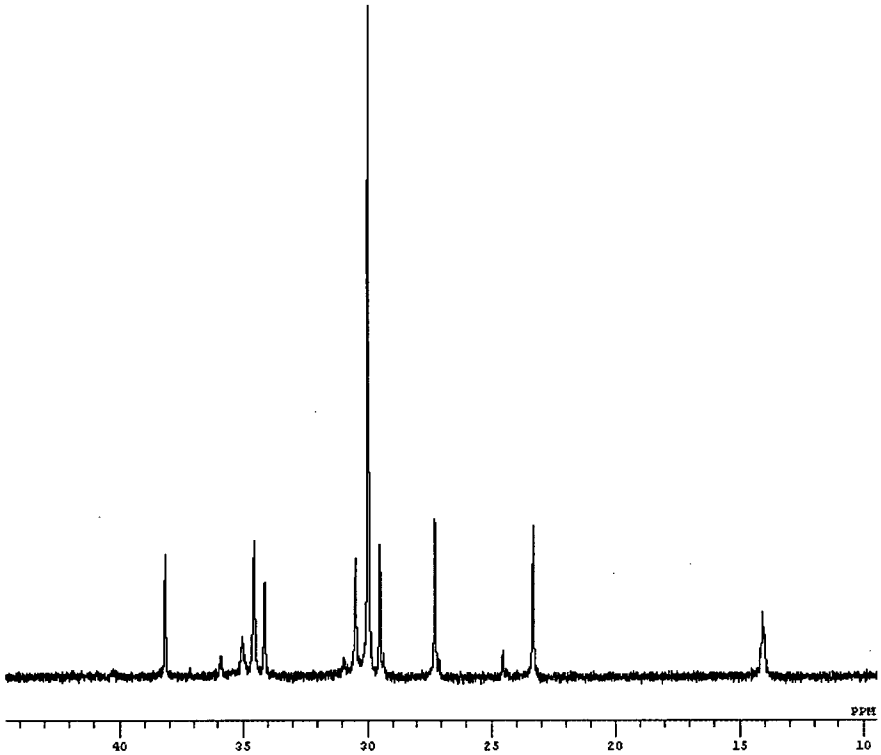
GPC trace for poly(ethylene-*co*-1-hexene) prepared by **6** - MAO catalyst system (ethylene 6 atm, 1-hexene 3 mL, run 43, **6** 10.0 μmol, Al/Ti = 500).



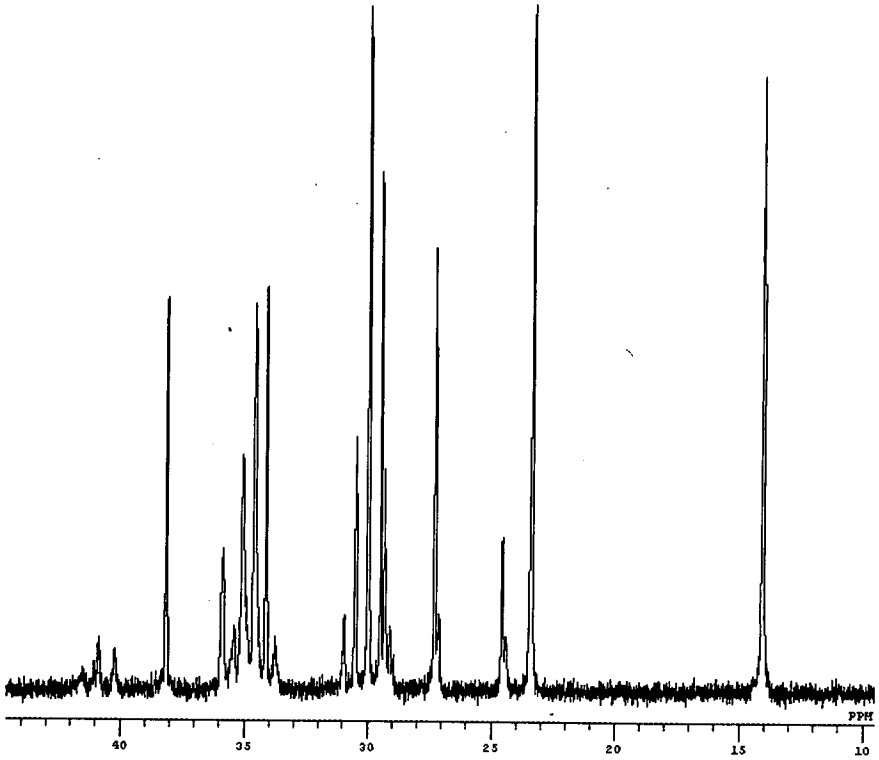
^{13}C NMR spectrum for poly(ethylene-*co*-1-hexene) by $(1,3\text{-}Me_2C_5H_3)TiCl_2N(Cy)Me$ (**4**) - MAO catalyst system (ethylene 6 atm, 1-hexene 10 mL, run 37, **4** 3.0 μmol, Al/Ti = 1000).



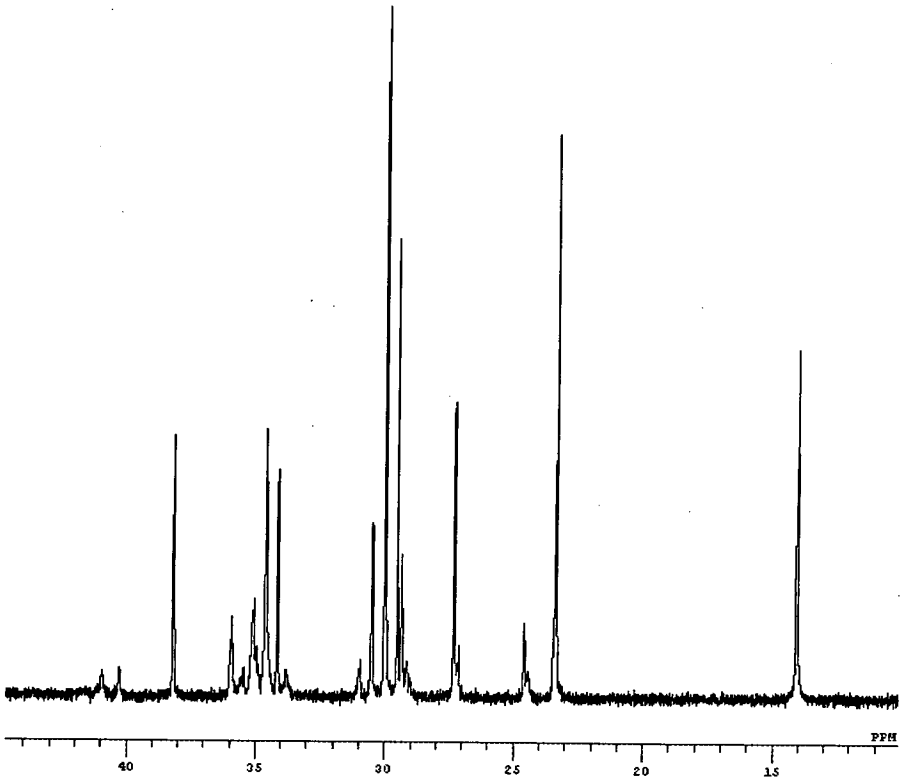
^{13}C NMR spectrum for poly(ethylene-*co*-1-hexene) by $(1,3\text{-}Me_2C_5H_3)TiCl_2N(Cy)Me$ (**4**) - MAO catalyst system (ethylene 6 atm, 1-hexene 3 mL, run 35, **4** 3.0 μmol, Al/Ti = 1000).



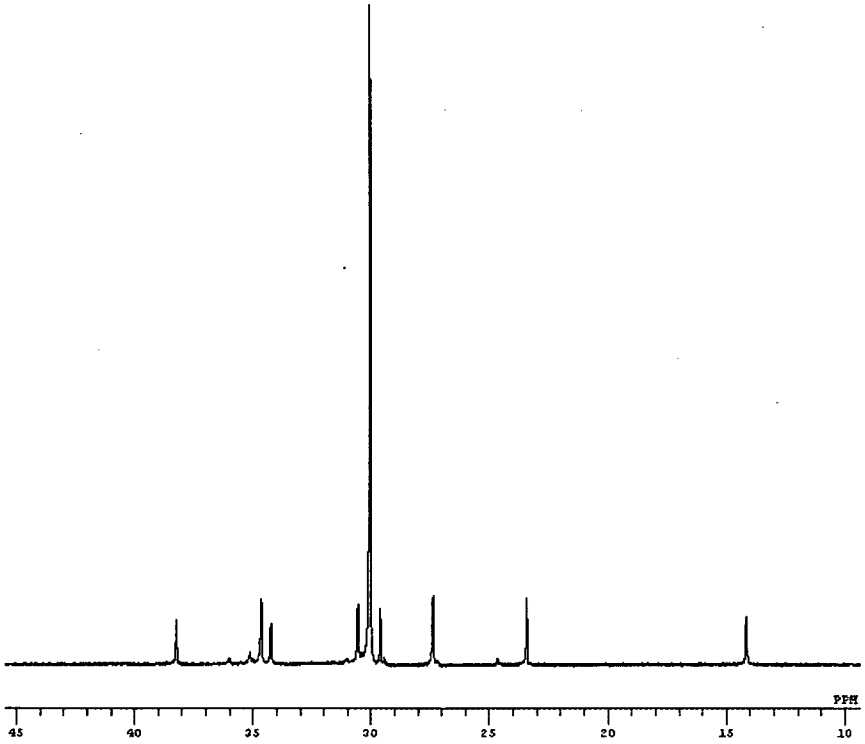
^{13}C NMR spectrum for poly(ethylene-*co*-1-hexene) by $(1,3\text{-}Me_2C_5H_3)TiCl_2N(Cy)Me$ (**4**) - MAO catalyst system (ethylene 4 atm, 1-hexene 10 mL, run 38, **4** 1.0 μmol, Al/Ti = 3000).



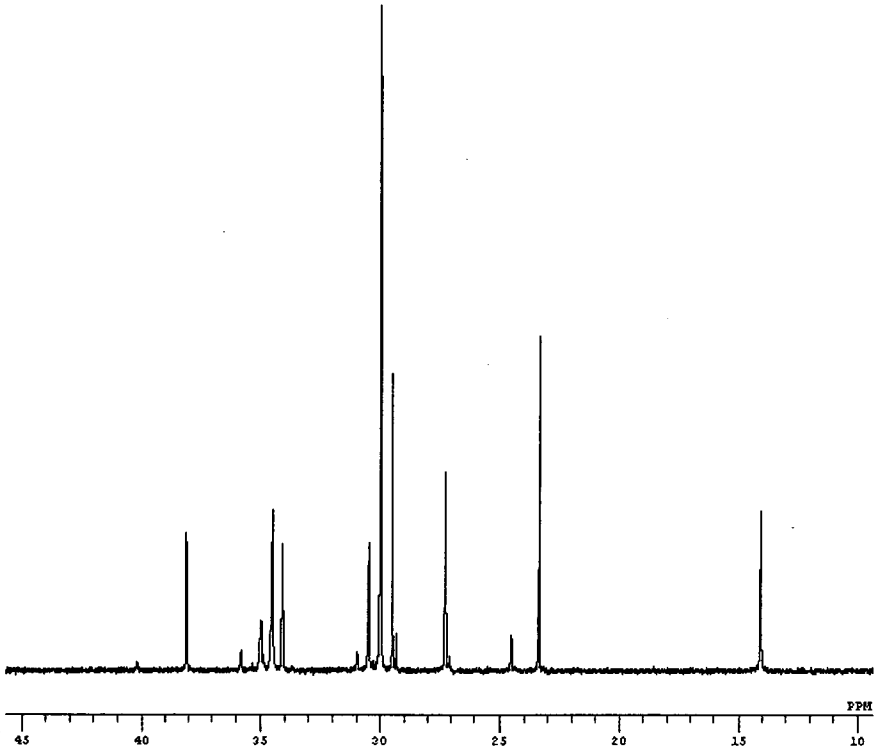
^{13}C NMR spectrum for poly(ethylene-*co*-1-hexene) by $(1,3\text{-}Me_2C_5H_3)TiCl_2NCy_2$ (**5**) - MAO catalyst system (ethylene 6 atm, 1-hexene 10 mL, run 39, **5** 3.0 μmol, Al/Ti = 1000).



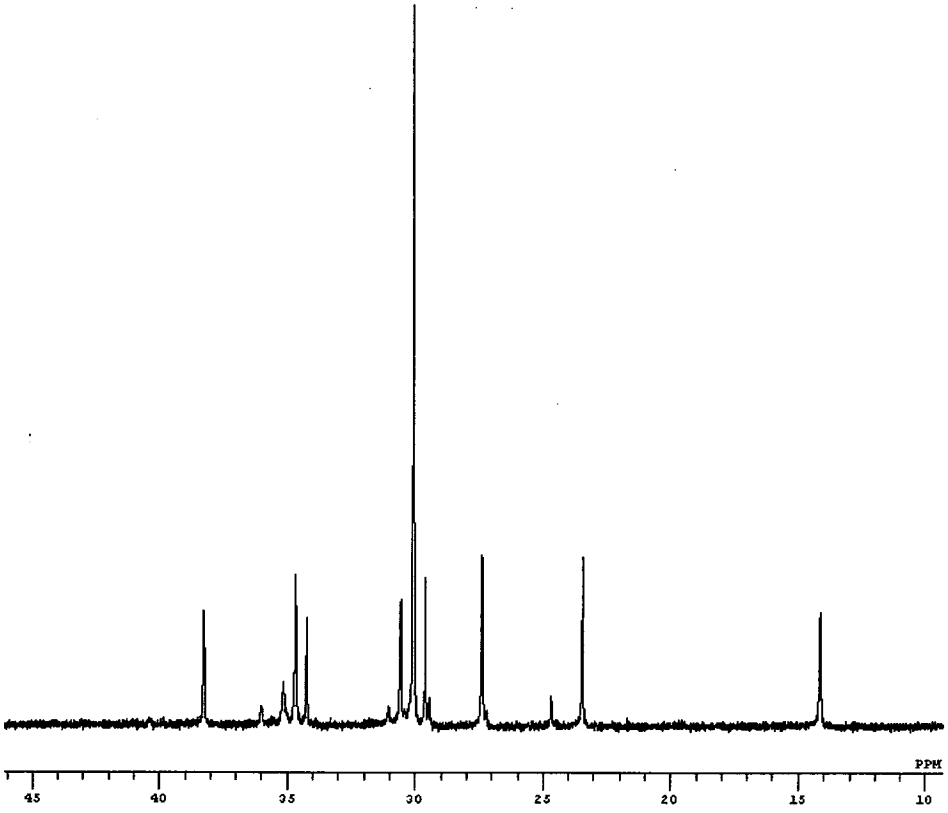
^{13}C NMR spectrum for poly(ethylene-*co*-1-hexene) by $Cp^*TiCl_2NMe_2$ (**1**) - MAO catalyst system (ethylene 8 atm, 1-hexene 10 mL, run 30, **1** 1.0 μmol, Al/Ti = 4000).



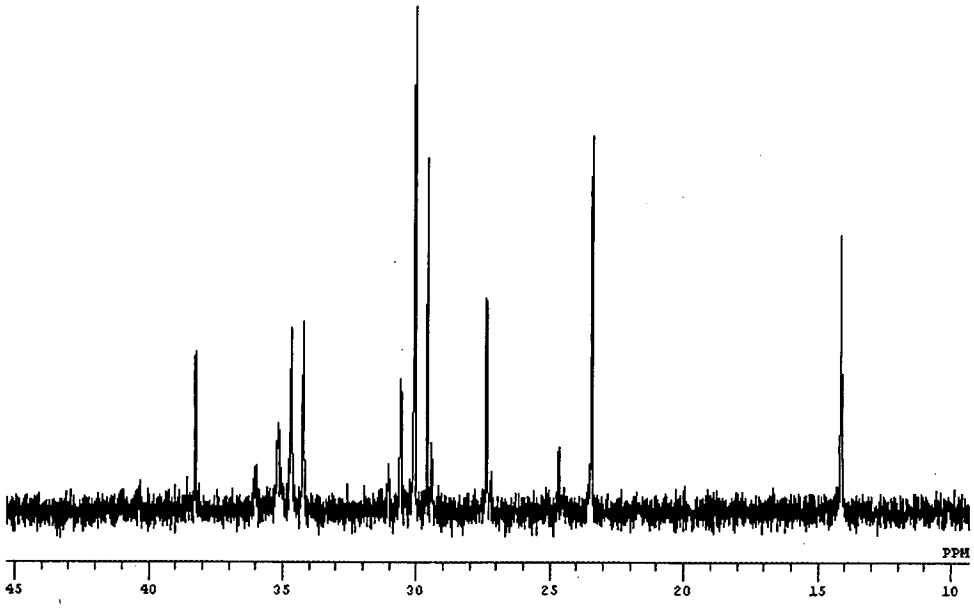
^{13}C NMR spectrum for poly(ethylene-*co*-1-hexene) by $Cp^*TiCl_2N(Cy)Me$ (**3**) - MAO catalyst system (ethylene 6 atm, 1-hexene 10 mL, run 31, **3** 3.0 μmol, Al/Ti = 1000).



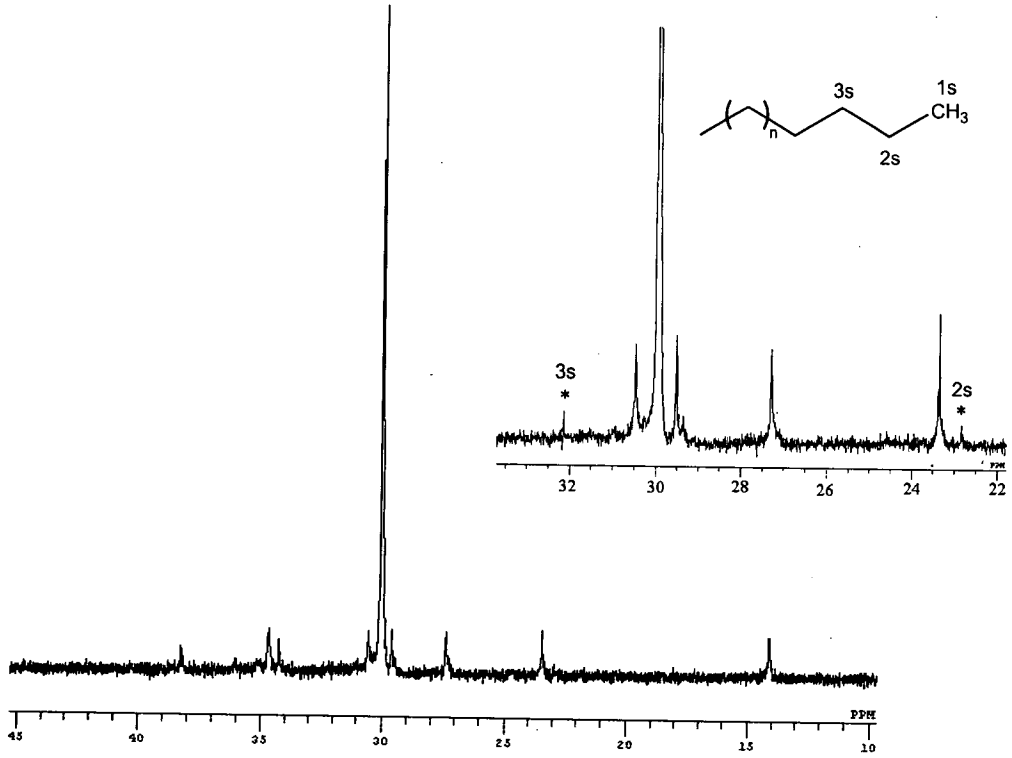
^{13}C NMR spectrum for poly(ethylene-*co*-1-hexene) by Cp*$TiCl_2N$(Cy)Me (**3**) - MAO catalyst system (ethylene 8 atm, 1-hexene 10 mL, run 33, **3** 1.0 μmol, Al/Ti = 3000).



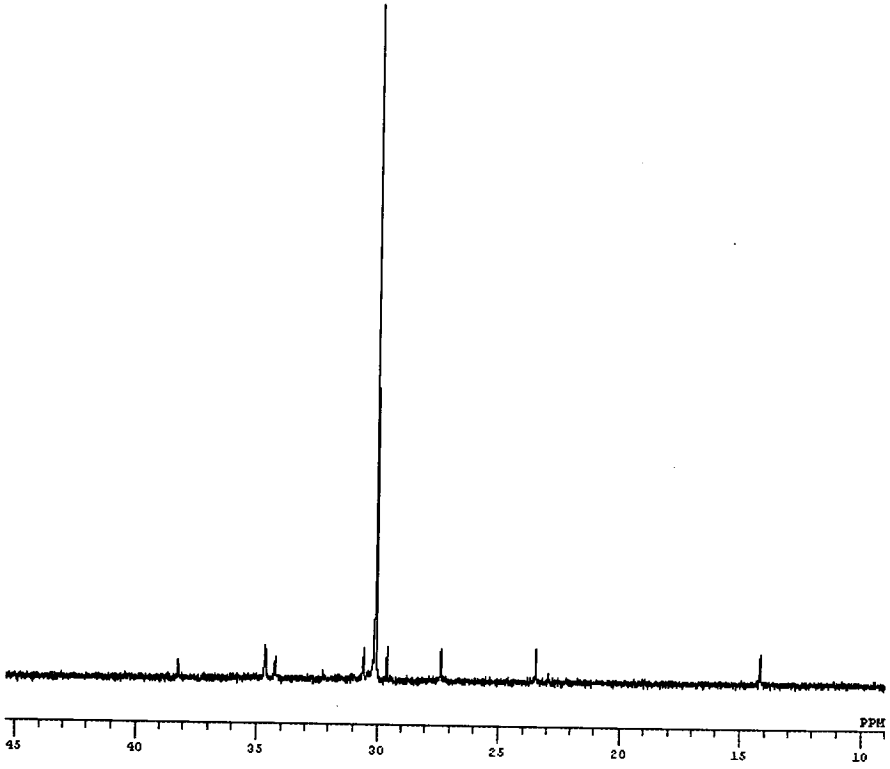
^{13}C NMR spectrum for poly(ethylene-*co*-1-hexene) by Cp*$TiCl_2N$(Cy)Me (**3**) - MAO catalyst system (ethylene 4 atm, 1-hexene 10 mL, run 34, **3** 1.0 μmol, Al/Ti = 3000).



^{13}C NMR spectrum for poly(ethylene-*co*-1-hexene) by $Cp^*TiCl_2[N(SiMe_3)(2,6\text{-}Me_2C_6H_3)]$ - MAO catalyst system (ethylene 6 atm, 1-hexene 5 mL, run 42, **6** 10.0 μmol, Al/Ti = 500).



^{13}C NMR spectrum for poly(ethylene-*co*-1-hexene) by $Cp^*TiCl_2[N(SiMe_3)(2,6\text{-}Me_2C_6H_3)]$ - MAO catalyst system (ethylene 6 atm, 1-hexene 3 mL, run 43, **6** 10.0 μmol, Al/Ti = 500).



X-ray Structure Report

for

$Cp^*TiCl_2[N(Me)Cy]$ (**3**)

Measured on Wed. October 23, 2002

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 12

Experimental

Data Collection

An orange needle crystal of $C_{34}H_{58}Cl_4N_2Ti_2$ having approximate dimensions of 0.80 x 0.21 x 0.17 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS-RAPID Imaging Plate diffractometer with graphite monochromated Mo-Kα radiation.

Indexing was performed from 3 oscillations which were exposed for 3.0 minutes. The camera radius was 127.40 mm. Readout was performed in the 0.200 mm pixel mode.

Cell constants and an orientation matrix for data collection corresponded to a primitive monoclinic cell with dimensions:

a = 8.1771(4) $\AA$
b = 28.245(2) $\AA$ β = 90.249(3)°
c = 16.317(2) $\AA$
V = 3768.6(4) $\AA^3$

For Z = 4 and F.W. = 732.46, the calculated density is 1.29 g/cm^3. The systematic absences of:

h0l: l $\neq$ 2n
0k0: k $\neq$ 2n

uniquely determine the space group to be:

$P2_1/c$ (#14)

The data were collected at a temperature of -30 $\pm$ 1°C to a maximum 2θ value of 55.0°. A total of 44 images, corresponding to 220.0 ° oscillation angles, were collected with 2 different goniometer settings. Exposure time was 2.00 minutes per degree. The camera radius was 127.40 mm. Readout was performed in the 0.200 mm pixel mode. Data were processed by the PROCESS-AUTO program package.

Data Reduction

Of the 31051 reflections which were collected, 8016 were unique (R_{int} = 0.060).

The linear absorption coefficient, μ, for Mo-Kα radiation is 7.3 cm^{-1}. A symmetry-related absorption correction using the program ABSCOR[1] was applied which resulted in transmission factors ranging from 0.49 to 0.88. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 13

The structure was solved by direct methods[2] and expanded using Fourier techniques[3]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[4] was based on 8016 observed reflections (I > -10.00σ(I)) and 379 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma(Fo^2 - Fc^2)/\Sigma Fo^2 = 0.083$$

$$R_w = \sqrt{\Sigma w(Fo^2 - Fc^2)^2/\Sigma w(Fo^2)^2} = 0.135$$

$$R1 = \Sigma||Fo| - |Fc||/\Sigma|Fo| = 0.050 \quad for \;\; I > 2.0\sigma(I) \;\; data$$

The standard deviation of an observation of unit weight[5] was 1.15. The weighting scheme was based on counting statistics and included a factor (p = 0.050) to downweight the intense reflections. Plots of $\Sigma w(Fo^2 - Fc^2)^2$ versus Fo^2, reflection order in data collection, sin θ/λ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.66 and -0.67 $e^-/\AA^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6] . Anomalous dispersion effects were included in Fcalc[7]; the values for Δf' and Δf" were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[9]. All calculations were performed using the teXsan[10] crystallographic software package of Molecular Structure Corporation.

References

(1) ABSCOR: Higashi T. (1995). Program for Absorption Correction, Rigaku Corporation, Tokyo, Japan.

(2) SIR92: Altomare, A., Burla, M.C., Camalli, M., Cascarano, M., Giacovazzo, C., Guagliardi, A., Polidori, G., (1994). J. Appl. Cryst. 27, 435.

(3) DIRDIF94: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M. (1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(4) Least-Squares:

Function minimized: $\Sigma w(Fo^2 - Fc^2)^2$

where w = $\frac{1}{\sigma^2(Fo^2)} = [\sigma_c^2(Fo^2) + (p(Max(Fo^2, 0) + 2Fc^2)/3)^2]^{-1}$

$\sigma_c(Fo^2)$ = e.s.d. based on counting statistics

p = p-factor

(5) Standard deviation of an observation of unit weight:

$$\sqrt{\Sigma w(|Fo| - |Fc|)^2/(No - Nv)}$$

where: No = number of observations

Nv = number of variables

(6) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(7) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(8) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(9) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(10) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1999).

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 15

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{34}H_{58}Cl_4N_2Ti_2$
Formula Weight	732.46
Crystal Color, Habit	orange, needle
Crystal Dimensions	0.80 X 0.21 X 0.17 mm
Crystal System	monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	22252 (5.0 - 55.0°)
Indexing Images	3 oscillations at 3.0 minutes
Camera Radius	127.40 mm
Lattice Parameters	a = 8.1771(4) Å b = 28.245(2) Å c = 16.317(2) Å β = 90.249(3)° V = 3768.6(4) $Å^3$
Space Group	$P2_1/c$ (#14)
Z value	4
D_{calc}	1.291 g/cm^3
F_{000}	1552.00
μ(MoKα)	7.32 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID Imaging Plate
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated

Temperature	-30.0 °C
Voltage, Current	50 kV, 30 mA
Collimator Size	0.8 mm
Detector Aperture	270.0 mm x 256.0 mm
Data Images	44 exposures at 2.0 minutes per degree
Oscillation Range (ϕ=0.0°,χ=45.0°)	ω 130.0 - 190.0° with 5.0° step
Oscillation Range (ϕ=180.0°,χ=45.0°)	ω 0.0 - 160.0° with 5.0° step
Camera Radius	127.40 mm
Pixel Size	0.200 mm
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 31051 Unique: 8016 (R_{int} = 0.060)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.4866 - 0.8830)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = \frac{1}{\sigma^2(Fo^2)}$
p-factor	0.0500
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>-10.00σ(I))	8016
No. Variables	379
Reflection/Parameter Ratio	21.15
Residuals: R; Rw	0.083 ; 0.135
Residuals: R1	0.050

No. of Reflections to calc R1	4842
Goodness of Fit Indicator	1.15
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.66 $e^-/\AA^3$
Minimum peak in Final Diff. Map	-0.67 $e^-/\AA^3$

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 18

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ti(1)	0.21169(7)	0.33452(2)	1.05989(4)	2.06(1)
Ti(2)	0.28023(7)	0.02754(2)	1.19145(4)	2.10(1)
Cl(1)	0.4288(1)	0.38338(4)	1.03013(8)	3.95(2)
Cl(2)	0.3338(1)	0.27751(4)	1.14049(7)	3.95(2)
Cl(3)	0.1346(1)	-0.01260(4)	1.09396(7)	3.95(2)
Cl(4)	0.0837(1)	0.04240(5)	1.28860(7)	4.75(3)
N(1)	0.1622(4)	0.3031(1)	0.9620(2)	2.58(6)
N(2)	0.3227(4)	0.0873(1)	1.1458(2)	2.71(6)
C(1)	-0.0720(4)	0.3377(1)	1.0952(2)	2.34(7)
C(2)	0.0195(4)	0.3397(1)	1.1680(2)	2.60(7)
C(3)	0.1125(4)	0.3820(1)	1.1682(2)	2.79(8)
C(4)	0.0773(4)	0.4062(1)	1.0943(2)	2.68(8)
C(5)	-0.0356(4)	0.3792(1)	1.0489(2)	2.46(7)
C(6)	-0.2030(5)	0.3019(1)	1.0779(3)	3.50(9)
C(7)	0.0043(6)	0.3059(2)	1.2389(3)	4.3(1)
C(8)	0.2224(6)	0.3976(2)	1.2374(3)	5.6(1)
C(9)	0.1359(6)	0.4550(2)	1.0736(4)	4.7(1)
C(10)	-0.1178(5)	0.3957(2)	0.9723(3)	3.80(10)
C(11)	0.0291(5)	0.2916(2)	0.9058(3)	3.97(10)
C(12)	0.3227(4)	0.2833(1)	0.9356(2)	2.57(7)
C(13)	0.3811(5)	0.3017(2)	0.8530(3)	3.62(9)
C(14)	0.5556(6)	0.2849(2)	0.8376(3)	5.2(1)
C(15)	0.5695(7)	0.2316(2)	0.8441(4)	5.9(1)
C(16)	0.5041(6)	0.2134(2)	0.9253(4)	4.8(1)

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 19

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(17)	0.3292(5)	0.2293(1)	0.9400(3)	3.65(9)
C(18)	0.5349(4)	0.0264(1)	1.2633(2)	2.62(7)
C(19)	0.4270(4)	-0.0055(1)	1.3028(2)	2.71(8)
C(20)	0.3890(4)	-0.0426(1)	1.2475(2)	2.65(7)
C(21)	0.4756(4)	-0.0337(1)	1.1741(2)	2.46(7)
C(22)	0.5658(4)	0.0085(1)	1.1836(2)	2.38(7)
C(23)	0.6155(6)	0.0677(2)	1.3040(3)	4.3(1)
C(24)	0.3764(6)	-0.0032(2)	1.3913(3)	4.6(1)
C(25)	0.2836(6)	-0.0846(2)	1.2649(4)	4.7(1)
C(26)	0.4856(6)	-0.0661(2)	1.1018(3)	3.99(10)
C(27)	0.6930(5)	0.0258(2)	1.1245(3)	3.99(10)
C(28)	0.4538(5)	0.1205(2)	1.1291(4)	4.4(1)
C(29)	0.1589(4)	0.1048(1)	1.1196(2)	2.64(7)
C(30)	0.1428(5)	0.1116(1)	1.0279(3)	3.48(9)
C(31)	-0.0299(6)	0.1264(2)	1.0053(3)	4.5(1)
C(32)	-0.0825(6)	0.1702(2)	1.0519(4)	4.9(1)
C(33)	-0.0677(5)	0.1627(2)	1.1433(4)	4.6(1)
C(34)	0.1072(5)	0.1491(1)	1.1668(3)	3.72(9)
H(1)	-0.2883	0.3043	1.1174	4.3482
H(2)	-0.2492	0.3071	1.0246	4.3482
H(3)	-0.1593	0.2705	1.0797	4.3482
H(4)	-0.1043	0.3063	1.2602	5.3536
H(5)	0.0280	0.2742	1.2212	5.3536
H(6)	0.0788	0.3141	1.2815	5.3536

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 20

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(7)	0.3048	0.3747	1.2479	6.8480
H(8)	0.2738	0.4271	1.2242	6.8480
H(9)	0.1595	0.4020	1.2863	6.8480
H(10)	0.2527	0.4561	1.0729	5.9827
H(11)	0.0962	0.4645	1.0208	5.9827
H(12)	0.0980	0.4776	1.1131	5.9827
H(13)	-0.1811	0.4236	0.9832	4.6780
H(14)	-0.0392	0.4031	0.9313	4.6780
H(15)	-0.1898	0.3719	0.9515	4.6780
H(16)	-0.0701	0.3050	0.9257	5.1140
H(17)	0.0516	0.3043	0.8530	5.1140
H(18)	0.0169	0.2583	0.9017	5.1140
H(19)	0.4013	0.2948	0.9748	3.0608
H(20)	0.3115	0.2893	0.8105	4.4083
H(21)	0.3732	0.3356	0.8513	4.4083
H(22)	0.5921	0.2966	0.7853	6.3792
H(23)	0.6264	0.3002	0.8787	6.3792
H(24)	0.5036	0.2177	0.8008	7.2336
H(25)	0.6789	0.2217	0.8370	7.2336
H(26)	0.5104	0.1794	0.9268	5.6528
H(27)	0.5729	0.2252	0.9688	5.6528
H(28)	0.2920	0.2186	0.9926	4.5308
H(29)	0.2589	0.2159	0.8990	4.5308
H(30)	0.6843	0.0571	1.3476	5.3606

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 21

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(31)	0.6820	0.0845	1.2651	5.3606
H(32)	0.5363	0.0890	1.3252	5.3606
H(33)	0.4704	-0.0054	1.4261	5.6267
H(34)	0.3232	0.0265	1.4021	5.6267
H(35)	0.3033	-0.0281	1.4039	5.6267
H(36)	0.2388	-0.0828	1.3180	5.8109
H(37)	0.1970	-0.0866	1.2254	5.8109
H(38)	0.3481	-0.1130	1.2607	5.8109
H(39)	0.4121	-0.0923	1.1086	4.9187
H(40)	0.4548	-0.0496	1.0530	4.9187
H(41)	0.5933	-0.0779	1.0958	4.9187
H(42)	0.7796	0.0033	1.1194	5.0492
H(43)	0.6459	0.0310	1.0715	5.0492
H(44)	0.7397	0.0553	1.1429	5.0492
H(45)	0.5553	0.1074	1.1469	5.5741
H(46)	0.4594	0.1261	1.0713	5.5741
H(47)	0.4345	0.1494	1.1564	5.5741
H(48)	0.0818	0.0805	1.1341	3.1991
H(49)	0.2175	0.1359	1.0106	4.1816
H(50)	0.1714	0.0830	1.0000	4.1816
H(51)	-0.0369	0.1321	0.9476	5.6351
H(52)	-0.1027	0.1007	1.0181	5.6351
H(53)	-0.0131	0.1963	1.0376	5.6910
H(54)	-0.1924	0.1784	1.0388	5.6910

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 22

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(55)	-0.1003	0.1906	1.1718	5.5193
H(56)	-0.1401	0.1374	1.1588	5.5193
H(57)	0.1151	0.1438	1.2245	4.7082
H(58)	0.1794	0.1749	1.1532	4.7082

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 23

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti(1)	0.0214(3)	0.0269(3)	0.0301(3)	0.0003(3)	-0.0021(2)	0.0013(3)
Ti(2)	0.0205(3)	0.0286(3)	0.0306(3)	0.0018(3)	0.0011(2)	0.0009(3)
Cl(1)	0.0318(4)	0.0378(5)	0.0808(8)	-0.0079(4)	0.0152(5)	-0.0096(5)
Cl(2)	0.0524(6)	0.0545(6)	0.0433(6)	0.0181(5)	-0.0063(5)	0.0125(5)
Cl(3)	0.0418(5)	0.0409(5)	0.0673(7)	0.0060(5)	-0.0224(5)	-0.0148(5)
Cl(4)	0.0461(5)	0.0853(8)	0.0493(7)	0.0293(6)	0.0208(5)	0.0168(6)
N(1)	0.028(1)	0.036(2)	0.033(2)	0.003(1)	-0.003(1)	-0.004(1)
N(2)	0.029(1)	0.028(1)	0.046(2)	0.000(1)	-0.005(1)	0.003(1)
C(1)	0.027(2)	0.030(2)	0.032(2)	-0.003(2)	0.001(1)	0.000(2)
C(2)	0.028(2)	0.038(2)	0.033(2)	0.003(2)	0.004(1)	0.006(2)
C(3)	0.031(2)	0.039(2)	0.035(2)	-0.004(2)	0.003(2)	-0.010(2)
C(4)	0.031(2)	0.029(2)	0.041(2)	0.000(2)	0.008(2)	-0.001(2)
C(5)	0.027(2)	0.032(2)	0.035(2)	0.004(2)	0.003(1)	0.002(2)
C(6)	0.030(2)	0.043(2)	0.060(3)	-0.007(2)	-0.001(2)	-0.006(2)
C(7)	0.050(2)	0.072(3)	0.043(3)	0.006(2)	0.004(2)	0.023(2)
C(8)	0.048(3)	0.097(4)	0.066(3)	-0.012(3)	-0.007(2)	-0.038(3)
C(9)	0.055(3)	0.030(2)	0.094(4)	0.000(2)	0.030(3)	0.004(2)
C(10)	0.047(2)	0.054(3)	0.044(3)	0.017(2)	-0.002(2)	0.010(2)
C(11)	0.037(2)	0.069(3)	0.045(3)	0.007(2)	-0.010(2)	-0.016(2)
C(12)	0.029(2)	0.034(2)	0.035(2)	0.004(2)	-0.002(1)	-0.007(2)
C(13)	0.042(2)	0.057(3)	0.038(2)	0.006(2)	0.003(2)	0.001(2)
C(14)	0.046(2)	0.104(4)	0.050(3)	0.007(3)	0.014(2)	0.003(3)
C(15)	0.055(3)	0.099(4)	0.071(4)	0.037(3)	-0.001(3)	-0.027(3)
C(16)	0.058(3)	0.047(2)	0.076(4)	0.022(2)	-0.014(3)	-0.018(2)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(17)	0.050(2)	0.032(2)	0.056(3)	0.003(2)	-0.007(2)	-0.011(2)
C(18)	0.025(2)	0.037(2)	0.038(2)	0.004(2)	-0.005(1)	-0.004(2)
C(19)	0.033(2)	0.045(2)	0.025(2)	0.012(2)	0.000(1)	0.003(2)
C(20)	0.027(2)	0.034(2)	0.040(2)	0.007(2)	0.001(2)	0.006(2)
C(21)	0.030(2)	0.033(2)	0.031(2)	0.011(2)	0.000(1)	-0.002(2)
C(22)	0.022(1)	0.037(2)	0.032(2)	0.006(2)	0.002(1)	0.003(2)
C(23)	0.049(2)	0.048(2)	0.064(3)	-0.001(2)	-0.022(2)	-0.015(2)
C(24)	0.058(3)	0.079(3)	0.036(2)	0.027(3)	0.004(2)	0.004(2)
C(25)	0.051(3)	0.044(2)	0.084(4)	-0.006(2)	0.007(3)	0.020(2)
C(26)	0.049(2)	0.055(3)	0.048(3)	0.016(2)	-0.008(2)	-0.019(2)
C(27)	0.032(2)	0.068(3)	0.051(3)	0.007(2)	0.011(2)	0.015(2)
C(28)	0.034(2)	0.046(2)	0.089(4)	-0.006(2)	-0.002(2)	0.011(3)
C(29)	0.032(2)	0.026(2)	0.042(2)	0.000(2)	-0.001(2)	0.002(2)
C(30)	0.047(2)	0.040(2)	0.045(2)	0.005(2)	-0.001(2)	0.009(2)
C(31)	0.060(3)	0.050(3)	0.059(3)	0.008(2)	-0.015(2)	0.008(2)
C(32)	0.043(2)	0.047(3)	0.095(4)	0.010(2)	-0.015(3)	0.014(3)
C(33)	0.041(2)	0.035(2)	0.098(4)	0.004(2)	0.004(2)	-0.013(2)
C(34)	0.048(2)	0.031(2)	0.062(3)	0.004(2)	-0.001(2)	-0.014(2)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 25

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Ti(1)	Cl(1)	2.302(1)	Ti(1)	Cl(2)	2.304(1)
Ti(1)	N(1)	1.870(3)	Ti(1)	C(1)	2.394(3)
Ti(1)	C(2)	2.372(3)	Ti(1)	C(3)	2.365(4)
Ti(1)	C(4)	2.372(4)	Ti(1)	C(5)	2.389(3)
Ti(2)	Cl(3)	2.284(1)	Ti(2)	Cl(4)	2.301(1)
Ti(2)	N(2)	1.879(3)	Ti(2)	C(18)	2.385(4)
Ti(2)	C(19)	2.366(4)	Ti(2)	C(20)	2.355(4)
Ti(2)	C(21)	2.372(3)	Ti(2)	C(22)	2.400(3)
N(1)	C(11)	1.457(5)	N(1)	C(12)	1.491(4)
N(2)	C(28)	1.451(5)	N(2)	C(29)	1.488(5)
C(1)	C(2)	1.403(5)	C(1)	C(5)	1.426(5)
C(1)	C(6)	1.499(5)	C(2)	C(3)	1.417(5)
C(2)	C(7)	1.507(6)	C(3)	C(4)	1.413(6)
C(3)	C(8)	1.505(6)	C(4)	C(5)	1.407(5)
C(4)	C(9)	1.499(5)	C(5)	C(10)	1.492(6)
C(12)	C(13)	1.523(6)	C(12)	C(17)	1.530(5)
C(13)	C(14)	1.525(6)	C(14)	C(15)	1.515(9)
C(15)	C(16)	1.521(8)	C(16)	C(17)	1.519(6)
C(18)	C(19)	1.419(5)	C(18)	C(22)	1.419(5)
C(18)	C(23)	1.495(6)	C(19)	C(20)	1.417(6)
C(19)	C(24)	1.504(6)	C(20)	C(21)	1.416(5)
C(20)	C(25)	1.494(6)	C(21)	C(22)	1.410(5)
C(21)	C(26)	1.496(5)	C(22)	C(27)	1.504(5)
C(29)	C(30)	1.513(6)	C(29)	C(34)	1.530(5)

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 26

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(30)	C(31)	1.517(6)	C(31)	C(32)	1.515(7)
C(32)	C(33)	1.512(8)	C(33)	C(34)	1.528(6)

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 27

Table 4. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
C(6)	H(1)	0.95	C(6)	H(2)	0.96
C(6)	H(3)	0.96	C(7)	H(4)	0.95
C(7)	H(5)	0.96	C(7)	H(6)	0.95
C(8)	H(7)	0.95	C(8)	H(8)	0.96
C(8)	H(9)	0.96	C(9)	H(10)	0.96
C(9)	H(11)	0.96	C(9)	H(12)	0.96
C(10)	H(13)	0.96	C(10)	H(14)	0.95
C(10)	H(15)	0.96	C(11)	H(16)	0.95
C(11)	H(17)	0.95	C(11)	H(18)	0.95
C(12)	H(19)	0.96	C(13)	H(20)	0.96
C(13)	H(21)	0.96	C(14)	H(22)	0.96
C(14)	H(23)	0.98	C(15)	H(24)	0.97
C(15)	H(25)	0.94	C(16)	H(26)	0.96
C(16)	H(27)	0.96	C(17)	H(28)	0.96
C(17)	H(29)	0.96	C(23)	H(30)	0.95
C(23)	H(31)	0.96	C(23)	H(32)	0.95
C(24)	H(33)	0.96	C(24)	H(34)	0.96
C(24)	H(35)	0.95	C(25)	H(36)	0.94
C(25)	H(37)	0.96	C(25)	H(38)	0.96
C(26)	H(39)	0.96	C(26)	H(40)	0.96
C(26)	H(41)	0.95	C(27)	H(42)	0.96
C(27)	H(43)	0.96	C(27)	H(44)	0.96
C(28)	H(45)	0.95	C(28)	H(46)	0.96
C(28)	H(47)	0.94	C(29)	H(48)	0.96

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 28

Table 4. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(30)	H(49)	0.96	C(30)	H(50)	0.96
C(31)	H(51)	0.96	C(31)	H(52)	0.96
C(32)	H(53)	0.96	C(32)	H(54)	0.95
C(33)	H(55)	0.95	C(33)	H(56)	0.96
C(34)	H(57)	0.96	C(34)	H(58)	0.96

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 29

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
Cl(1)	Ti(1)	Cl(2)	101.92(5)	Cl(1)	Ti(1)	N(1)	105.6(1)
Cl(1)	Ti(1)	C(1)	140.99(9)	Cl(1)	Ti(1)	C(2)	129.3(1)
Cl(1)	Ti(1)	C(3)	94.86(10)	Cl(1)	Ti(1)	C(4)	84.08(9)
Cl(1)	Ti(1)	C(5)	108.72(9)	Cl(2)	Ti(1)	N(1)	104.3(1)
Cl(2)	Ti(1)	C(1)	107.89(9)	Cl(2)	Ti(1)	C(2)	84.58(9)
Cl(2)	Ti(1)	C(3)	96.9(1)	Cl(2)	Ti(1)	C(4)	131.4(1)
Cl(2)	Ti(1)	C(5)	140.94(9)	N(1)	Ti(1)	C(1)	91.0(1)
N(1)	Ti(1)	C(2)	121.5(1)	N(1)	Ti(1)	C(3)	146.5(1)
N(1)	Ti(1)	C(4)	120.6(1)	N(1)	Ti(1)	C(5)	90.4(1)
C(1)	Ti(1)	C(2)	34.2(1)	C(1)	Ti(1)	C(3)	57.5(1)
C(1)	Ti(1)	C(4)	57.4(1)	C(1)	Ti(1)	C(5)	34.7(1)
C(2)	Ti(1)	C(3)	34.8(1)	C(2)	Ti(1)	C(4)	57.4(1)
C(2)	Ti(1)	C(5)	57.3(1)	C(3)	Ti(1)	C(4)	34.7(1)
C(3)	Ti(1)	C(5)	57.6(1)	C(4)	Ti(1)	C(5)	34.4(1)
Cl(3)	Ti(2)	Cl(4)	101.93(5)	Cl(3)	Ti(2)	N(2)	105.5(1)
Cl(3)	Ti(2)	C(18)	141.90(10)	Cl(3)	Ti(2)	C(19)	126.9(1)
Cl(3)	Ti(2)	C(20)	92.7(1)	Cl(3)	Ti(2)	C(21)	84.51(9)
Cl(3)	Ti(2)	C(22)	110.86(10)	Cl(4)	Ti(2)	N(2)	103.9(1)
Cl(4)	Ti(2)	C(18)	105.94(10)	Cl(4)	Ti(2)	C(19)	84.03(9)
Cl(4)	Ti(2)	C(20)	98.61(9)	Cl(4)	Ti(2)	C(21)	133.47(10)
Cl(4)	Ti(2)	C(22)	139.47(10)	N(2)	Ti(2)	C(18)	92.6(1)
N(2)	Ti(2)	C(19)	124.4(1)	N(2)	Ti(2)	C(20)	147.2(1)
N(2)	Ti(2)	C(21)	118.8(1)	N(2)	Ti(2)	C(22)	89.9(1)
C(18)	Ti(2)	C(19)	34.7(1)	C(18)	Ti(2)	C(20)	58.0(1)

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 30

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(18)	Ti(2)	C(21)	57.5(1)	C(18)	Ti(2)	C(22)	34.5(1)
C(19)	Ti(2)	C(20)	34.9(1)	C(19)	Ti(2)	C(21)	57.6(1)
C(19)	Ti(2)	C(22)	57.5(1)	C(20)	Ti(2)	C(21)	34.9(1)
C(20)	Ti(2)	C(22)	57.7(1)	C(21)	Ti(2)	C(22)	34.4(1)
Ti(1)	N(1)	C(11)	143.2(3)	Ti(1)	N(1)	C(12)	103.7(2)
C(11)	N(1)	C(12)	113.1(3)	Ti(2)	N(2)	C(28)	142.5(3)
Ti(2)	N(2)	C(29)	104.1(2)	C(28)	N(2)	C(29)	113.4(3)
Ti(1)	C(1)	C(2)	72.0(2)	Ti(1)	C(1)	C(5)	72.5(2)
Ti(1)	C(1)	C(6)	128.4(3)	C(2)	C(1)	C(5)	107.7(3)
C(2)	C(1)	C(6)	124.3(3)	C(5)	C(1)	C(6)	127.3(3)
Ti(1)	C(2)	C(1)	73.7(2)	Ti(1)	C(2)	C(3)	72.3(2)
Ti(1)	C(2)	C(7)	126.1(3)	C(1)	C(2)	C(3)	108.7(3)
C(1)	C(2)	C(7)	125.4(4)	C(3)	C(2)	C(7)	125.5(4)
Ti(1)	C(3)	C(2)	72.9(2)	Ti(1)	C(3)	C(4)	72.9(2)
Ti(1)	C(3)	C(8)	121.4(3)	C(2)	C(3)	C(4)	107.4(3)
C(2)	C(3)	C(8)	124.5(4)	C(4)	C(3)	C(8)	128.1(4)
Ti(1)	C(4)	C(3)	72.4(2)	Ti(1)	C(4)	C(5)	73.5(2)
Ti(1)	C(4)	C(9)	125.7(2)	C(3)	C(4)	C(5)	108.6(3)
C(3)	C(4)	C(9)	124.9(4)	C(5)	C(4)	C(9)	126.1(4)
Ti(1)	C(5)	C(1)	72.9(2)	Ti(1)	C(5)	C(4)	72.2(2)
Ti(1)	C(5)	C(10)	127.4(3)	C(1)	C(5)	C(4)	107.7(3)
C(1)	C(5)	C(10)	127.4(3)	C(4)	C(5)	C(10)	124.3(3)
N(1)	C(12)	C(13)	114.1(3)	N(1)	C(12)	C(17)	112.9(3)
C(13)	C(12)	C(17)	111.7(3)	C(12)	C(13)	C(14)	109.8(4)

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 31

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(13)	C(14)	C(15)	111.5(4)	C(14)	C(15)	C(16)	111.7(4)
C(15)	C(16)	C(17)	111.9(4)	C(12)	C(17)	C(16)	108.6(4)
Ti(2)	C(18)	C(19)	71.9(2)	Ti(2)	C(18)	C(22)	73.3(2)
Ti(2)	C(18)	C(23)	126.2(3)	C(19)	C(18)	C(22)	107.7(3)
C(19)	C(18)	C(23)	124.6(4)	C(22)	C(18)	C(23)	127.3(4)
Ti(2)	C(19)	C(18)	73.4(2)	Ti(2)	C(19)	C(20)	72.1(2)
Ti(2)	C(19)	C(24)	125.4(3)	C(18)	C(19)	C(20)	108.4(3)
C(18)	C(19)	C(24)	125.6(4)	C(20)	C(19)	C(24)	125.7(4)
Ti(2)	C(20)	C(19)	72.9(2)	Ti(2)	C(20)	C(21)	73.2(2)
Ti(2)	C(20)	C(25)	121.6(3)	C(19)	C(20)	C(21)	107.4(3)
C(19)	C(20)	C(25)	126.2(4)	C(21)	C(20)	C(25)	126.4(4)
Ti(2)	C(21)	C(20)	71.9(2)	Ti(2)	C(21)	C(22)	73.9(2)
Ti(2)	C(21)	C(26)	125.4(3)	C(20)	C(21)	C(22)	108.7(3)
C(20)	C(21)	C(26)	125.9(4)	C(22)	C(21)	C(26)	125.0(3)
Ti(2)	C(22)	C(18)	72.2(2)	Ti(2)	C(22)	C(21)	71.7(2)
Ti(2)	C(22)	C(27)	129.6(3)	C(18)	C(22)	C(21)	107.9(3)
C(18)	C(22)	C(27)	126.7(4)	C(21)	C(22)	C(27)	124.6(3)
N(2)	C(29)	C(30)	113.6(3)	N(2)	C(29)	C(34)	112.1(3)
C(30)	C(29)	C(34)	111.8(3)	C(29)	C(30)	C(31)	110.7(4)
C(30)	C(31)	C(32)	111.7(4)	C(31)	C(32)	C(33)	111.0(4)
C(32)	C(33)	C(34)	110.7(4)	C(29)	C(34)	C(33)	109.8(4)

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 32

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	C(6)	H(1)	110.5	C(1)	C(6)	H(2)	110.3
C(1)	C(6)	H(3)	110.7	H(1)	C(6)	H(2)	108.4
H(1)	C(6)	H(3)	108.6	H(2)	C(6)	H(3)	108.3
C(2)	C(7)	H(4)	110.5	C(2)	C(7)	H(5)	110.1
C(2)	C(7)	H(6)	110.6	H(4)	C(7)	H(5)	108.1
H(4)	C(7)	H(6)	109.0	H(5)	C(7)	H(6)	108.5
C(3)	C(8)	H(7)	110.9	C(3)	C(8)	H(8)	110.3
C(3)	C(8)	H(9)	110.0	H(7)	C(8)	H(8)	108.8
H(7)	C(8)	H(9)	108.8	H(8)	C(8)	H(9)	108.0
C(4)	C(9)	H(10)	110.5	C(4)	C(9)	H(11)	110.6
C(4)	C(9)	H(12)	110.8	H(10)	C(9)	H(11)	108.4
H(10)	C(9)	H(12)	108.3	H(11)	C(9)	H(12)	108.2
C(5)	C(10)	H(13)	110.1	C(5)	C(10)	H(14)	110.6
C(5)	C(10)	H(15)	110.5	H(13)	C(10)	H(14)	108.6
H(13)	C(10)	H(15)	108.2	H(14)	C(10)	H(15)	108.8
N(1)	C(11)	H(16)	109.5	N(1)	C(11)	H(17)	109.8
N(1)	C(11)	H(18)	110.0	H(16)	C(11)	H(17)	109.0
H(16)	C(11)	H(18)	109.2	H(17)	C(11)	H(18)	109.3
N(1)	C(12)	H(19)	105.6	C(13)	C(12)	H(19)	105.2
C(17)	C(12)	H(19)	106.5	C(12)	C(13)	H(20)	109.2
C(12)	C(13)	H(21)	110.1	C(14)	C(13)	H(20)	108.7
C(14)	C(13)	H(21)	111.6	H(20)	C(13)	H(21)	107.5
C(13)	C(14)	H(22)	109.5	C(13)	C(14)	H(23)	107.5
C(15)	C(14)	H(22)	112.3	C(15)	C(14)	H(23)	110.2

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 33

Table 6. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
H(22)	C(14)	H(23)	105.6	C(14)	C(15)	H(24)	108.0
C(14)	C(15)	H(25)	110.9	C(16)	C(15)	H(24)	107.6
C(16)	C(15)	H(25)	110.1	H(24)	C(15)	H(25)	108.4
C(15)	C(16)	H(26)	109.8	C(15)	C(16)	H(27)	108.6
C(17)	C(16)	H(26)	110.0	C(17)	C(16)	H(27)	109.2
H(26)	C(16)	H(27)	107.2	C(12)	C(17)	H(28)	110.2
C(12)	C(17)	H(29)	109.9	C(16)	C(17)	H(28)	110.5
C(16)	C(17)	H(29)	109.6	H(28)	C(17)	H(29)	108.0
C(18)	C(23)	H(30)	110.1	C(18)	C(23)	H(31)	109.9
C(18)	C(23)	H(32)	110.8	H(30)	C(23)	H(31)	108.2
H(30)	C(23)	H(32)	109.3	H(31)	C(23)	H(32)	108.4
C(19)	C(24)	H(33)	110.1	C(19)	C(24)	H(34)	110.0
C(19)	C(24)	H(35)	110.7	H(33)	C(24)	H(34)	108.0
H(33)	C(24)	H(35)	109.2	H(34)	C(24)	H(35)	108.8
C(20)	C(25)	H(36)	110.9	C(20)	C(25)	H(37)	110.1
C(20)	C(25)	H(38)	109.3	H(36)	C(25)	H(37)	109.4
H(36)	C(25)	H(38)	109.0	H(37)	C(25)	H(38)	107.9
C(21)	C(26)	H(39)	110.2	C(21)	C(26)	H(40)	110.0
C(21)	C(26)	H(41)	110.5	H(39)	C(26)	H(40)	108.1
H(39)	C(26)	H(41)	108.9	H(40)	C(26)	H(41)	109.2
C(22)	C(27)	H(42)	110.7	C(22)	C(27)	H(43)	110.6
C(22)	C(27)	H(44)	110.9	H(42)	C(27)	H(43)	108.6
H(42)	C(27)	H(44)	108.0	H(43)	C(27)	H(44)	108.0
N(2)	C(28)	H(45)	109.6	N(2)	C(28)	H(46)	109.2

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 34

Table 6. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
N(2)	C(28)	H(47)	110.2	H(45)	C(28)	H(46)	108.6
H(45)	C(28)	H(47)	109.8	H(46)	C(28)	H(47)	109.5
N(2)	C(29)	H(48)	106.5	C(30)	C(29)	H(48)	106.1
C(34)	C(29)	H(48)	106.0	C(29)	C(30)	H(49)	109.1
C(29)	C(30)	H(50)	110.2	C(31)	C(30)	H(49)	108.8
C(31)	C(30)	H(50)	110.3	H(49)	C(30)	H(50)	107.8
C(30)	C(31)	H(51)	109.8	C(30)	C(31)	H(52)	108.3
C(32)	C(31)	H(51)	109.8	C(32)	C(31)	H(52)	109.2
H(51)	C(31)	H(52)	107.9	C(31)	C(32)	H(53)	109.7
C(31)	C(32)	H(54)	110.9	C(33)	C(32)	H(53)	107.6
C(33)	C(32)	H(54)	109.0	H(53)	C(32)	H(54)	108.5
C(32)	C(33)	H(55)	110.1	C(32)	C(33)	H(56)	108.5
C(34)	C(33)	H(55)	110.4	C(34)	C(33)	H(56)	108.9
H(55)	C(33)	H(56)	108.1	C(29)	C(34)	H(57)	110.4
C(29)	C(34)	H(58)	109.3	C(33)	C(34)	H(57)	110.3
C(33)	C(34)	H(58)	109.1	H(57)	C(34)	H(58)	107.9

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 35

Table 7. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Ti(1)	N(1)	C(12)	C(13)	-119.0(3)	Ti(1)	N(1)	C(12)	C(17)	112.0(3)
Ti(1)	C(1)	C(2)	C(3)	64.4(2)	Ti(1)	C(1)	C(2)	C(7)	-123.1(4)
Ti(1)	C(1)	C(5)	C(4)	-64.2(2)	Ti(1)	C(1)	C(5)	C(10)	124.3(4)
Ti(1)	C(2)	C(1)	C(5)	-64.1(2)	Ti(1)	C(2)	C(1)	C(6)	124.8(3)
Ti(1)	C(2)	C(3)	C(4)	65.3(2)	Ti(1)	C(2)	C(3)	C(8)	-116.7(4)
Ti(1)	C(3)	C(2)	C(1)	-65.3(2)	Ti(1)	C(3)	C(2)	C(7)	122.2(4)
Ti(1)	C(3)	C(4)	C(5)	65.1(2)	Ti(1)	C(3)	C(4)	C(9)	-121.6(4)
Ti(1)	C(4)	C(3)	C(2)	-65.3(2)	Ti(1)	C(4)	C(3)	C(8)	116.8(4)
Ti(1)	C(4)	C(5)	C(1)	64.7(2)	Ti(1)	C(4)	C(5)	C(10)	-123.5(3)
Ti(1)	C(5)	C(1)	C(2)	63.9(2)	Ti(1)	C(5)	C(1)	C(6)	-125.4(4)
Ti(1)	C(5)	C(4)	C(3)	-64.3(2)	Ti(1)	C(5)	C(4)	C(9)	122.4(4)
Ti(2)	N(2)	C(29)	C(30)	-116.2(3)	Ti(2)	N(2)	C(29)	C(34)	115.9(3)
Ti(2)	C(18)	C(19)	C(20)	64.1(3)	Ti(2)	C(18)	C(19)	C(24)	-122.0(4)
Ti(2)	C(18)	C(22)	C(21)	-63.3(2)	Ti(2)	C(18)	C(22)	C(27)	126.5(4)
Ti(2)	C(19)	C(18)	C(22)	-65.1(2)	Ti(2)	C(19)	C(18)	C(23)	121.9(4)
Ti(2)	C(19)	C(20)	C(21)	65.7(2)	Ti(2)	C(19)	C(20)	C(25)	-117.1(4)
Ti(2)	C(20)	C(19)	C(18)	-64.9(3)	Ti(2)	C(20)	C(19)	C(24)	121.2(4)
Ti(2)	C(20)	C(21)	C(22)	65.3(2)	Ti(2)	C(20)	C(21)	C(26)	-121.1(4)
Ti(2)	C(21)	C(20)	C(19)	-65.5(2)	Ti(2)	C(21)	C(20)	C(25)	117.3(4)
Ti(2)	C(21)	C(22)	C(18)	63.6(2)	Ti(2)	C(21)	C(22)	C(27)	-126.0(4)
Ti(2)	C(22)	C(18)	C(19)	64.1(2)	Ti(2)	C(22)	C(18)	C(23)	-123.1(4)
Ti(2)	C(22)	C(21)	C(20)	-64.0(2)	Ti(2)	C(22)	C(21)	C(26)	122.3(4)
Cl(1)	Ti(1)	N(1)	C(11)	-128.6(5)	Cl(1)	Ti(1)	N(1)	C(12)	51.6(2)
Cl(1)	Ti(1)	C(1)	C(2)	-88.6(2)	Cl(1)	Ti(1)	C(1)	C(5)	27.4(3)

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 36

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Cl(1)	Ti(1)	C(1)	C(6)	151.4(3)	Cl(1)	Ti(1)	C(2)	C(1)	125.6(2)
Cl(1)	Ti(1)	C(2)	C(3)	9.3(3)	Cl(1)	Ti(1)	C(2)	C(7)	-112.1(3)
Cl(1)	Ti(1)	C(3)	C(2)	-172.8(2)	Cl(1)	Ti(1)	C(3)	C(4)	72.3(2)
Cl(1)	Ti(1)	C(3)	C(8)	-52.4(4)	Cl(1)	Ti(1)	C(4)	C(3)	-107.4(2)
Cl(1)	Ti(1)	C(4)	C(5)	136.3(2)	Cl(1)	Ti(1)	C(4)	C(9)	13.3(4)
Cl(1)	Ti(1)	C(5)	C(1)	-162.2(2)	Cl(1)	Ti(1)	C(5)	C(4)	-46.5(2)
Cl(1)	Ti(1)	C(5)	C(10)	73.5(3)	Cl(2)	Ti(1)	N(1)	C(11)	124.4(5)
Cl(2)	Ti(1)	N(1)	C(12)	-55.4(2)	Cl(2)	Ti(1)	C(1)	C(2)	49.4(2)
Cl(2)	Ti(1)	C(1)	C(5)	165.4(2)	Cl(2)	Ti(1)	C(1)	C(6)	-70.6(3)
Cl(2)	Ti(1)	C(2)	C(1)	-133.4(2)	Cl(2)	Ti(1)	C(2)	C(3)	110.3(2)
Cl(2)	Ti(1)	C(2)	C(7)	-11.2(4)	Cl(2)	Ti(1)	C(3)	C(2)	-70.2(2)
Cl(2)	Ti(1)	C(3)	C(4)	174.9(2)	Cl(2)	Ti(1)	C(3)	C(8)	50.2(4)
Cl(2)	Ti(1)	C(4)	C(3)	-6.7(3)	Cl(2)	Ti(1)	C(4)	C(5)	-123.0(2)
Cl(2)	Ti(1)	C(4)	C(9)	114.0(4)	Cl(2)	Ti(1)	C(5)	C(1)	-22.4(3)
Cl(2)	Ti(1)	C(5)	C(4)	93.3(2)	Cl(2)	Ti(1)	C(5)	C(10)	-146.7(3)
Cl(3)	Ti(2)	N(2)	C(28)	-128.1(5)	Cl(3)	Ti(2)	N(2)	C(29)	52.7(2)
Cl(3)	Ti(2)	C(18)	C(19)	-82.4(2)	Cl(3)	Ti(2)	C(18)	C(22)	33.2(3)
Cl(3)	Ti(2)	C(18)	C(23)	157.5(3)	Cl(3)	Ti(2)	C(19)	C(18)	130.1(2)
Cl(3)	Ti(2)	C(19)	C(20)	13.9(2)	Cl(3)	Ti(2)	C(19)	C(24)	-107.6(4)
Cl(3)	Ti(2)	C(20)	C(19)	-168.9(2)	Cl(3)	Ti(2)	C(20)	C(21)	76.4(2)
Cl(3)	Ti(2)	C(20)	C(25)	-46.4(4)	Cl(3)	Ti(2)	C(21)	C(20)	-102.8(2)
Cl(3)	Ti(2)	C(21)	C(22)	140.8(2)	Cl(3)	Ti(2)	C(21)	C(26)	18.9(3)
Cl(3)	Ti(2)	C(22)	C(18)	-158.8(2)	Cl(3)	Ti(2)	C(22)	C(21)	-42.3(2)
Cl(3)	Ti(2)	C(22)	C(27)	77.8(4)	Cl(4)	Ti(2)	N(2)	C(28)	125.1(5)

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 37

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Cl(4)	Ti(2)	N(2)	C(29)	-54.2(2)	Cl(4)	Ti(2)	C(18)	C(19)	53.0(2)
Cl(4)	Ti(2)	C(18)	C(22)	168.6(2)	Cl(4)	Ti(2)	C(18)	C(23)	-67.0(4)
Cl(4)	Ti(2)	C(19)	C(18)	-129.4(2)	Cl(4)	Ti(2)	C(19)	C(20)	114.4(2)
Cl(4)	Ti(2)	C(19)	C(24)	-7.2(4)	Cl(4)	Ti(2)	C(20)	C(19)	-66.4(2)
Cl(4)	Ti(2)	C(20)	C(21)	178.9(2)	Cl(4)	Ti(2)	C(20)	C(25)	56.1(4)
Cl(4)	Ti(2)	C(21)	C(20)	-1.6(3)	Cl(4)	Ti(2)	C(21)	C(22)	-118.0(2)
Cl(4)	Ti(2)	C(21)	C(26)	120.1(3)	Cl(4)	Ti(2)	C(22)	C(18)	-17.0(3)
Cl(4)	Ti(2)	C(22)	C(21)	99.5(2)	Cl(4)	Ti(2)	C(22)	C(27)	-140.3(3)
N(1)	Ti(1)	C(1)	C(2)	154.8(2)	N(1)	Ti(1)	C(1)	C(5)	-89.3(2)
N(1)	Ti(1)	C(1)	C(6)	34.8(4)	N(1)	Ti(1)	C(2)	C(1)	-30.0(3)
N(1)	Ti(1)	C(2)	C(3)	-146.3(2)	N(1)	Ti(1)	C(2)	C(7)	92.3(4)
N(1)	Ti(1)	C(3)	C(2)	59.1(4)	N(1)	Ti(1)	C(3)	C(4)	-55.9(3)
N(1)	Ti(1)	C(3)	C(8)	179.4(4)	N(1)	Ti(1)	C(4)	C(3)	148.0(2)
N(1)	Ti(1)	C(4)	C(5)	31.7(3)	N(1)	Ti(1)	C(4)	C(9)	-91.3(4)
N(1)	Ti(1)	C(5)	C(1)	91.1(2)	N(1)	Ti(1)	C(5)	C(4)	-153.1(2)
N(1)	Ti(1)	C(5)	C(10)	-33.2(3)	N(1)	C(12)	C(13)	C(14)	172.0(4)
N(1)	C(12)	C(17)	C(16)	-171.0(4)	N(2)	Ti(2)	C(18)	C(19)	158.2(2)
N(2)	Ti(2)	C(18)	C(22)	-86.2(2)	N(2)	Ti(2)	C(18)	C(23)	38.2(4)
N(2)	Ti(2)	C(19)	C(18)	-26.7(3)	N(2)	Ti(2)	C(19)	C(20)	-142.9(2)
N(2)	Ti(2)	C(19)	C(24)	95.6(4)	N(2)	Ti(2)	C(20)	C(19)	66.6(3)
N(2)	Ti(2)	C(20)	C(21)	-48.2(4)	N(2)	Ti(2)	C(20)	C(25)	-170.9(3)
N(2)	Ti(2)	C(21)	C(20)	152.5(2)	N(2)	Ti(2)	C(21)	C(22)	36.1(3)
N(2)	Ti(2)	C(21)	C(26)	-85.8(4)	N(2)	Ti(2)	C(22)	C(18)	94.6(2)
N(2)	Ti(2)	C(22)	C(21)	-148.9(2)	N(2)	Ti(2)	C(22)	C(27)	-28.7(4)

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 38

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
N(2)	C(29)	C(30)	C(31)	176.5(3)	N(2)	C(29)	C(34)	C(33)	-174.7(4)
C(1)	Ti(1)	N(1)	C(11)	15.7(5)	C(1)	Ti(1)	N(1)	C(12)	-164.1(2)
C(1)	Ti(1)	C(2)	C(3)	-116.3(3)	C(1)	Ti(1)	C(2)	C(7)	122.3(5)
C(1)	Ti(1)	C(3)	C(2)	36.7(2)	C(1)	Ti(1)	C(3)	C(4)	-78.2(2)
C(1)	Ti(1)	C(3)	C(8)	157.1(4)	C(1)	Ti(1)	C(4)	C(3)	78.8(2)
C(1)	Ti(1)	C(4)	C(5)	-37.5(2)	C(1)	Ti(1)	C(4)	C(9)	-160.5(5)
C(1)	Ti(1)	C(5)	C(4)	115.7(3)	C(1)	Ti(1)	C(5)	C(10)	-124.3(4)
C(1)	C(2)	Ti(1)	C(3)	116.3(3)	C(1)	C(2)	Ti(1)	C(4)	78.5(2)
C(1)	C(2)	Ti(1)	C(5)	37.4(2)	C(1)	C(2)	C(3)	C(4)	0.0(4)
C(1)	C(2)	C(3)	C(8)	178.0(4)	C(1)	C(5)	Ti(1)	C(2)	-36.9(2)
C(1)	C(5)	Ti(1)	C(3)	-78.5(2)	C(1)	C(5)	Ti(1)	C(4)	-115.7(3)
C(1)	C(5)	C(4)	C(3)	0.3(4)	C(1)	C(5)	C(4)	C(9)	-172.9(3)
C(2)	Ti(1)	N(1)	C(11)	32.0(5)	C(2)	Ti(1)	N(1)	C(12)	-147.8(2)
C(2)	Ti(1)	C(1)	C(5)	115.9(3)	C(2)	Ti(1)	C(1)	C(6)	-120.0(4)
C(2)	Ti(1)	C(3)	C(4)	-114.9(3)	C(2)	Ti(1)	C(3)	C(8)	120.4(5)
C(2)	Ti(1)	C(4)	C(3)	37.9(2)	C(2)	Ti(1)	C(4)	C(5)	-78.4(2)
C(2)	Ti(1)	C(4)	C(9)	158.6(5)	C(2)	Ti(1)	C(5)	C(4)	78.8(2)
C(2)	Ti(1)	C(5)	C(10)	-161.2(4)	C(2)	C(1)	Ti(1)	C(3)	-37.3(2)
C(2)	C(1)	Ti(1)	C(4)	-78.8(2)	C(2)	C(1)	Ti(1)	C(5)	-115.9(3)
C(2)	C(1)	C(5)	C(4)	-0.4(4)	C(2)	C(1)	C(5)	C(10)	-171.8(4)
C(2)	C(3)	Ti(1)	C(4)	114.9(3)	C(2)	C(3)	Ti(1)	C(5)	78.1(2)
C(2)	C(3)	C(4)	C(5)	-0.2(4)	C(2)	C(3)	C(4)	C(9)	173.1(3)
C(3)	Ti(1)	N(1)	C(11)	-3.1(6)	C(3)	Ti(1)	N(1)	C(12)	177.1(2)
C(3)	Ti(1)	C(1)	C(5)	78.6(2)	C(3)	Ti(1)	C(1)	C(6)	-157.3(4)

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 39

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(3)	Ti(1)	C(2)	C(7)	-121.4(5)	C(3)	Ti(1)	C(4)	C(5)	-116.3(3)
C(3)	Ti(1)	C(4)	C(9)	120.7(5)	C(3)	Ti(1)	C(5)	C(4)	37.2(2)
C(3)	Ti(1)	C(5)	C(10)	157.2(4)	C(3)	C(2)	Ti(1)	C(4)	-37.8(2)
C(3)	C(2)	Ti(1)	C(5)	-78.9(2)	C(3)	C(2)	C(1)	C(5)	0.2(4)
C(3)	C(2)	C(1)	C(6)	-170.9(3)	C(3)	C(4)	Ti(1)	C(5)	116.3(3)
C(3)	C(4)	C(5)	C(10)	172.2(3)	C(4)	Ti(1)	N(1)	C(11)	-36.3(5)
C(4)	Ti(1)	N(1)	C(12)	143.9(2)	C(4)	Ti(1)	C(1)	C(5)	37.2(2)
C(4)	Ti(1)	C(1)	C(6)	161.2(4)	C(4)	Ti(1)	C(2)	C(7)	-159.2(4)
C(4)	Ti(1)	C(3)	C(8)	-124.7(5)	C(4)	Ti(1)	C(5)	C(10)	120.0(4)
C(4)	C(3)	Ti(1)	C(5)	-36.8(2)	C(4)	C(3)	C(2)	C(7)	-172.6(4)
C(4)	C(5)	C(1)	C(6)	170.4(3)	C(5)	Ti(1)	N(1)	C(11)	-19.0(5)
C(5)	Ti(1)	N(1)	C(12)	161.2(2)	C(5)	Ti(1)	C(1)	C(6)	124.1(4)
C(5)	Ti(1)	C(2)	C(7)	159.7(4)	C(5)	Ti(1)	C(3)	C(8)	-161.6(4)
C(5)	Ti(1)	C(4)	C(9)	-123.0(5)	C(5)	C(1)	C(2)	C(7)	172.8(4)
C(5)	C(4)	C(3)	C(8)	-178.1(4)	C(6)	C(1)	C(2)	C(7)	1.7(6)
C(6)	C(1)	C(5)	C(10)	-1.1(6)	C(7)	C(2)	C(3)	C(8)	5.5(6)
C(8)	C(3)	C(4)	C(9)	-4.8(6)	C(9)	C(4)	C(5)	C(10)	-1.1(6)
C(11)	N(1)	C(12)	C(13)	61.1(4)	C(11)	N(1)	C(12)	C(17)	-67.9(4)
C(12)	C(13)	C(14)	C(15)	55.1(6)	C(12)	C(17)	C(16)	C(15)	-56.6(5)
C(13)	C(12)	C(17)	C(16)	58.7(5)	C(13)	C(14)	C(15)	C(16)	-54.0(6)
C(14)	C(13)	C(12)	C(17)	-58.3(5)	C(14)	C(15)	C(16)	C(17)	55.3(6)
C(18)	Ti(2)	N(2)	C(28)	18.0(5)	C(18)	Ti(2)	N(2)	C(29)	-161.3(2)
C(18)	Ti(2)	C(19)	C(20)	-116.2(3)	C(18)	Ti(2)	C(19)	C(24)	122.3(5)
C(18)	Ti(2)	C(20)	C(19)	37.1(2)	C(18)	Ti(2)	C(20)	C(21)	-77.7(2)

© 2003 American Chemical Society, Macromolecules, Nomura ma030053b Supporting Info Page 40

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(18)	Ti(2)	C(20)	C(25)	159.5(4)	C(18)	Ti(2)	C(21)	C(20)	79.5(2)
C(18)	Ti(2)	C(21)	C(22)	-37.0(2)	C(18)	Ti(2)	C(21)	C(26)	-158.8(4)
C(18)	Ti(2)	C(22)	C(21)	116.5(3)	C(18)	Ti(2)	C(22)	C(27)	-123.3(5)
C(18)	C(19)	Ti(2)	C(20)	116.2(3)	C(18)	C(19)	Ti(2)	C(21)	78.3(2)
C(18)	C(19)	Ti(2)	C(22)	37.3(2)	C(18)	C(19)	C(20)	C(21)	0.7(4)
C(18)	C(19)	C(20)	C(25)	178.0(4)	C(18)	C(22)	Ti(2)	C(19)	-37.6(2)
C(18)	C(22)	Ti(2)	C(20)	-79.2(2)	C(18)	C(22)	Ti(2)	C(21)	-116.5(3)
C(18)	C(22)	C(21)	C(20)	-0.4(4)	C(18)	C(22)	C(21)	C(26)	-174.1(4)
C(19)	Ti(2)	N(2)	C(28)	32.8(6)	C(19)	Ti(2)	N(2)	C(29)	-146.4(2)
C(19)	Ti(2)	C(18)	C(22)	115.6(3)	C(19)	Ti(2)	C(18)	C(23)	-120.0(4)
C(19)	Ti(2)	C(20)	C(21)	-114.7(3)	C(19)	Ti(2)	C(20)	C(25)	122.5(4)
C(19)	Ti(2)	C(21)	C(20)	38.0(2)	C(19)	Ti(2)	C(21)	C(22)	-78.4(2)
C(19)	Ti(2)	C(21)	C(26)	159.7(4)	C(19)	Ti(2)	C(22)	C(21)	78.9(2)
C(19)	Ti(2)	C(22)	C(27)	-160.9(4)	C(19)	C(18)	Ti(2)	C(20)	-37.3(2)
C(19)	C(18)	Ti(2)	C(21)	-78.8(2)	C(19)	C(18)	Ti(2)	C(22)	-115.6(3)
C(19)	C(18)	C(22)	C(21)	0.8(4)	C(19)	C(18)	C(22)	C(27)	-169.4(3)
C(19)	C(20)	Ti(2)	C(21)	114.7(3)	C(19)	C(20)	Ti(2)	C(22)	78.0(2)
C(19)	C(20)	C(21)	C(22)	-0.2(4)	C(19)	C(20)	C(21)	C(26)	173.5(4)
C(20)	Ti(2)	N(2)	C(28)	-6.7(7)	C(20)	Ti(2)	N(2)	C(29)	174.0(2)
C(20)	Ti(2)	C(18)	C(22)	78.3(2)	C(20)	Ti(2)	C(18)	C(23)	-157.3(4)
C(20)	Ti(2)	C(19)	C(24)	-121.5(5)	C(20)	Ti(2)	C(21)	C(22)	-116.4(3)
C(20)	Ti(2)	C(21)	C(26)	121.7(4)	C(20)	Ti(2)	C(22)	C(21)	37.3(2)
C(20)	Ti(2)	C(22)	C(27)	157.4(4)	C(20)	C(19)	Ti(2)	C(21)	-37.9(2)
C(20)	C(19)	Ti(2)	C(22)	-78.9(2)	C(20)	C(19)	C(18)	C(22)	-1.0(4)