Ethylene Trimerization Catalysts Based on Chromium Complexes with a Nitrogen-Bridged Diphosphine Ligand Having *ortho*-Methoxyaryl or *ortho*-Thiomethoxy Substituents: Well Defined Catalyst Precursors and Investigations of the Mechanism

Susan J. Schofer, Michael W. Day, Lawrence M. Henling, Jay A. Labinger,* and John E. Bercaw*

Arnold and Mabel Beckman Laboratories of Chemical Synthesis, California Institute of Technology, Pasadena, CA 91125 (U. S. A.)

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Supporting Information

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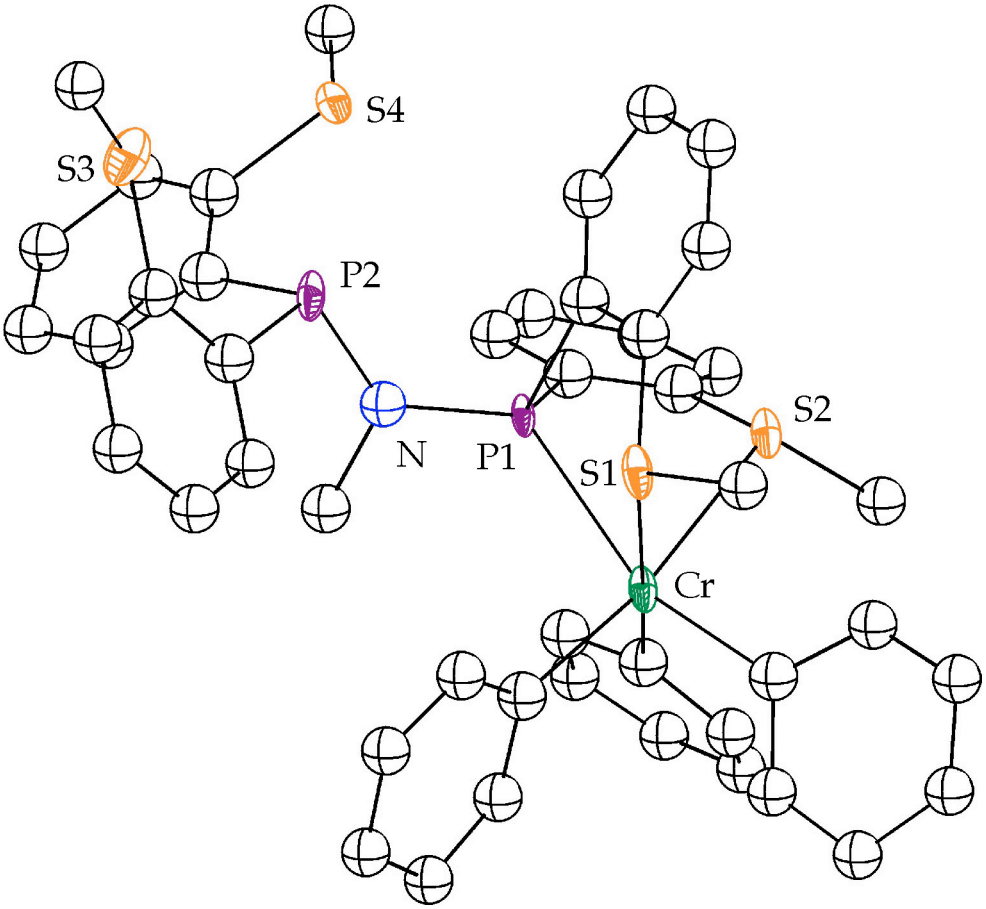

Figure 1. Molecular structure of **5**. Heteratoms have been refined anisotropically and are displayed with 50% probability ellipsoids. All carbons were refined isotropically.

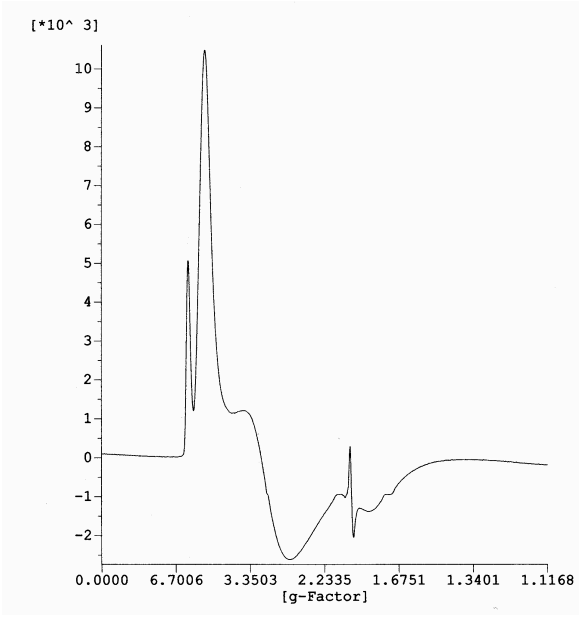

Figure 2. EPR spectrum of a glassy toluene solution of **4** at 20 K.

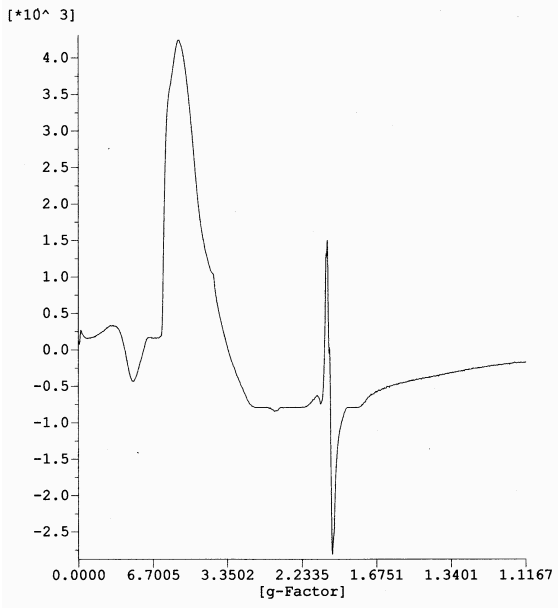

Figure 3. EPR spectrum of a glassy toluene solution of **5** at 20 K.

Table 1. Crystal data and structure refinement for 7 (CCDC 228269).

Empirical formula	$C_{41}H_{41}NO_4P_2Cr \bullet \_(C_6H_5Cl)$
Formula weight	799.69
Crystallization Solvent	Chlorobenzene

Crystal Habit	Thin hexagon
Crystal size	0.33 x 0.24 x 0.07 mm^3
Crystal color	Dichroic Green/brown

Data Collection

Preliminary Photos	Rotation	
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	98(2) K	
θ range for 11713 reflections used in lattice determination	2.19 to 32.17°	
Unit cell dimensions	a = 10.5083(6) Å b = 11.2424(7) Å c = 18.3603(10) Å	α = 93.9640(10)° β = 92.9940(10)° γ = 115.0850(10)°
Volume	1951.8(2) $Å^3$	
Z	2	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.361 Mg/m^3	
F(000)	835	
Data collection program	Bruker SMART v5.054	
θ range for data collection	2.01 to 32.75°	
Completeness to θ = 32.75°	83.2 %	
Index ranges	$-15 \le h \le 15$, $-14 \le k \le 16$, $-27 \le l \le 27$	
Data collection scan type	ω scans at 5 ϕ settings	
Data reduction program	Bruker SAINT v6.45	
Reflections collected	32181	
Independent reflections	11984 [R_{int}= 0.0704]	
Absorption coefficient	0.488 mm^{-1}	
Absorption correction	None	
Max. and min. transmission	0.9667 and 0.8556	
Structure solution program	SHELXS-97 (Sheldrick, 1990)	
Primary solution method	Direct methods	
Secondary solution method	Difference Fourier map	
Hydrogen placement	Geometric positions	
Structure refinement program	SHELXL-97 (Sheldrick, 1997)	
Refinement method	Full matrix least-squares on F^2	
Data / restraints / parameters	11984 / 0 / 507	

Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.472
Final R indices [I>2σ(I), 7848 reflections]	R1 = 0.0509, *w*R2 = 0.0985
R indices (all data)	R1 = 0.0836, *w*R2 = 0.1030
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.005
Average shift/error	0.000
Largest diff. peak and hole	1.071 and -0.562 e.Å^{-3}

Special Refinement Details

Chlorobenzene is included in the crystals as the solvent of crystallization. The molecule sits on an inversion center, therefore it was assigned half occupancy in the model.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 7 (CCDC 228269). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cr	1160(1)	8949(1)	1926(1)	15(1)
Cl(1)	-736(1)	9117(1)	1328(1)	23(1)
P(1)	3623(1)	9389(1)	2214(1)	15(1)
P(2)	2890(1)	11447(1)	2177(1)	15(1)
O(1)	2267(1)	9058(1)	783(1)	18(1)
O(2)	3454(2)	6854(1)	2575(1)	24(1)
O(3)	614(2)	11863(2)	2690(1)	26(1)
O(4)	5249(2)	14226(1)	2174(1)	25(1)
N(1)	4304(2)	11060(2)	2232(1)	15(1)
C(1)	5786(2)	11876(2)	2102(1)	22(1)
C(2)	4200(2)	8847(2)	1396(1)	16(1)
C(3)	5357(2)	8557(2)	1382(1)	18(1)
C(4)	5713(2)	8143(2)	728(1)	21(1)
C(5)	4907(2)	8007(2)	88(1)	23(1)
C(6)	3750(2)	8301(2)	79(1)	22(1)
C(7)	3396(2)	8726(2)	733(1)	16(1)
C(8)	1571(2)	9084(2)	95(1)	21(1)
C(9)	4520(2)	9078(2)	2999(1)	19(1)

C(10)	5329(2)	10106(2)	3540(1)	24(1)
C(11)	5832(3)	9848(3)	4193(1)	30(1)
C(12)	5498(3)	8554(3)	4318(1)	31(1)
C(13)	4704(2)	7509(2)	3793(1)	28(1)
C(14)	4227(2)	7786(2)	3129(1)	20(1)
C(15)	2932(3)	5487(2)	2719(2)	34(1)
C(16)	2964(2)	12375(2)	3043(1)	18(1)
C(17)	4144(2)	12960(2)	3554(1)	23(1)
C(18)	4066(3)	13554(2)	4227(1)	28(1)
C(19)	2808(3)	13544(2)	4401(1)	30(1)
C(20)	1610(3)	12977(2)	3912(1)	27(1)
C(21)	1707(2)	12407(2)	3230(1)	21(1)
C(22)	-796(2)	11434(2)	2910(2)	33(1)
C(23)	3183(2)	12634(2)	1509(1)	16(1)
C(24)	2160(2)	12280(2)	919(1)	21(1)
C(25)	2255(3)	13135(2)	396(1)	25(1)
C(26)	3360(3)	14371(2)	469(1)	28(1)
C(27)	4395(2)	14773(2)	1053(1)	25(1)
C(28)	4293(2)	13906(2)	1573(1)	20(1)
C(29)	6433(3)	15497(2)	2251(2)	37(1)
C(30)	378(2)	6905(2)	1790(1)	19(1)
C(31)	-10(3)	6208(2)	1101(1)	28(1)
C(32)	-616(3)	4827(2)	985(1)	33(1)
C(33)	-822(3)	4098(2)	1573(1)	30(1)
C(34)	-441(3)	4748(2)	2271(1)	32(1)
C(35)	145(2)	6117(2)	2379(1)	26(1)
C(36)	567(2)	8930(2)	2966(1)	19(1)
C(37)	-877(2)	8354(2)	3063(1)	24(1)
C(38)	-1379(3)	8203(2)	3749(1)	28(1)
C(39)	-463(3)	8655(2)	4364(1)	32(1)
C(40)	980(3)	9251(2)	4300(1)	27(1)
C(41)	1483(2)	9384(2)	3614(1)	22(1)
Cl(5)	-2392(3)	3575(3)	4415(2)	70(1)
C(51)	-731(4)	4569(4)	4820(3)	36(1)
C(52)	85(5)	5697(5)	4496(2)	44(5)
C(53)	1439(5)	6524(4)	4804(3)	46(2)
C(54)	1978(4)	6224(5)	5437(3)	51(3)
C(55)	1163(6)	5096(5)	5761(2)	52(2)
C(56)	-191(5)	4269(4)	5453(2)	35(4)

Table 3. Selected bond lengths [Å] and angles [°] for 7 (CCDC 228269).

Cr-C(36)	2.039(2)	C(36)-Cr-C(30)	92.04(8)
Cr-C(30)	2.077(2)	C(36)-Cr-Cl(1)	98.45(6)
Cr-Cl(1)	2.3078(6)	C(30)-Cr-Cl(1)	97.71(6)
Cr-O(1)	2.4371(14)	C(36)-Cr-O(1)	170.17(7)
Cr-P(1)	2.4414(6)	C(30)-Cr-O(1)	89.39(7)
Cr-P(2)	2.6096(6)	Cl(1)-Cr-O(1)	90.99(4)
		C(36)-Cr-P(1)	98.84(6)
		C(30)-Cr-P(1)	96.26(6)
		Cl(1)-Cr-P(1)	157.30(3)
		O(1)-Cr-P(1)	71.34(3)
		C(36)-Cr-P(2)	90.97(6)
		C(30)-Cr-P(2)	161.72(6)
		Cl(1)-Cr-P(2)	99.67(2)
		O(1)-Cr-P(2)	84.71(4)
		P(1)-Cr-P(2)	65.458(19)

Table 4. Bond lengths [Å] and angles [°] for 7 (CCDC 228269).

Cr-C(36)	2.039(2)	C(36)-C(37)	1.402(3)
Cr-C(30)	2.077(2)	C(36)-C(41)	1.408(3)
Cr-Cl(1)	2.3078(6)	C(37)-C(38)	1.384(3)
Cr-O(1)	2.4371(14)	C(38)-C(39)	1.361(3)
Cr-P(1)	2.4414(6)	C(39)-C(40)	1.390(3)
Cr-P(2)	2.6096(6)	C(40)-C(41)	1.384(3)
P(1)-N(1)	1.6995(17)	Cl(5)-C(54)#1	0.459(6)
P(1)-C(2)	1.809(2)	Cl(5)-C(55)#1	1.574(8)
P(1)-C(9)	1.815(2)	Cl(5)-C(51)	1.717(4)
P(2)-N(1)	1.7168(17)	Cl(5)-C(53)#1	1.744(8)
P(2)-C(23)	1.816(2)	C(51)-C(54)#1	1.274(7)
P(2)-C(16)	1.820(2)	C(51)-C(55)#1	1.279(10)
O(1)-C(7)	1.392(2)	C(51)-C(53)#1	1.392(10)
O(1)-C(8)	1.434(2)	C(51)-C(52)	1.3900
O(2)-C(14)	1.356(2)	C(51)-C(56)	1.3900
O(2)-C(15)	1.446(3)	C(51)-C(56)#1	1.401(9)
O(3)-C(21)	1.370(3)	C(51)-C(52)#1	1.505(9)
O(3)-C(22)	1.440(3)	C(51)-C(51)#1	1.509(7)
O(4)-C(28)	1.371(2)	C(52)-C(56)#1	0.133(8)
O(4)-C(29)	1.434(3)	C(52)-C(55)#1	1.274(10)
N(1)-C(1)	1.477(3)	C(52)-C(53)	1.3900
C(2)-C(3)	1.386(3)	C(52)-C(51)#1	1.505(7)
C(2)-C(7)	1.411(3)	C(53)-C(56)#1	1.274(9)
C(3)-C(4)	1.383(3)	C(53)-C(51)#1	1.392(7)
C(4)-C(5)	1.373(3)	C(53)-C(54)	1.3900
C(5)-C(6)	1.388(3)	C(53)-Cl(5)#1	1.744(7)
C(6)-C(7)	1.387(3)	C(54)-Cl(5)#1	0.459(5)
C(9)-C(14)	1.392(3)	C(54)-C(51)#1	1.274(7)
C(9)-C(10)	1.402(3)	C(54)-C(55)	1.3900
C(10)-C(11)	1.383(3)	C(55)-C(52)#1	1.274(11)
C(11)-C(12)	1.384(3)	C(55)-C(51)#1	1.279(7)
C(12)-C(13)	1.390(3)	C(55)-C(56)	1.3900
C(13)-C(14)	1.397(3)	C(55)-Cl(5)#1	1.574(8)
C(16)-C(21)	1.396(3)	C(56)-C(52)#1	0.133(11)
C(16)-C(17)	1.397(3)	C(56)-C(53)#1	1.274(11)
C(17)-C(18)	1.386(3)	C(56)-C(51)#1	1.401(7)
C(18)-C(19)	1.372(3)		
C(19)-C(20)	1.385(3)	C(36)-Cr-C(30)	92.04(8)
C(20)-C(21)	1.396(3)	C(36)-Cr-Cl(1)	98.45(6)
C(23)-C(24)	1.394(3)	C(30)-Cr-Cl(1)	97.71(6)
C(23)-C(28)	1.403(3)	C(36)-Cr-O(1)	170.17(7)
C(24)-C(25)	1.383(3)	C(30)-Cr-O(1)	89.39(7)
C(25)-C(26)	1.374(3)	Cl(1)-Cr-O(1)	90.99(4)
C(26)-C(27)	1.390(3)	C(36)-Cr-P(1)	98.84(6)
C(27)-C(28)	1.387(3)	C(30)-Cr-P(1)	96.26(6)
C(30)-C(31)	1.385(3)	Cl(1)-Cr-P(1)	157.30(3)
C(30)-C(35)	1.411(3)	O(1)-Cr-P(1)	71.34(3)
C(31)-C(32)	1.401(3)	C(36)-Cr-P(2)	90.97(6)
C(32)-C(33)	1.371(3)	C(30)-Cr-P(2)	161.72(6)
C(33)-C(34)	1.379(3)	Cl(1)-Cr-P(2)	99.67(2)
C(34)-C(35)	1.388(3)	O(1)-Cr-P(2)	84.71(4)

P(1)-Cr-P(2)	65.458(19)	C(28)-C(23)-P(2)	124.96(16)
N(1)-P(1)-C(2)	105.22(9)	C(25)-C(24)-C(23)	121.4(2)
N(1)-P(1)-C(9)	105.45(9)	C(26)-C(25)-C(24)	119.4(2)
C(2)-P(1)-C(9)	107.58(9)	C(25)-C(26)-C(27)	121.3(2)
N(1)-P(1)-Cr	96.84(6)	C(28)-C(27)-C(26)	118.9(2)
C(2)-P(1)-Cr	106.80(7)	O(4)-C(28)-C(27)	123.0(2)
C(9)-P(1)-Cr	131.83(7)	O(4)-C(28)-C(23)	116.00(19)
N(1)-P(2)-C(23)	108.39(9)	C(27)-C(28)-C(23)	121.0(2)
N(1)-P(2)-C(16)	106.82(9)	C(31)-C(30)-C(35)	114.8(2)
C(23)-P(2)-C(16)	103.91(9)	C(31)-C(30)-Cr	121.56(16)
N(1)-P(2)-Cr	90.51(6)	C(35)-C(30)-Cr	123.60(16)
C(23)-P(2)-Cr	124.03(7)	C(30)-C(31)-C(32)	123.5(2)
C(16)-P(2)-Cr	120.53(7)	C(33)-C(32)-C(31)	119.7(2)
C(7)-O(1)-C(8)	115.19(15)	C(32)-C(33)-C(34)	118.9(2)
C(7)-O(1)-Cr	120.74(11)	C(33)-C(34)-C(35)	120.9(2)
C(8)-O(1)-Cr	121.71(12)	C(34)-C(35)-C(30)	122.2(2)
C(14)-O(2)-C(15)	117.53(17)	C(37)-C(36)-C(41)	115.7(2)
C(21)-O(3)-C(22)	117.39(18)	C(37)-C(36)-Cr	118.32(16)
C(28)-O(4)-C(29)	118.16(18)	C(41)-C(36)-Cr	125.87(16)
C(1)-N(1)-P(1)	122.44(13)	C(38)-C(37)-C(36)	122.5(2)
C(1)-N(1)-P(2)	129.00(14)	C(39)-C(38)-C(37)	120.2(2)
P(1)-N(1)-P(2)	106.35(9)	C(38)-C(39)-C(40)	119.6(2)
C(3)-C(2)-C(7)	119.00(18)	C(41)-C(40)-C(39)	120.2(2)
C(3)-C(2)-P(1)	124.92(16)	C(40)-C(41)-C(36)	121.7(2)
C(7)-C(2)-P(1)	116.09(15)	C(54)#1-Cl(5)-C(55)#1	58.4(9)
C(4)-C(3)-C(2)	120.7(2)	C(54)#1-Cl(5)-C(51)	13.0(12)
C(5)-C(4)-C(3)	119.7(2)	C(55)#1-Cl(5)-C(51)	45.5(3)
C(4)-C(5)-C(6)	121.3(2)	C(54)#1-Cl(5)-C(53)#1	34.5(9)
C(7)-C(6)-C(5)	119.1(2)	C(55)#1-Cl(5)-C(53)#1	92.9(3)
C(6)-C(7)-O(1)	123.71(18)	C(51)-Cl(5)-C(53)#1	47.4(3)
C(6)-C(7)-C(2)	120.14(19)	C(54)#1-C(51)-C(55)#1	66.0(4)
O(1)-C(7)-C(2)	116.15(17)	C(54)#1-C(51)-C(53)#1	62.7(4)
C(14)-C(9)-C(10)	118.85(19)	C(55)#1-C(51)-C(53)#1	128.7(6)
C(14)-C(9)-P(1)	119.95(16)	C(54)#1-C(51)-C(52)	122.8(8)
C(10)-C(9)-P(1)	120.40(16)	C(55)#1-C(51)-C(52)	56.8(6)
C(11)-C(10)-C(9)	120.8(2)	C(53)#1-C(51)-C(52)	174.5(6)
C(10)-C(11)-C(12)	119.3(2)	C(54)#1-C(51)-C(56)	117.2(8)
C(11)-C(12)-C(13)	121.5(2)	C(55)#1-C(51)-C(56)	176.8(6)
C(12)-C(13)-C(14)	118.6(2)	C(53)#1-C(51)-C(56)	54.5(6)
O(2)-C(14)-C(9)	115.02(18)	C(52)-C(51)-C(56)	120.0
O(2)-C(14)-C(13)	124.0(2)	C(54)#1-C(51)-C(56)#1	128.3(7)
C(9)-C(14)-C(13)	120.9(2)	C(55)#1-C(51)-C(56)#1	62.3(4)
C(21)-C(16)-C(17)	118.09(19)	C(53)#1-C(51)-C(56)#1	169.1(7)
C(21)-C(16)-P(2)	116.71(16)	C(52)-C(51)-C(56)#1	5.5(3)
C(17)-C(16)-P(2)	124.99(16)	C(56)-C(51)-C(56)#1	114.5(3)
C(18)-C(17)-C(16)	120.9(2)	C(54)#1-C(51)-C(52)#1	119.9(7)
C(19)-C(18)-C(17)	119.7(2)	C(55)#1-C(51)-C(52)#1	174.1(7)
C(18)-C(19)-C(20)	121.5(2)	C(53)#1-C(51)-C(52)#1	57.2(4)
C(19)-C(20)-C(21)	118.3(2)	C(52)-C(51)-C(52)#1	117.3(4)
O(3)-C(21)-C(16)	114.72(19)	C(56)-C(51)-C(52)#1	2.7(4)
O(3)-C(21)-C(20)	123.8(2)	C(56)#1-C(51)-C(52)#1	111.9(5)
C(16)-C(21)-C(20)	121.4(2)	C(54)#1-C(51)-C(51)#1	174.8(10)
C(24)-C(23)-C(28)	118.02(19)	C(55)#1-C(51)-C(51)#1	119.2(8)
C(24)-C(23)-P(2)	116.82(16)	C(53)#1-C(51)-C(51)#1	112.1(8)

C(52)-C(51)-C(51)#1	62.4(3)	C(52)#1-C(56)-C(51)#1	83(3)
C(56)-C(51)-C(51)#1	57.6(3)	C(53)#1-C(56)-C(51)#1	128.3(8)
C(56)#1-C(51)-C(51)#1	56.9(4)	C(55)-C(56)-C(51)#1	54.5(3)
C(52)#1-C(51)-C(51)#1	54.9(4)	C(51)-C(56)-C(51)#1	65.5(3)
C(54)#1-C(51)-Cl(5)	4.6(4)		
C(55)#1-C(51)-Cl(5)	61.3(3)		
C(53)#1-C(51)-Cl(5)	67.3(3)		
C(52)-C(51)-Cl(5)	118.2(4)		
C(56)-C(51)-Cl(5)	121.8(4)		
C(56)#1-C(51)-Cl(5)	123.6(4)		
C(52)#1-C(51)-Cl(5)	124.5(4)		
C(51)#1-C(51)-Cl(5)	179.4(6)		
C(56)#1-C(52)-C(55)#1	149(4)		
C(56)#1-C(52)-C(53)	28(4)		
C(55)#1-C(52)-C(53)	177.2(6)		
C(56)#1-C(52)-C(51)	92(4)		
C(55)#1-C(52)-C(51)	57.2(6)		
C(53)-C(52)-C(51)	120.0		
C(56)#1-C(52)-C(51)#1	29(4)		
C(55)#1-C(52)-C(51)#1	119.9(7)		
C(53)-C(52)-C(51)#1	57.3(3)		
C(51)-C(52)-C(51)#1	62.7(3)		
C(56)#1-C(53)-C(51)#1	62.7(3)		
C(56)#1-C(53)-C(52)	2.8(3)		
C(51)#1-C(53)-C(52)	65.5(3)		
C(56)#1-C(53)-C(54)	117.2(3)		
C(51)#1-C(53)-C(54)	54.5(3)		
C(52)-C(53)-C(54)	120.0		
C(56)#1-C(53)-Cl(5)#1	127.9(4)		
C(51)#1-C(53)-Cl(5)#1	65.3(3)		
C(52)-C(53)-Cl(5)#1	130.8(2)		
C(54)-C(53)-Cl(5)#1	10.8(2)		
Cl(5)#1-C(54)-C(51)#1	162.3(11)		
Cl(5)#1-C(54)-C(55)	105.2(11)		
C(51)#1-C(54)-C(55)	57.2(3)		
Cl(5)#1-C(54)-C(53)	134.8(11)		
C(51)#1-C(54)-C(53)	62.8(3)		
C(55)-C(54)-C(53)	120.0		
C(52)#1-C(55)-C(51)#1	66.0(3)		
C(52)#1-C(55)-C(54)	122.8(3)		
C(51)#1-C(55)-C(54)	56.8(3)		
C(52)#1-C(55)-C(56)	2.8(3)		
C(51)#1-C(55)-C(56)	63.2(3)		
C(54)-C(55)-C(56)	120.0		
C(52)#1-C(55)-Cl(5)#1	139.1(4)		
C(51)#1-C(55)-Cl(5)#1	73.2(4)		
C(54)-C(55)-Cl(5)#1	16.3(2)		
C(56)-C(55)-Cl(5)#1	136.3(2)		
C(52)#1-C(56)-C(53)#1	149(3)		
C(52)#1-C(56)-C(55)	28(3)		
C(53)#1-C(56)-C(55)	177.2(6)		
C(52)#1-C(56)-C(51)	148(3)		
C(53)#1-C(56)-C(51)	62.8(6)		
C(55)-C(56)-C(51)	120.0		

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

Table 5. Anisotropic displacement parameters ($Å^2$ x 10^4) for 7 (CCDC 228269). 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}
Cr	142(2)	138(2)	164(2)	15(1)	7(1)	44(1)
Cl(1)	184(3)	264(3)	236(3)	19(2)	-24(2)	97(2)
P(1)	150(3)	128(3)	159(3)	18(2)	14(2)	56(2)
P(2)	148(3)	129(3)	173(3)	16(2)	13(2)	56(2)
O(1)	173(8)	191(8)	139(7)	-1(6)	7(6)	59(6)
O(2)	294(9)	148(8)	270(9)	49(7)	35(7)	96(7)
O(3)	208(8)	262(9)	326(9)	32(7)	52(7)	109(7)
O(4)	225(8)	146(8)	295(9)	16(7)	-21(7)	7(7)
N(1)	135(9)	113(9)	194(9)	-2(7)	1(7)	44(7)
C(1)	150(11)	179(11)	300(13)	38(10)	31(9)	49(9)
C(2)	178(11)	116(10)	156(10)	0(8)	34(8)	39(9)
C(3)	153(11)	142(11)	227(11)	13(9)	10(9)	41(9)
C(4)	185(11)	157(11)	298(13)	48(10)	106(10)	59(9)
C(5)	268(12)	176(12)	226(12)	4(9)	105(10)	80(10)
C(6)	226(12)	213(12)	174(11)	13(9)	25(9)	61(10)
C(7)	144(10)	119(10)	207(11)	33(9)	38(9)	29(9)
C(8)	209(12)	251(12)	180(11)	60(9)	8(9)	97(10)
C(9)	178(11)	235(12)	185(11)	37(9)	31(9)	112(10)
C(10)	238(12)	248(13)	246(12)	18(10)	-5(10)	109(10)
C(11)	304(13)	428(16)	188(12)	-43(11)	-81(10)	202(12)
C(12)	338(14)	435(16)	205(12)	88(11)	-5(11)	223(13)
C(13)	309(13)	330(14)	303(13)	124(11)	65(11)	205(12)
C(14)	183(11)	243(12)	209(11)	32(10)	45(9)	116(10)
C(15)	379(15)	177(12)	488(16)	87(12)	90(13)	119(12)
C(16)	237(12)	116(10)	176(11)	34(8)	47(9)	71(9)
C(17)	257(12)	207(12)	214(12)	3(9)	-3(10)	103(10)
C(18)	420(15)	182(12)	190(12)	-23(10)	-39(11)	100(11)
C(19)	521(17)	208(13)	173(12)	11(10)	76(11)	141(12)
C(20)	367(14)	196(12)	307(13)	78(10)	146(11)	145(11)
C(21)	265(12)	121(11)	254(12)	70(9)	63(10)	77(10)
C(22)	174(12)	307(14)	542(17)	54(12)	107(11)	128(11)
C(23)	207(11)	137(10)	161(10)	24(8)	68(9)	87(9)
C(24)	217(12)	192(12)	206(11)	4(9)	26(9)	87(10)
C(25)	290(13)	273(13)	236(12)	39(10)	7(10)	164(11)
C(26)	394(15)	260(13)	260(13)	124(10)	114(11)	185(12)
C(27)	283(13)	161(12)	301(13)	57(10)	101(11)	84(10)
C(28)	229(11)	166(11)	217(11)	14(9)	75(9)	102(10)
C(29)	255(13)	183(13)	523(17)	40(12)	-18(12)	-30(11)
C(30)	134(10)	171(11)	249(12)	21(9)	28(9)	56(9)
C(31)	349(14)	198(12)	226(12)	34(10)	43(11)	54(11)
C(32)	438(16)	207(13)	269(13)	-44(11)	41(12)	75(12)
C(33)	319(14)	135(12)	378(15)	2(11)	58(11)	31(11)
C(34)	387(15)	218(13)	334(14)	107(11)	77(12)	90(12)
C(35)	298(13)	214(12)	237(12)	18(10)	12(10)	89(11)
C(36)	260(12)	115(10)	187(11)	33(9)	59(9)	80(9)
C(37)	208(12)	196(12)	266(12)	-8(10)	-5(10)	41(10)
C(38)	232(12)	233(13)	343(14)	27(11)	126(11)	59(11)

C(39)	424(16)	275(14)	260(13)	64(11)	153(12)	141(12)
C(40)	339(14)	293(13)	162(11)	31(10)	24(10)	126(11)
C(41)	213(12)	195(12)	223(12)	-2(9)	27(9)	75(10)
Cl(5)	435(12)	502(12)	966(18)	-277(12)	-59(13)	91(9)
C(51)	350(30)	310(30)	430(30)	-110(30)	120(30)	160(30)
C(52)	580(110)	450(130)	440(80)	160(80)	180(80)	340(100)
C(53)	430(40)	330(30)	680(40)	110(30)	220(30)	200(30)
C(54)	560(80)	500(70)	540(50)	-10(50)	-100(50)	320(60)
C(55)	790(50)	750(50)	330(30)	80(30)	80(30)	640(50)
C(56)	560(100)	260(100)	290(70)	70(60)	150(70)	210(80)

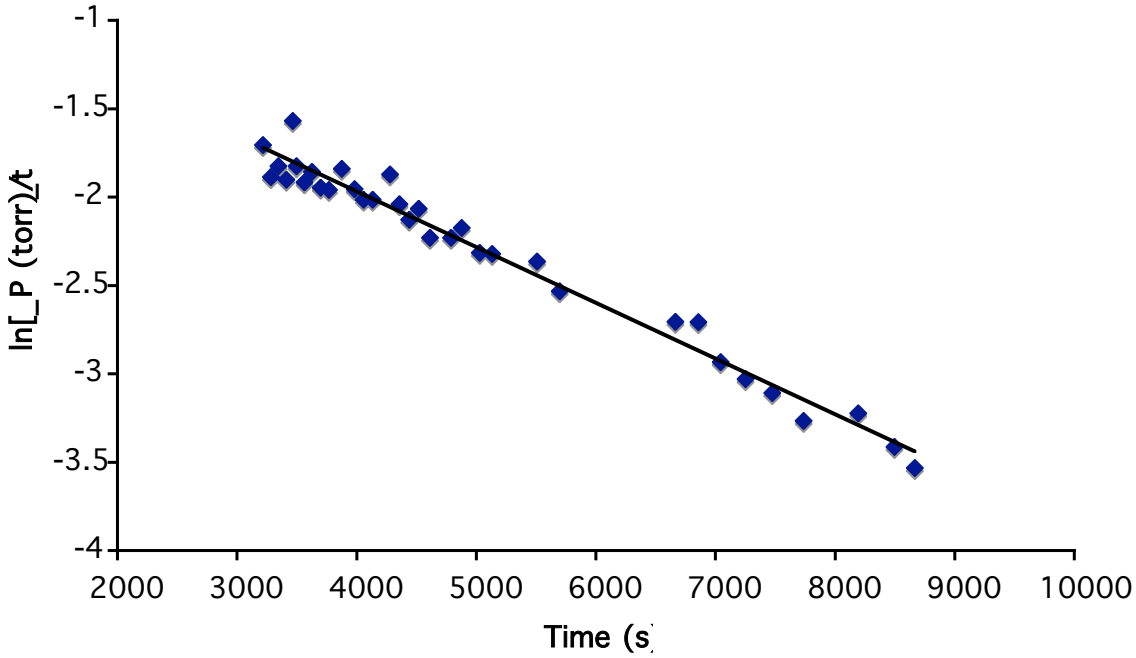

Figure 4. Plot of the natural log of the rate of ethylene consumption *versus* time during the decomposition period in trimerization catalyzed by **4**/$H^+(OEt_2)_2B[C_6H_3(CF_3)_2]_4^-$. 20 μmol **4**, 20 μmol $H^+(OEt_2)_2B[C_6H_3(CF_3)_2]_4^-$ in a mixture of 2 mL Et_2O and 48 mL toluene at room temperature; 1 atm ethylene.

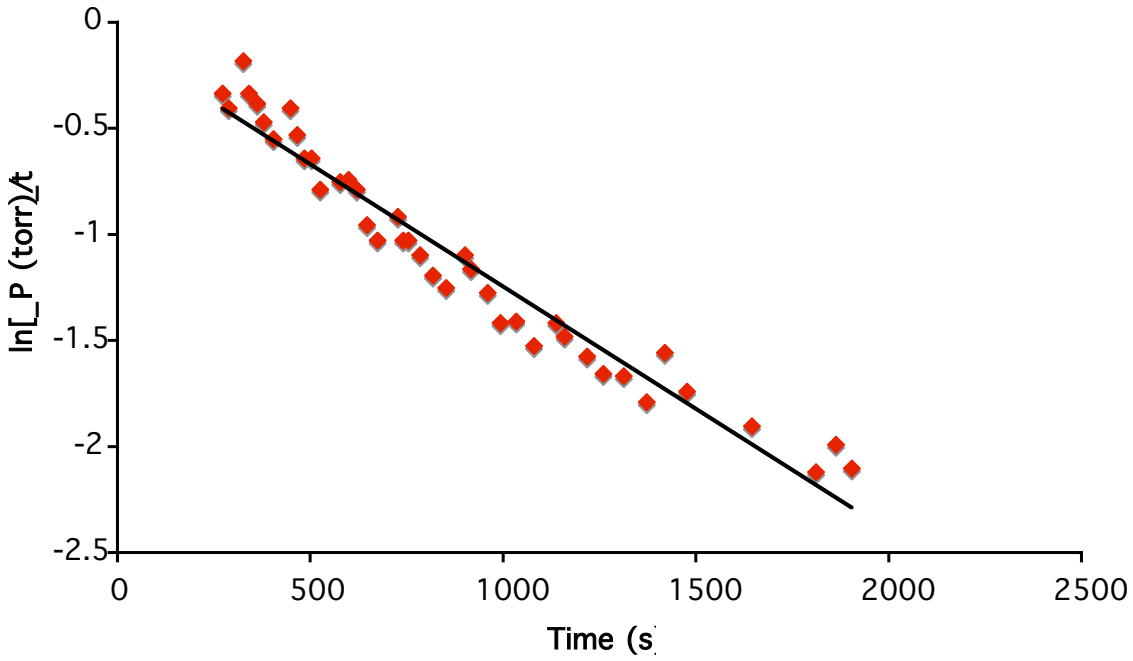

Figure 5. Plot of the natural log of the rate of ethylene consumption *versus* time during the decomposition period in trimerization generated from **1** and $CrCl_3(THF)_3$ and activated by MAO after exposure to ethylene. 21 μmol **1**, 21 μmol $CrCl_3(THF)_3$, 6 mmol MAO in 50 mL toluene at room temperature; 1 atm ethylene.