Electronic Supplementary Material (ESI) for Chemical Science.

Supporting Information

Formation of quaternary centres by copper catalysed asymmetric conjugate addition to β-substituted cyclopentenones with the aid of a quantitative structure-selectivity relationship

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Table 1. Crystal data and structure refinement for 6790.

Identification code	6790	
Empirical formula	C42.45 H36.90 Cl0.90 N O2 P1	
Formula weight	655.85	
Temperature	150 K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 2	
Unit cell dimensions	a = 24.2085(3) Å	α= 90°.
	b = 16.0031(2) Å	β= 90°.
	c = 8.82830(10) Å	γ = 90°.
Volume	3420.18(7) $Å^3$	
Z	4	
Density (calculated)	1.274 Mg/m^3	
Absorption coefficient	1.649 mm^{-1}	
F(000)	1379.412	
Crystal size	0.22 x 0.20 x 0.07 mm^3	
Theta range for data collection	3.652 to 76.378°.	
Index ranges	-29<=h<=30, -19<=k<=20, -11<=l<=7	
Reflections collected	36120	
Independent reflections	7115 [R(int) = 0.045]	
Completeness to theta = 74.850°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.89 and 0.79	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7115 / 0 / 438	
Goodness-of-fit on F^2	1.0024	
Final R indices [I>2sigma(I)]	R1 = 0.0358, wR2 = 0.0929	
R indices (all data)	R1 = 0.0375, wR2 = 0.0949	
Absolute structure parameter	-0.008(15)	
Largest diff. peak and hole	0.34 and -0.28 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 6790. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	2842(1)	6239(1)	6543(1)	30
O(2)	2163(1)	6445(1)	6455(1)	28
C(3)	1833(1)	6092(1)	7561(2)	26
C(4)	1523(1)	5374(1)	7157(2)	30
C(5)	1185(1)	5004(1)	8199(2)	32
C(6)	1158(1)	5316(1)	9704(2)	28
C(7)	837(1)	4916(1)	10833(2)	38
C(8)	834(1)	5191(1)	12289(3)	44
C(9)	1157(1)	5886(1)	12698(2)	40
C(10)	1466(1)	6298(1)	11632(2)	33
C(11)	1474(1)	6033(1)	10099(2)	26
C(12)	1803(1)	6448(1)	8975(2)	25
C(13)	2129(1)	7216(1)	9296(2)	27
C(14)	1888(1)	7956(1)	9911(2)	33
C(15)	1315(1)	8039(1)	10175(3)	43
C(16)	1110(1)	8750(2)	10830(4)	68
C(17)	1464(2)	9417(2)	11227(4)	82
C(18)	2009(2)	9366(2)	10936(3)	66
C(19)	2236(1)	8651(1)	10264(2)	45
C(20)	2804(1)	8602(2)	9944(2)	49
C(21)	3026(1)	7918(2)	9296(2)	43
C(22)	2686(1)	7224(1)	8961(2)	32
O(23)	2940(1)	6539(1)	8325(1)	35
N(24)	3043(1)	7030(1)	5438(2)	28
C(25)	3476(1)	6868(1)	4276(2)	27
C(26)	2711(1)	7818(1)	5285(2)	30
C(27)	3053(1)	8614(1)	5228(3)	46
C(28)	2321(1)	7771(1)	3932(2)	44
C(29)	3997(1)	7391(1)	4514(2)	29
C(30)	4167(1)	7619(1)	5934(2)	39
C(31)	4641(1)	8114(1)	6157(2)	44

C(32)	4940(1)	8380(1)	4944(3)	45
C(33)	4796(1)	8142(1)	3463(2)	36
C(34)	5118(1)	8391(1)	2194(3)	45
C(35)	4989(1)	8134(2)	771(3)	50
C(36)	4527(1)	7625(2)	539(2)	46
C(37)	4201(1)	7373(1)	1728(2)	37
C(38)	4321(1)	7632(1)	3231(2)	30
C(43)	3623(1)	5936(1)	4152(2)	30
C(44)	3295(1)	5392(1)	3291(2)	35
C(45)	3430(1)	4543(1)	3250(3)	42
C(46)	3879(1)	4221(1)	4030(3)	43
C(47)	4203(1)	4764(1)	4864(3)	45
C(48)	4078(1)	5612(1)	4917(2)	38
C(49)	2790(1)	5688(1)	2458(3)	48
C(50)	4014(1)	3295(2)	3959(4)	64
C(61)	5339(3)	4647(5)	874(9)	70
Cl(62)	4891(1)	5492(1)	1137(2)	65
Cl(63)	5403(1)	4333(1)	-1001(2)	70

Table 3. Bond lengths [Å] and angles [°] for 6790.

P(1)-O(2)	1.6785(12)	C(19)-C(20)	1.406(3)
P(1)-O(23)	1.6619(14)	C(20)-C(21)	1.346(4)
P(1)-N(24)	1.6702(14)	C(20)-H(201)	0.949
O(2)-C(3)	1.3830(19)	C(21)-C(22)	1.414(3)
C(3)-C(4)	1.417(2)	C(21)-H(211)	0.940
C(3)-C(12)	1.374(2)	C(22)-O(23)	1.377(2)
C(4)-C(5)	1.366(3)	N(24)-C(25)	1.490(2)
C(4)-H(41)	0.942	N(24)-C(26)	1.501(2)
C(5)-C(6)	1.421(3)	C(25)-C(29)	1.527(2)
C(5)-H(51)	0.931	C(25)-C(43)	1.537(2)
C(6)-C(7)	1.417(2)	C(25)-H(251)	0.986
C(6)-C(11)	1.422(2)	C(26)-C(27)	1.520(3)
C(7)-C(8)	1.359(3)	C(26)-C(28)	1.525(3)
C(7)-H(71)	0.947	C(26)-H(261)	0.981
C(8)-C(9)	1.407(3)	C(27)-H(273)	0.958
C(8)-H(81)	0.919	C(27)-H(271)	0.977
C(9)-C(10)	1.370(2)	C(27)-H(272)	0.963
C(9)-H(91)	0.944	C(28)-H(281)	0.944
C(10)-C(11)	1.419(2)	C(28)-H(282)	0.933
C(10)-H(101)	0.917	C(28)-H(283)	0.972
C(11)-C(12)	1.435(2)	C(29)-C(30)	1.369(3)
C(12)-C(13)	1.489(2)	C(29)-C(38)	1.431(2)
C(13)-C(14)	1.428(2)	C(30)-C(31)	1.409(3)
C(13)-C(22)	1.380(2)	C(30)-H(301)	0.935
C(14)-C(15)	1.412(3)	C(31)-C(32)	1.361(3)
C(14)-C(19)	1.430(2)	C(31)-H(311)	0.939
C(15)-C(16)	1.369(3)	C(32)-C(33)	1.406(3)
C(15)-H(151)	0.925	C(32)-H(321)	0.950
C(16)-C(17)	1.413(4)	C(33)-C(34)	1.422(3)
C(16)-H(161)	0.931	C(33)-C(38)	1.425(3)
C(17)-C(18)	1.346(5)	C(34)-C(35)	1.357(4)
C(17)-H(171)	0.943	C(34)-H(341)	0.927
C(18)-C(19)	1.402(3)	C(35)-C(36)	1.399(3)
C(18)-H(181)	0.962	C(35)-H(351)	0.970

C(36)-C(37)	1.374(3)	C(4)-C(5)-C(6)	120.33(15)
C(36)-H(361)	0.950	C(4)-C(5)-H(51)	121.7
C(37)-C(38)	1.421(3)	C(6)-C(5)-H(51)	118.0
C(37)-H(371)	0.958	C(5)-C(6)-C(7)	121.60(16)
C(43)-C(44)	1.404(3)	C(5)-C(6)-C(11)	119.20(15)
C(43)-C(48)	1.392(3)	C(7)-C(6)-C(11)	119.18(17)
C(44)-C(45)	1.398(3)	C(6)-C(7)-C(8)	121.45(17)
C(44)-C(49)	1.502(3)	C(6)-C(7)-H(71)	116.8
C(45)-C(46)	1.385(3)	C(8)-C(7)-H(71)	121.7
C(45)-H(451)	0.947	C(7)-C(8)-C(9)	119.72(17)
C(46)-C(47)	1.384(3)	C(7)-C(8)-H(81)	120.0
C(46)-C(50)	1.519(3)	C(9)-C(8)-H(81)	120.2
C(47)-C(48)	1.392(3)	C(8)-C(9)-C(10)	120.47(19)
C(47)-H(471)	0.932	C(8)-C(9)-H(91)	120.5
C(48)-H(481)	0.938	C(10)-C(9)-H(91)	119.1
C(49)-H(492)	0.948	C(9)-C(10)-C(11)	121.31(17)
C(49)-H(493)	0.981	C(9)-C(10)-H(101)	119.5
C(49)-H(491)	0.961	C(11)-C(10)-H(101)	119.2
C(50)-H(503)	0.948	C(6)-C(11)-C(10)	117.84(15)
C(50)-H(501)	0.979	C(6)-C(11)-C(12)	120.11(15)
C(50)-H(502)	0.955	C(10)-C(11)-C(12)	122.01(15)
C(61)-Cl(62)	1.748(8)	C(11)-C(12)-C(3)	117.79(14)
C(61)-Cl(63)	1.736(8)	C(11)-C(12)-C(13)	122.98(14)
C(61)-H(611)	0.998	C(3)-C(12)-C(13)	119.17(14)
C(61)-H(612)	0.957	C(12)-C(13)-C(14)	122.68(15)
		C(12)-C(13)-C(22)	119.03(15)
O(2)-P(1)-O(23)	97.30(6)	C(14)-C(13)-C(22)	118.28(16)
O(2)-P(1)-N(24)	96.26(6)	C(13)-C(14)-C(15)	122.90(16)
O(23)-P(1)-N(24)	107.03(7)	C(13)-C(14)-C(19)	119.06(18)
P(1)-O(2)-C(3)	116.89(10)	C(15)-C(14)-C(19)	118.03(18)
O(2)-C(3)-C(4)	117.35(15)	C(14)-C(15)-C(16)	120.3(2)
O(2)-C(3)-C(12)	120.17(14)	C(14)-C(15)-H(151)	120.4
C(4)-C(3)-C(12)	122.45(15)	C(16)-C(15)-H(151)	119.3
C(3)-C(4)-C(5)	119.90(16)	C(15)-C(16)-C(17)	120.8(3)
C(3)-C(4)-H(41)	120.2	C(15)-C(16)-H(161)	119.9
C(5)-C(4)-H(41)	119.9	C(17)-C(16)-H(161)	119.1

C(16)-C(17)-C(18)	120.1(2)	H(273)-C(27)-H(271)	107.3
C(16)-C(17)-H(171)	119.6	C(26)-C(27)-H(272)	109.3
C(18)-C(17)-H(171)	120.4	H(273)-C(27)-H(272)	109.5
C(17)-C(18)-C(19)	121.1(2)	H(271)-C(27)-H(272)	109.3
C(17)-C(18)-H(181)	118.7	C(26)-C(28)-H(281)	111.1
C(19)-C(18)-H(181)	120.2	C(26)-C(28)-H(282)	111.6
C(14)-C(19)-C(18)	119.6(2)	H(281)-C(28)-H(282)	107.0
C(14)-C(19)-C(20)	119.33(19)	C(26)-C(28)-H(283)	108.5
C(18)-C(19)-C(20)	121.0(2)	H(281)-C(28)-H(283)	108.5
C(19)-C(20)-C(21)	121.43(18)	H(282)-C(28)-H(283)	110.0
C(19)-C(20)-H(201)	118.4	C(25)-C(29)-C(30)	121.37(16)
C(21)-C(20)-H(201)	120.1	C(25)-C(29)-C(38)	119.43(15)
C(20)-C(21)-C(22)	119.61(19)	C(30)-C(29)-C(38)	119.19(17)
C(20)-C(21)-H(211)	121.7	C(29)-C(30)-C(31)	121.53(19)
C(22)-C(21)-H(211)	118.7	C(29)-C(30)-H(301)	121.0
C(21)-C(22)-C(13)	122.12(19)	C(31)-C(30)-H(301)	117.4
C(21)-C(22)-O(23)	116.77(17)	C(30)-C(31)-C(32)	119.99(19)
C(13)-C(22)-O(23)	121.08(16)	C(30)-C(31)-H(311)	118.3
C(22)-O(23)-P(1)	123.53(11)	C(32)-C(31)-H(311)	121.7
P(1)-N(24)-C(25)	118.39(11)	C(31)-C(32)-C(33)	120.98(18)
P(1)-N(24)-C(26)	122.19(11)	C(31)-C(32)-H(321)	120.3
C(25)-N(24)-C(26)	117.48(13)	C(33)-C(32)-H(321)	118.7
N(24)-C(25)-C(29)	113.01(14)	C(32)-C(33)-C(34)	121.43(18)
N(24)-C(25)-C(43)	112.37(13)	C(32)-C(33)-C(38)	119.29(18)
C(29)-C(25)-C(43)	110.53(14)	C(34)-C(33)-C(38)	119.3(2)
N(24)-C(25)-H(251)	106.5	C(33)-C(34)-C(35)	121.29(19)
C(29)-C(25)-H(251)	106.2	C(33)-C(34)-H(341)	118.1
C(43)-C(25)-H(251)	107.8	C(35)-C(34)-H(341)	120.6
N(24)-C(26)-C(27)	114.55(15)	C(34)-C(35)-C(36)	119.68(18)
N(24)-C(26)-C(28)	111.15(14)	C(34)-C(35)-H(351)	121.7
C(27)-C(26)-C(28)	110.62(16)	C(36)-C(35)-H(351)	118.6
N(24)-C(26)-H(261)	104.2	C(35)-C(36)-C(37)	121.2(2)
C(27)-C(26)-H(261)	107.5	C(35)-C(36)-H(361)	120.0
C(28)-C(26)-H(261)	108.4	C(37)-C(36)-H(361)	118.7
C(26)-C(27)-H(273)	109.0	C(36)-C(37)-C(38)	120.69(19)
C(26)-C(27)-H(271)	112.4	C(36)-C(37)-H(371)	119.1

C(38)-C(37)-H(371)	120.2	C(47)-C(48)-H(481)	118.3
C(29)-C(38)-C(33)	118.91(17)	C(43)-C(48)-H(481)	120.5
C(29)-C(38)-C(37)	123.26(16)	C(44)-C(49)-H(492)	109.9
C(33)-C(38)-C(37)	117.81(17)	C(44)-C(49)-H(493)	109.4
C(25)-C(43)-C(44)	120.62(16)	H(492)-C(49)-H(493)	110.1
C(25)-C(43)-C(48)	120.63(16)	C(44)-C(49)-H(491)	108.0
C(44)-C(43)-C(48)	118.73(17)	H(492)-C(49)-H(491)	109.3
C(43)-C(44)-C(45)	118.92(18)	H(493)-C(49)-H(491)	110.2
C(43)-C(44)-C(49)	122.02(16)	C(46)-C(50)-H(503)	110.1
C(45)-C(44)-C(49)	119.03(18)	C(46)-C(50)-H(501)	107.0
C(44)-C(45)-C(46)	122.2(2)	H(503)-C(50)-H(501)	108.6
C(44)-C(45)-H(451)	117.9	C(46)-C(50)-H(502)	113.6
C(46)-C(45)-H(451)	119.9	H(503)-C(50)-H(502)	107.8
C(45)-C(46)-C(47)	118.44(18)	H(501)-C(50)-H(502)	109.7
C(45)-C(46)-C(50)	120.8(2)	Cl(62)-C(61)-Cl(63)	113.9(5)
C(47)-C(46)-C(50)	120.8(2)	Cl(62)-C(61)-H(611)	105.2
C(46)-C(47)-C(48)	120.5(2)	Cl(63)-C(61)-H(611)	111.5
C(46)-C(47)-H(471)	120.2	Cl(62)-C(61)-H(612)	107.0
C(48)-C(47)-H(471)	119.2	Cl(63)-C(61)-H(612)	109.4
C(47)-C(48)-C(43)	121.26(19)	H(611)-C(61)-H(612)	109.6

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 6790. 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}
P(1)	30(1)	26(1)	35(1)	8(1)	9(1)	4(1)
O(2)	28(1)	27(1)	29(1)	1(1)	3(1)	-2(1)
C(3)	23(1)	22(1)	34(1)	1(1)	2(1)	1(1)
C(4)	32(1)	21(1)	37(1)	-5(1)	1(1)	1(1)
C(5)	28(1)	19(1)	48(1)	-3(1)	0(1)	-3(1)
C(6)	22(1)	22(1)	40(1)	3(1)	3(1)	1(1)
C(7)	28(1)	28(1)	57(1)	4(1)	9(1)	-8(1)
C(8)	39(1)	41(1)	51(1)	8(1)	18(1)	-7(1)
C(9)	37(1)	48(1)	35(1)	2(1)	10(1)	-6(1)
C(10)	30(1)	34(1)	34(1)	1(1)	5(1)	-6(1)
C(11)	20(1)	25(1)	33(1)	3(1)	3(1)	0(1)
C(12)	20(1)	21(1)	33(1)	1(1)	1(1)	-1(1)
C(13)	28(1)	27(1)	25(1)	2(1)	-1(1)	-8(1)
C(14)	42(1)	25(1)	31(1)	-2(1)	3(1)	-8(1)
C(15)	46(1)	27(1)	55(1)	-6(1)	11(1)	0(1)
C(16)	73(2)	38(1)	94(2)	-11(1)	31(2)	6(1)
C(17)	119(3)	33(1)	96(2)	-27(1)	42(2)	-4(1)
C(18)	108(2)	34(1)	56(1)	-16(1)	19(2)	-25(1)
C(19)	70(1)	35(1)	30(1)	-5(1)	2(1)	-19(1)
C(20)	60(1)	56(1)	32(1)	1(1)	-6(1)	-39(1)
C(21)	36(1)	62(1)	30(1)	6(1)	-5(1)	-25(1)
C(22)	30(1)	41(1)	25(1)	8(1)	-3(1)	-8(1)
O(23)	24(1)	47(1)	33(1)	11(1)	2(1)	4(1)
N(24)	29(1)	24(1)	30(1)	4(1)	8(1)	2(1)
C(25)	27(1)	27(1)	28(1)	2(1)	5(1)	0(1)
C(26)	33(1)	25(1)	32(1)	4(1)	6(1)	4(1)
C(27)	46(1)	25(1)	65(1)	8(1)	16(1)	3(1)
C(28)	54(1)	42(1)	36(1)	2(1)	-3(1)	17(1)
C(29)	29(1)	26(1)	33(1)	2(1)	3(1)	1(1)
C(30)	37(1)	41(1)	37(1)	0(1)	0(1)	1(1)
C(31)	42(1)	46(1)	45(1)	-8(1)	-9(1)	0(1)

C(32)	31(1)	38(1)	66(1)	-2(1)	-7(1)	-4(1)
C(33)	25(1)	31(1)	52(1)	10(1)	-1(1)	3(1)
C(34)	24(1)	44(1)	68(1)	24(1)	4(1)	-1(1)
C(35)	28(1)	67(1)	55(1)	30(1)	12(1)	8(1)
C(36)	35(1)	67(1)	37(1)	14(1)	8(1)	9(1)
C(37)	30(1)	45(1)	36(1)	6(1)	5(1)	2(1)
C(38)	25(1)	27(1)	38(1)	7(1)	3(1)	2(1)
C(43)	27(1)	28(1)	35(1)	0(1)	8(1)	1(1)
C(44)	32(1)	31(1)	41(1)	-5(1)	4(1)	3(1)
C(45)	44(1)	30(1)	53(1)	-7(1)	6(1)	2(1)
C(46)	41(1)	30(1)	57(1)	-1(1)	11(1)	7(1)
C(47)	34(1)	40(1)	60(1)	6(1)	2(1)	10(1)
C(48)	29(1)	35(1)	51(1)	2(1)	3(1)	0(1)
C(49)	45(1)	37(1)	61(1)	-14(1)	-12(1)	6(1)
C(50)	65(2)	35(1)	92(2)	-4(1)	5(1)	14(1)
C(61)	67(1)	59(1)	85(1)	-11(1)	24(1)	-24(1)
Cl(62)	61(1)	59(1)	73(1)	-6(1)	-1(1)	12(1)
Cl(63)	67(1)	59(1)	85(1)	-11(1)	24(1)	-24(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 6790.

	x	y	z	U(eq)
H(41)	1550	5152	6172	35
H(51)	969	4543	7956	38
H(71)	631	4442	10528	45
H(81)	625	4919	13006	52
H(91)	1168	6071	13713	49
H(101)	1675	6750	11915	39
H(151)	1074	7617	9900	51
H(161)	730	8811	10960	82
H(171)	1315	9898	11689	99
H(181)	2239	9838	11168	80
H(201)	3032	9063	10200	58
H(211)	3405	7886	9068	52
H(251)	3321	7046	3296	32
H(261)	2489	7837	6214	34
H(273)	2809	9085	5196	67
H(271)	3288	8680	6119	66
H(272)	3279	8609	4331	67
H(281)	2097	8253	3871	65
H(282)	2514	7732	3020	67
H(283)	2082	7287	4057	65
H(301)	3969	7457	6794	46
H(311)	4742	8252	7153	53
H(321)	5254	8728	5086	55
H(341)	5425	8724	2366	54
H(351)	5213	8288	-96	60
H(361)	4431	7453	-456	57
H(371)	3888	7023	1529	43
H(451)	3200	4181	2683	52
H(471)	4494	4559	5450	54
H(481)	4304	5962	5505	45

H(492)	2609	5229	2000	72
H(493)	2900	6095	1684	73
H(491)	2547	5945	3181	72
H(503)	4133	3103	4922	96
H(501)	4319	3230	3240	97
H(502)	3710	2955	3651	97
H(611)	5188	4190	1521	85
H(612)	5693	4814	1249	85