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 6791.

Identification code	6791	
Empirical formula	C93 H78 Cl2 N2 O4 P2	
Formula weight	1420.51	
Temperature	150 K	
Wavelength	1.54180 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 13.92750(10) Å	α= 90°.
	b = 18.66730(10) Å	β= 110.7566(8)°.
	c = 15.27460(10) Å	γ = 90°.
Volume	3713.47(5) $Å^3$	
Z	2	
Density (calculated)	1.270 Mg/m^3	
Absorption coefficient	1.627 mm^{-1}	
F(000)	1492	
Crystal size	0.22 x 0.08 x 0.02 mm^3	
Theta range for data collection	3.094 to 76.281°.	
Index ranges	-17<=h<=17, -23<=k<=23, -19<=l<=19	
Reflections collected	102352	
Independent reflections	15438 [R(int) = 0.066]	
Completeness to theta = 76.281°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.97 and 0.68	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15438 / 1 / 929	
Goodness-of-fit on F^2	1.0071	
Final R indices [I>2sigma(I)]	R1 = 0.0453, wR2 = 0.1169	
R indices (all data)	R1 = 0.0475, wR2 = 0.1194	
Absolute structure parameter	0.001(11)	
Largest diff. peak and hole	0.42 and -0.41 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 6791. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	4624(1)	5001(1)	6088(1)	21
O(2)	4093(1)	4243(1)	6272(1)	24
C(3)	3364(2)	4188(1)	6694(2)	22
C(4)	3631(2)	3793(1)	7535(2)	26
C(5)	2952(2)	3742(1)	7991(2)	29
C(6)	1998(2)	4097(1)	7649(2)	26
C(7)	1323(2)	4100(2)	8158(2)	34
C(8)	420(2)	4466(2)	7841(2)	37
C(9)	132(2)	4841(2)	6993(2)	32
C(10)	755(2)	4839(1)	6471(2)	25
C(11)	1711(2)	4466(1)	6783(2)	21
C(12)	2404(2)	4488(1)	6281(2)	20
C(13)	2143(2)	4864(1)	5368(2)	20
C(14)	1271(2)	4674(1)	4565(2)	23
C(15)	658(2)	4064(1)	4543(2)	28
C(16)	-168(2)	3900(2)	3763(2)	35
C(17)	-432(2)	4333(2)	2963(2)	39
C(18)	148(2)	4915(2)	2946(2)	34
C(19)	1026(2)	5098(1)	3736(2)	26
C(20)	1656(2)	5687(2)	3721(2)	30
C(21)	2520(2)	5836(1)	4474(2)	27
C(22)	2766(2)	5413(1)	5286(2)	23
O(23)	3663(1)	5560(1)	6028(1)	23
N(24)	5429(2)	5265(1)	7124(1)	23
C(25)	6519(2)	5388(1)	7257(2)	24
C(26)	5107(2)	5360(2)	7950(2)	29
C(27)	5211(3)	6128(2)	8297(3)	54
C(28)	5677(2)	4849(2)	8748(2)	47
C(29)	6772(2)	6171(1)	7146(2)	23
C(30)	6055(2)	6627(1)	6599(2)	25
C(31)	6277(2)	7359(1)	6471(2)	25

C(32)	5520(2)	7800(2)	5843(2)	30
C(33)	5732(2)	8499(2)	5692(2)	35
C(34)	6702(2)	8779(2)	6177(2)	38
C(35)	7455(2)	8362(1)	6799(2)	33
C(36)	7267(2)	7637(1)	6947(2)	26
C(37)	8062(2)	7151(1)	7534(2)	26
C(38)	9079(2)	7380(2)	7982(2)	33
C(39)	9837(2)	6914(2)	8479(2)	36
C(40)	9612(2)	6193(2)	8531(2)	35
C(41)	8617(2)	5952(2)	8117(2)	29
C(42)	7816(2)	6424(1)	7608(2)	24
C(43)	6883(2)	4886(1)	6640(2)	25
C(44)	7226(2)	5137(1)	5952(2)	27
C(45)	7574(2)	4673(2)	5413(2)	30
C(46)	7555(2)	3941(2)	5578(2)	33
C(47)	7198(2)	3670(2)	6254(2)	32
C(48)	6877(2)	4150(1)	6792(2)	30
C(49)	7972(2)	4965(2)	4693(2)	39
C(50)	7161(3)	2872(2)	6413(3)	48
P(51)	4478(1)	11163(1)	8475(1)	20
O(52)	3445(1)	10644(1)	7973(1)	22
C(53)	2624(2)	10867(1)	8221(2)	22
C(54)	2462(2)	10518(2)	8971(2)	28
C(55)	1695(2)	10746(2)	9265(2)	30
C(56)	1070(2)	11339(2)	8829(2)	28
C(57)	282(2)	11589(2)	9139(2)	36
C(58)	-298(2)	12170(2)	8730(2)	41
C(59)	-108(2)	12535(2)	8001(2)	39
C(60)	641(2)	12301(1)	7676(2)	29
C(61)	1232(2)	11688(1)	8061(2)	23
C(62)	2017(2)	11423(1)	7737(2)	20
C(63)	2235(2)	11750(1)	6942(2)	20
C(64)	1462(2)	11801(1)	6023(2)	21
C(65)	470(2)	11502(1)	5800(2)	25
C(66)	-245(2)	11546(2)	4912(2)	31
C(67)	5(2)	11884(2)	4197(2)	37
C(68)	949(2)	12174(2)	4385(2)	33

C(69)	1711(2)	12136(1)	5295(2)	24
C(70)	2707(2)	12417(1)	5488(2)	27
C(71)	3446(2)	12338(1)	6349(2)	24
C(72)	3212(2)	11983(1)	7065(2)	21
O(73)	3999(1)	11923(1)	7927(1)	23
N(74)	5214(2)	10825(1)	7930(1)	23
C(75)	6298(2)	10666(1)	8474(2)	23
C(76)	4839(2)	10706(2)	6901(2)	29
C(77)	4846(3)	9918(2)	6657(2)	50
C(78)	5422(3)	11160(2)	6427(2)	51
C(79)	6501(2)	9890(1)	8800(2)	23
C(80)	5772(2)	9480(1)	8942(2)	24
C(81)	5956(2)	8761(1)	9288(2)	23
C(82)	5193(2)	8369(2)	9487(2)	30
C(83)	5377(2)	7681(2)	9827(2)	31
C(84)	6332(2)	7365(1)	9975(2)	30
C(85)	7089(2)	7733(1)	9783(2)	27
C(86)	6927(2)	8446(1)	9447(2)	23
C(87)	7731(2)	8875(1)	9308(2)	22
C(88)	8729(2)	8605(1)	9501(2)	29
C(89)	9502(2)	9021(2)	9428(2)	34
C(90)	9306(2)	9737(2)	9147(2)	33
C(91)	8341(2)	10018(2)	8941(2)	29
C(92)	7525(2)	9600(1)	9006(2)	22
C(93)	6734(2)	11190(1)	9288(2)	26
C(94)	6997(2)	10979(1)	10215(2)	29
C(95)	7350(2)	11469(2)	10946(2)	35
C(96)	7430(2)	12184(2)	10724(2)	40
C(97)	7196(2)	12412(2)	9812(3)	41
C(98)	6850(2)	11911(2)	9092(2)	33
C(99)	7648(3)	11221(2)	11945(2)	48
C(100)	7309(3)	13186(2)	9588(4)	66
Cl(101)	2949(1)	8595(1)	7369(1)	58
C(102)	3752(3)	7991(3)	7081(4)	70
Cl(103)	3069(1)	7356(1)	6254(1)	63

Table 3. Bond lengths [Å] and angles [°] for 6791.

P(1)-O(2)	1.6640(18)	C(19)-C(20)	1.412(4)
P(1)-O(23)	1.6739(17)	C(20)-C(21)	1.366(4)
P(1)-N(24)	1.658(2)	C(20)-H(201)	0.939
O(2)-C(3)	1.387(3)	C(21)-C(22)	1.406(3)
C(3)-C(4)	1.411(3)	C(21)-H(211)	0.944
C(3)-C(12)	1.379(3)	C(22)-O(23)	1.385(3)
C(4)-C(5)	1.363(4)	N(24)-C(25)	1.476(3)
C(4)-H(41)	0.930	N(24)-C(26)	1.492(3)
C(5)-C(6)	1.410(4)	C(25)-C(29)	1.526(3)
C(5)-H(51)	0.916	C(25)-C(43)	1.537(3)
C(6)-C(7)	1.416(4)	C(25)-H(251)	1.013
C(6)-C(11)	1.419(3)	C(26)-C(27)	1.517(4)
C(7)-C(8)	1.360(4)	C(26)-C(28)	1.529(4)
C(7)-H(71)	0.941	C(26)-H(261)	0.984
C(8)-C(9)	1.399(4)	C(27)-H(271)	0.953
C(8)-H(81)	0.933	C(27)-H(272)	0.958
C(9)-C(10)	1.372(3)	C(27)-H(273)	0.969
C(9)-H(91)	0.943	C(28)-H(281)	0.978
C(10)-C(11)	1.426(3)	C(28)-H(282)	0.971
C(10)-H(101)	0.946	C(28)-H(283)	0.973
C(11)-C(12)	1.431(3)	C(29)-C(30)	1.354(3)
C(12)-C(13)	1.486(3)	C(29)-C(42)	1.452(3)
C(13)-C(14)	1.432(3)	C(30)-C(31)	1.429(3)
C(13)-C(22)	1.378(3)	C(30)-H(301)	0.950
C(14)-C(15)	1.417(4)	C(31)-C(32)	1.412(4)
C(14)-C(19)	1.427(3)	C(31)-C(36)	1.410(3)
C(15)-C(16)	1.367(4)	C(32)-C(33)	1.374(4)
C(15)-H(151)	0.935	C(32)-H(321)	0.927
C(16)-C(17)	1.400(4)	C(33)-C(34)	1.393(4)
C(16)-H(161)	0.953	C(33)-H(331)	0.935
C(17)-C(18)	1.360(5)	C(34)-C(35)	1.379(4)
C(17)-H(171)	0.941	C(34)-H(341)	0.928
C(18)-C(19)	1.421(4)	C(35)-C(36)	1.412(4)
C(18)-H(181)	0.944	C(35)-H(351)	0.961

C(36)-C(37)	1.465(4)	C(55)-C(56)	1.421(4)
C(37)-C(38)	1.404(3)	C(55)-H(551)	0.938
C(37)-C(42)	1.414(4)	C(56)-C(57)	1.420(4)
C(38)-C(39)	1.372(4)	C(56)-C(61)	1.427(3)
C(38)-H(381)	0.946	C(57)-C(58)	1.364(5)
C(39)-C(40)	1.390(5)	C(57)-H(571)	0.938
C(39)-H(391)	0.924	C(58)-C(59)	1.408(5)
C(40)-C(41)	1.379(4)	C(58)-H(581)	0.948
C(40)-H(401)	0.937	C(59)-C(60)	1.376(4)
C(41)-C(42)	1.417(4)	C(59)-H(591)	0.945
C(41)-H(411)	0.932	C(60)-C(61)	1.411(4)
C(43)-C(44)	1.381(4)	C(60)-H(601)	0.932
C(43)-C(48)	1.394(4)	C(61)-C(62)	1.439(3)
C(44)-C(45)	1.395(4)	C(62)-C(63)	1.483(3)
C(44)-H(441)	0.950	C(63)-C(64)	1.439(3)
C(45)-C(46)	1.390(4)	C(63)-C(72)	1.376(3)
C(45)-C(49)	1.499(4)	C(64)-C(65)	1.416(3)
C(46)-C(47)	1.390(4)	C(64)-C(69)	1.421(3)
C(46)-H(461)	0.927	C(65)-C(66)	1.371(3)
C(47)-C(48)	1.392(4)	C(65)-H(651)	0.925
C(47)-C(50)	1.513(4)	C(66)-C(67)	1.407(4)
C(48)-H(481)	0.934	C(66)-H(661)	0.945
C(49)-H(491)	0.953	C(67)-C(68)	1.356(4)
C(49)-H(492)	0.953	C(67)-H(671)	0.936
C(49)-H(493)	0.948	C(68)-C(69)	1.420(3)
C(50)-H(501)	0.959	C(68)-H(681)	0.930
C(50)-H(502)	0.965	C(69)-C(70)	1.414(4)
C(50)-H(503)	0.972	C(70)-C(71)	1.361(4)
P(51)-O(52)	1.6774(17)	C(70)-H(701)	0.942
P(51)-O(73)	1.6634(17)	C(71)-C(72)	1.412(3)
P(51)-N(74)	1.658(2)	C(71)-H(711)	0.935
O(52)-C(53)	1.391(3)	C(72)-O(73)	1.388(3)
C(53)-C(54)	1.403(3)	N(74)-C(75)	1.473(3)
C(53)-C(62)	1.377(3)	N(74)-C(76)	1.486(3)
C(54)-C(55)	1.365(4)	C(75)-C(79)	1.524(3)
C(54)-H(541)	0.942	C(75)-C(93)	1.529(3)

C(75)-H(751)	0.997	C(93)-C(98)	1.399(4)
C(76)-C(77)	1.518(4)	C(94)-C(95)	1.390(4)
C(76)-C(78)	1.522(4)	C(94)-H(941)	0.932
C(76)-H(761)	0.998	C(95)-C(96)	1.392(5)
C(77)-H(771)	0.965	C(95)-C(99)	1.506(5)
C(77)-H(772)	0.964	C(96)-C(97)	1.380(5)
C(77)-H(773)	0.960	C(96)-H(961)	0.936
C(78)-H(781)	0.969	C(97)-C(98)	1.393(4)
C(78)-H(782)	0.966	C(97)-C(100)	1.506(5)
C(78)-H(783)	0.980	C(98)-H(981)	0.955
C(79)-C(80)	1.349(3)	C(99)-H(991)	0.958
C(79)-C(92)	1.452(3)	C(99)-H(992)	0.967
C(80)-C(81)	1.432(3)	C(99)-H(993)	0.963
C(80)-H(801)	0.953	C(100)-H(1001)	0.954
C(81)-C(82)	1.409(4)	C(100)-H(1002)	0.954
C(81)-C(86)	1.414(3)	C(100)-H(1003)	0.956
C(82)-C(83)	1.376(4)	Cl(101)-C(102)	1.751(4)
C(82)-H(821)	0.931	C(102)-Cl(103)	1.747(4)
C(83)-C(84)	1.398(4)	C(102)-H(1021)	0.962
C(83)-H(831)	0.946	C(102)-H(1022)	0.983
C(84)-C(85)	1.374(4)		
C(84)-H(841)	0.947	O(2)-P(1)-O(23)	98.34(8)
C(85)-C(86)	1.415(3)	O(2)-P(1)-N(24)	106.40(10)
C(85)-H(851)	0.934	O(23)-P(1)-N(24)	97.13(10)
C(86)-C(87)	1.452(3)	P(1)-O(2)-C(3)	125.72(15)
C(87)-C(88)	1.408(3)	O(2)-C(3)-C(4)	117.5(2)
C(87)-C(92)	1.425(3)	O(2)-C(3)-C(12)	120.5(2)
C(88)-C(89)	1.364(4)	C(4)-C(3)-C(12)	122.0(2)
C(88)-H(881)	0.936	C(3)-C(4)-C(5)	119.7(2)
C(89)-C(90)	1.400(4)	C(3)-C(4)-H(41)	120.3
C(89)-H(891)	0.943	C(5)-C(4)-H(41)	120.0
C(90)-C(91)	1.373(4)	C(4)-C(5)-C(6)	120.8(2)
C(90)-H(901)	0.947	C(4)-C(5)-H(51)	119.5
C(91)-C(92)	1.411(3)	C(6)-C(5)-H(51)	119.7
C(91)-H(911)	0.959	C(5)-C(6)-C(7)	121.4(2)
C(93)-C(94)	1.387(4)	C(5)-C(6)-C(11)	119.4(2)

C(7)-C(6)-C(11)	119.2(2)	C(19)-C(18)-H(181)	120.1
C(6)-C(7)-C(8)	121.1(2)	C(14)-C(19)-C(18)	118.9(2)
C(6)-C(7)-H(71)	118.5	C(14)-C(19)-C(20)	119.4(2)
C(8)-C(7)-H(71)	120.4	C(18)-C(19)-C(20)	121.7(2)
C(7)-C(8)-C(9)	120.4(3)	C(19)-C(20)-C(21)	120.8(2)
C(7)-C(8)-H(81)	120.1	C(19)-C(20)-H(201)	118.9
C(9)-C(8)-H(81)	119.5	C(21)-C(20)-H(201)	120.4
C(8)-C(9)-C(10)	120.3(3)	C(20)-C(21)-C(22)	119.7(2)
C(8)-C(9)-H(91)	120.1	C(20)-C(21)-H(211)	120.7
C(10)-C(9)-H(91)	119.7	C(22)-C(21)-H(211)	119.6
C(9)-C(10)-C(11)	121.0(2)	C(21)-C(22)-C(13)	122.2(2)
C(9)-C(10)-H(101)	119.7	C(21)-C(22)-O(23)	118.6(2)
C(11)-C(10)-H(101)	119.3	C(13)-C(22)-O(23)	119.2(2)
C(10)-C(11)-C(6)	118.0(2)	C(22)-O(23)-P(1)	113.14(15)
C(10)-C(11)-C(12)	122.3(2)	P(1)-N(24)-C(25)	119.49(16)
C(6)-C(11)-C(12)	119.6(2)	P(1)-N(24)-C(26)	122.58(16)
C(11)-C(12)-C(3)	118.1(2)	C(25)-N(24)-C(26)	117.90(19)
C(11)-C(12)-C(13)	122.0(2)	N(24)-C(25)-C(29)	113.64(19)
C(3)-C(12)-C(13)	119.8(2)	N(24)-C(25)-C(43)	111.57(19)
C(12)-C(13)-C(14)	122.6(2)	C(29)-C(25)-C(43)	112.1(2)
C(12)-C(13)-C(22)	118.9(2)	N(24)-C(25)-H(251)	106.0
C(14)-C(13)-C(22)	118.4(2)	C(29)-C(25)-H(251)	106.9
C(13)-C(14)-C(15)	122.6(2)	C(43)-C(25)-H(251)	105.9
C(13)-C(14)-C(19)	119.1(2)	N(24)-C(26)-C(27)	112.8(2)
C(15)-C(14)-C(19)	118.2(2)	N(24)-C(26)-C(28)	111.9(2)
C(14)-C(15)-C(16)	120.9(2)	C(27)-C(26)-C(28)	110.6(3)
C(14)-C(15)-H(151)	119.0	N(24)-C(26)-H(261)	105.5
C(16)-C(15)-H(151)	120.0	C(27)-C(26)-H(261)	107.7
C(15)-C(16)-C(17)	120.8(3)	C(28)-C(26)-H(261)	108.0
C(15)-C(16)-H(161)	118.5	C(26)-C(27)-H(271)	109.8
C(17)-C(16)-H(161)	120.8	C(26)-C(27)-H(272)	111.0
C(16)-C(17)-C(18)	120.2(2)	H(271)-C(27)-H(272)	109.5
C(16)-C(17)-H(171)	120.0	C(26)-C(27)-H(273)	106.9
C(18)-C(17)-H(171)	119.7	H(271)-C(27)-H(273)	109.9
C(17)-C(18)-C(19)	120.9(2)	H(272)-C(27)-H(273)	109.7
C(17)-C(18)-H(181)	119.0	C(26)-C(28)-H(281)	108.3

C(26)-C(28)-H(282)	109.0	C(38)-C(39)-H(391)	119.7
H(281)-C(28)-H(282)	110.1	C(40)-C(39)-H(391)	120.3
C(26)-C(28)-H(283)	109.4	C(39)-C(40)-C(41)	120.0(3)
H(281)-C(28)-H(283)	109.2	C(39)-C(40)-H(401)	121.2
H(282)-C(28)-H(283)	110.9	C(41)-C(40)-H(401)	118.8
C(25)-C(29)-C(30)	121.5(2)	C(40)-C(41)-C(42)	121.1(3)
C(25)-C(29)-C(42)	119.3(2)	C(40)-C(41)-H(411)	119.8
C(30)-C(29)-C(42)	119.2(2)	C(42)-C(41)-H(411)	119.2
C(29)-C(30)-C(31)	122.5(2)	C(29)-C(42)-C(41)	121.5(2)
C(29)-C(30)-H(301)	119.3	C(29)-C(42)-C(37)	120.1(2)
C(31)-C(30)-H(301)	118.1	C(41)-C(42)-C(37)	118.4(2)
C(30)-C(31)-C(32)	120.3(2)	C(25)-C(43)-C(44)	122.5(2)
C(30)-C(31)-C(36)	120.0(2)	C(25)-C(43)-C(48)	118.5(2)
C(32)-C(31)-C(36)	119.6(2)	C(44)-C(43)-C(48)	119.0(2)
C(31)-C(32)-C(33)	121.0(3)	C(43)-C(44)-C(45)	121.6(2)
C(31)-C(32)-H(321)	119.3	C(43)-C(44)-H(441)	119.4
C(33)-C(32)-H(321)	119.7	C(45)-C(44)-H(441)	119.1
C(32)-C(33)-C(34)	119.5(3)	C(44)-C(45)-C(46)	118.1(3)
C(32)-C(33)-H(331)	119.5	C(44)-C(45)-C(49)	120.2(3)
C(34)-C(33)-H(331)	121.0	C(46)-C(45)-C(49)	121.7(3)
C(33)-C(34)-C(35)	120.7(3)	C(45)-C(46)-C(47)	121.8(3)
C(33)-C(34)-H(341)	120.5	C(45)-C(46)-H(461)	118.2
C(35)-C(34)-H(341)	118.7	C(47)-C(46)-H(461)	120.0
C(34)-C(35)-C(36)	120.9(3)	C(46)-C(47)-C(48)	118.5(3)
C(34)-C(35)-H(351)	119.2	C(46)-C(47)-C(50)	121.3(3)
C(36)-C(35)-H(351)	119.8	C(48)-C(47)-C(50)	120.1(3)
C(35)-C(36)-C(31)	118.2(2)	C(43)-C(48)-C(47)	120.9(3)
C(35)-C(36)-C(37)	123.3(2)	C(43)-C(48)-H(481)	117.5
C(31)-C(36)-C(37)	118.5(2)	C(47)-C(48)-H(481)	121.5
C(36)-C(37)-C(38)	121.5(2)	C(45)-C(49)-H(491)	109.5
C(36)-C(37)-C(42)	119.4(2)	C(45)-C(49)-H(492)	109.4
C(38)-C(37)-C(42)	119.0(2)	H(491)-C(49)-H(492)	107.5
C(37)-C(38)-C(39)	121.5(3)	C(45)-C(49)-H(493)	113.5
C(37)-C(38)-H(381)	117.4	H(491)-C(49)-H(493)	109.0
C(39)-C(38)-H(381)	121.1	H(492)-C(49)-H(493)	107.7
C(38)-C(39)-C(40)	120.1(2)	C(47)-C(50)-H(501)	111.2

C(47)-C(50)-H(502)	111.9	C(61)-C(62)-C(53)	118.1(2)
H(501)-C(50)-H(502)	108.5	C(61)-C(62)-C(63)	122.7(2)
C(47)-C(50)-H(503)	112.5	C(53)-C(62)-C(63)	119.1(2)
H(501)-C(50)-H(503)	105.8	C(62)-C(63)-C(64)	121.8(2)
H(502)-C(50)-H(503)	106.8	C(62)-C(63)-C(72)	119.8(2)
O(52)-P(51)-O(73)	97.85(8)	C(64)-C(63)-C(72)	118.3(2)
O(52)-P(51)-N(74)	97.64(9)	C(63)-C(64)-C(65)	122.5(2)
O(73)-P(51)-N(74)	106.31(10)	C(63)-C(64)-C(69)	119.2(2)
P(51)-O(52)-C(53)	110.92(14)	C(65)-C(64)-C(69)	118.2(2)
O(52)-C(53)-C(54)	118.0(2)	C(64)-C(65)-C(66)	121.2(2)
O(52)-C(53)-C(62)	119.1(2)	C(64)-C(65)-H(651)	118.0
C(54)-C(53)-C(62)	122.9(2)	C(66)-C(65)-H(651)	120.8
C(53)-C(54)-C(55)	119.6(2)	C(65)-C(66)-C(67)	120.1(2)
C(53)-C(54)-H(541)	120.2	C(65)-C(66)-H(661)	119.9
C(55)-C(54)-H(541)	120.1	C(67)-C(66)-H(661)	120.0
C(54)-C(55)-C(56)	120.7(2)	C(66)-C(67)-C(68)	120.2(2)
C(54)-C(55)-H(551)	119.1	C(66)-C(67)-H(671)	119.7
C(56)-C(55)-H(551)	120.2	C(68)-C(67)-H(671)	120.1
C(55)-C(56)-C(57)	121.1(2)	C(67)-C(68)-C(69)	121.2(2)
C(55)-C(56)-C(61)	119.5(2)	C(67)-C(68)-H(681)	118.9
C(57)-C(56)-C(61)	119.4(3)	C(69)-C(68)-H(681)	119.9
C(56)-C(57)-C(58)	120.6(3)	C(64)-C(69)-C(68)	118.9(2)
C(56)-C(57)-H(571)	118.2	C(64)-C(69)-C(70)	119.6(2)
C(58)-C(57)-H(571)	121.1	C(68)-C(69)-C(70)	121.5(2)
C(57)-C(58)-C(59)	120.1(3)	C(69)-C(70)-C(71)	120.8(2)
C(57)-C(58)-H(581)	119.6	C(69)-C(70)-H(701)	120.3
C(59)-C(58)-H(581)	120.3	C(71)-C(70)-H(701)	118.9
C(58)-C(59)-C(60)	120.7(3)	C(70)-C(71)-C(72)	119.7(2)
C(58)-C(59)-H(591)	120.3	C(70)-C(71)-H(711)	121.3
C(60)-C(59)-H(591)	119.0	C(72)-C(71)-H(711)	118.9
C(59)-C(60)-C(61)	120.8(3)	C(71)-C(72)-C(63)	122.1(2)
C(59)-C(60)-H(601)	121.6	C(71)-C(72)-O(73)	116.8(2)
C(61)-C(60)-H(601)	117.6	C(63)-C(72)-O(73)	120.9(2)
C(56)-C(61)-C(60)	118.3(2)	C(72)-O(73)-P(51)	125.98(15)
C(56)-C(61)-C(62)	119.1(2)	P(51)-N(74)-C(75)	119.07(16)
C(60)-C(61)-C(62)	122.5(2)	P(51)-N(74)-C(76)	122.68(16)

C(75)-N(74)-C(76)	118.18(19)	C(83)-C(82)-H(821)	120.2
N(74)-C(75)-C(79)	114.20(19)	C(82)-C(83)-C(84)	119.6(2)
N(74)-C(75)-C(93)	111.22(19)	C(82)-C(83)-H(831)	120.2
C(79)-C(75)-C(93)	111.57(19)	C(84)-C(83)-H(831)	120.2
N(74)-C(75)-H(751)	105.1	C(83)-C(84)-C(85)	120.8(2)
C(79)-C(75)-H(751)	106.3	C(83)-C(84)-H(841)	121.3
C(93)-C(75)-H(751)	107.9	C(85)-C(84)-H(841)	117.9
N(74)-C(76)-C(77)	111.9(2)	C(84)-C(85)-C(86)	120.8(2)
N(74)-C(76)-C(78)	111.9(2)	C(84)-C(85)-H(851)	120.1
C(77)-C(76)-C(78)	111.8(3)	C(86)-C(85)-H(851)	119.2
N(74)-C(76)-H(761)	106.0	C(85)-C(86)-C(81)	118.3(2)
C(77)-C(76)-H(761)	108.0	C(85)-C(86)-C(87)	122.6(2)
C(78)-C(76)-H(761)	106.8	C(81)-C(86)-C(87)	119.0(2)
C(76)-C(77)-H(771)	107.7	C(86)-C(87)-C(88)	121.8(2)
C(76)-C(77)-H(772)	109.5	C(86)-C(87)-C(92)	119.6(2)
H(771)-C(77)-H(772)	111.1	C(88)-C(87)-C(92)	118.5(2)
C(76)-C(77)-H(773)	108.7	C(87)-C(88)-C(89)	121.9(2)
H(771)-C(77)-H(773)	109.8	C(87)-C(88)-H(881)	118.8
H(772)-C(77)-H(773)	109.9	C(89)-C(88)-H(881)	119.3
C(76)-C(78)-H(781)	109.8	C(88)-C(89)-C(90)	119.6(2)
C(76)-C(78)-H(782)	110.1	C(88)-C(89)-H(891)	120.1
H(781)-C(78)-H(782)	109.2	C(90)-C(89)-H(891)	120.3
C(76)-C(78)-H(783)	108.5	C(89)-C(90)-C(91)	120.2(3)
H(781)-C(78)-H(783)	108.6	C(89)-C(90)-H(901)	119.3
H(782)-C(78)-H(783)	110.6	C(91)-C(90)-H(901)	120.5
C(75)-C(79)-C(80)	122.0(2)	C(90)-C(91)-C(92)	121.4(3)
C(75)-C(79)-C(92)	118.6(2)	C(90)-C(91)-H(911)	119.7
C(80)-C(79)-C(92)	119.3(2)	C(92)-C(91)-H(911)	118.9
C(79)-C(80)-C(81)	123.0(2)	C(79)-C(92)-C(87)	119.6(2)
C(79)-C(80)-H(801)	119.5	C(79)-C(92)-C(91)	122.1(2)
C(81)-C(80)-H(801)	117.5	C(87)-C(92)-C(91)	118.2(2)
C(80)-C(81)-C(82)	121.1(2)	C(75)-C(93)-C(94)	122.2(2)
C(80)-C(81)-C(86)	119.3(2)	C(75)-C(93)-C(98)	118.9(2)
C(82)-C(81)-C(86)	119.7(2)	C(94)-C(93)-C(98)	118.8(2)
C(81)-C(82)-C(83)	120.9(2)	C(93)-C(94)-C(95)	121.5(3)
C(81)-C(82)-H(821)	118.9	C(93)-C(94)-H(941)	120.1

C(95)-C(94)-H(941)	118.3	C(95)-C(99)-H(993)	111.3
C(94)-C(95)-C(96)	118.1(3)	H(991)-C(99)-H(993)	110.1
C(94)-C(95)-C(99)	120.3(3)	H(992)-C(99)-H(993)	105.8
C(96)-C(95)-C(99)	121.6(3)	C(97)-C(100)-H(1001)	112.1
C(95)-C(96)-C(97)	122.0(3)	C(97)-C(100)-H(1002)	110.0
C(95)-C(96)-H(961)	119.6	H(1001)-C(100)-H(1002)	107.0
C(97)-C(96)-H(961)	118.4	C(97)-C(100)-H(1003)	112.9
C(96)-C(97)-C(98)	118.8(3)	H(1001)-C(100)-H(1003)	107.0
C(96)-C(97)-C(100)	121.2(3)	H(1002)-C(100)-H(1003)	107.6
C(98)-C(97)-C(100)	120.0(3)	Cl(101)-C(102)-Cl(103)	112.7(2)
C(93)-C(98)-C(97)	120.6(3)	Cl(101)-C(102)-H(1021)	108.9
C(93)-C(98)-H(981)	119.6	Cl(103)-C(102)-H(1021)	109.7
C(97)-C(98)-H(981)	119.7	Cl(101)-C(102)-H(1022)	107.5
C(95)-C(99)-H(991)	111.5	Cl(103)-C(102)-H(1022)	108.4
C(95)-C(99)-H(992)	110.4	H(1021)-C(102)-H(1022)	109.7
H(991)-C(99)-H(992)	107.5		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 6791. 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)	20(1)	22(1)	21(1)	-2(1)	6(1)	-1(1)
O(2)	21(1)	20(1)	30(1)	-4(1)	8(1)	0(1)
C(3)	22(1)	18(1)	22(1)	-3(1)	4(1)	-2(1)
C(4)	26(1)	19(1)	27(1)	2(1)	-1(1)	2(1)
C(5)	36(1)	25(1)	20(1)	8(1)	2(1)	-3(1)
C(6)	31(1)	25(1)	21(1)	-2(1)	7(1)	-8(1)
C(7)	45(2)	34(1)	23(1)	3(1)	13(1)	-6(1)
C(8)	40(1)	44(2)	31(1)	-2(1)	20(1)	-9(1)
C(9)	28(1)	39(2)	30(1)	-3(1)	12(1)	-1(1)
C(10)	25(1)	30(1)	20(1)	2(1)	6(1)	-1(1)
C(11)	24(1)	21(1)	17(1)	-2(1)	4(1)	-4(1)
C(12)	22(1)	17(1)	20(1)	-1(1)	4(1)	-1(1)
C(13)	19(1)	21(1)	19(1)	0(1)	7(1)	2(1)
C(14)	22(1)	26(1)	19(1)	-1(1)	5(1)	6(1)
C(15)	24(1)	32(1)	23(1)	0(1)	3(1)	1(1)
C(16)	28(1)	39(2)	31(1)	-6(1)	2(1)	-3(1)
C(17)	31(1)	49(2)	26(1)	-3(1)	-4(1)	5(1)
C(18)	34(1)	45(2)	19(1)	3(1)	2(1)	11(1)
C(19)	26(1)	34(1)	19(1)	4(1)	8(1)	11(1)
C(20)	32(1)	38(1)	21(1)	10(1)	11(1)	10(1)
C(21)	29(1)	27(1)	31(1)	7(1)	16(1)	4(1)
C(22)	21(1)	23(1)	23(1)	1(1)	8(1)	5(1)
O(23)	22(1)	21(1)	26(1)	0(1)	7(1)	-1(1)
N(24)	23(1)	24(1)	24(1)	-1(1)	8(1)	-4(1)
C(25)	22(1)	24(1)	24(1)	1(1)	6(1)	1(1)
C(26)	31(1)	34(1)	23(1)	-9(1)	11(1)	-11(1)
C(27)	73(2)	44(2)	62(2)	-28(2)	46(2)	-23(2)
C(28)	41(2)	73(2)	23(1)	5(1)	6(1)	-12(2)
C(29)	21(1)	26(1)	22(1)	-3(1)	8(1)	0(1)
C(30)	21(1)	26(1)	27(1)	-3(1)	7(1)	-2(1)
C(31)	28(1)	24(1)	27(1)	-2(1)	14(1)	-1(1)

C(32)	32(1)	29(1)	34(1)	1(1)	17(1)	3(1)
C(33)	45(2)	29(1)	39(1)	5(1)	25(1)	9(1)
C(34)	54(2)	24(1)	50(2)	-2(1)	35(2)	-3(1)
C(35)	41(1)	25(1)	39(1)	-9(1)	23(1)	-8(1)
C(36)	32(1)	26(1)	26(1)	-7(1)	16(1)	-5(1)
C(37)	28(1)	31(1)	22(1)	-8(1)	13(1)	-6(1)
C(38)	31(1)	39(2)	30(1)	-11(1)	13(1)	-14(1)
C(39)	22(1)	56(2)	31(1)	-14(1)	9(1)	-13(1)
C(40)	21(1)	54(2)	26(1)	-9(1)	4(1)	0(1)
C(41)	24(1)	36(1)	25(1)	-5(1)	5(1)	0(1)
C(42)	22(1)	28(1)	22(1)	-7(1)	8(1)	-3(1)
C(43)	18(1)	26(1)	28(1)	-2(1)	3(1)	2(1)
C(44)	23(1)	26(1)	30(1)	-3(1)	6(1)	-2(1)
C(45)	23(1)	34(1)	30(1)	-7(1)	5(1)	-2(1)
C(46)	29(1)	28(1)	38(1)	-11(1)	7(1)	4(1)
C(47)	29(1)	26(1)	35(1)	-2(1)	2(1)	3(1)
C(48)	28(1)	25(1)	34(1)	2(1)	7(1)	1(1)
C(49)	39(1)	44(2)	36(1)	-10(1)	18(1)	-2(1)
C(50)	55(2)	26(2)	56(2)	-2(1)	12(2)	2(1)
P(51)	19(1)	22(1)	19(1)	0(1)	6(1)	1(1)
O(52)	21(1)	22(1)	23(1)	1(1)	7(1)	2(1)
C(53)	22(1)	23(1)	20(1)	-1(1)	7(1)	-4(1)
C(54)	26(1)	32(1)	21(1)	5(1)	3(1)	-4(1)
C(55)	27(1)	43(2)	20(1)	2(1)	7(1)	-13(1)
C(56)	26(1)	38(1)	20(1)	-8(1)	9(1)	-10(1)
C(57)	36(1)	47(2)	31(1)	-11(1)	20(1)	-12(1)
C(58)	37(2)	44(2)	53(2)	-17(1)	28(1)	-6(1)
C(59)	32(1)	35(2)	52(2)	-9(1)	19(1)	3(1)
C(60)	27(1)	28(1)	35(1)	-5(1)	13(1)	-1(1)
C(61)	20(1)	27(1)	21(1)	-6(1)	7(1)	-6(1)
C(62)	19(1)	21(1)	19(1)	-2(1)	5(1)	-2(1)
C(63)	23(1)	17(1)	20(1)	0(1)	8(1)	1(1)
C(64)	23(1)	19(1)	22(1)	1(1)	7(1)	3(1)
C(65)	25(1)	25(1)	22(1)	0(1)	8(1)	-1(1)
C(66)	26(1)	34(1)	28(1)	-2(1)	2(1)	-3(1)
C(67)	35(1)	47(2)	22(1)	3(1)	1(1)	0(1)
C(68)	41(2)	37(1)	22(1)	4(1)	12(1)	0(1)

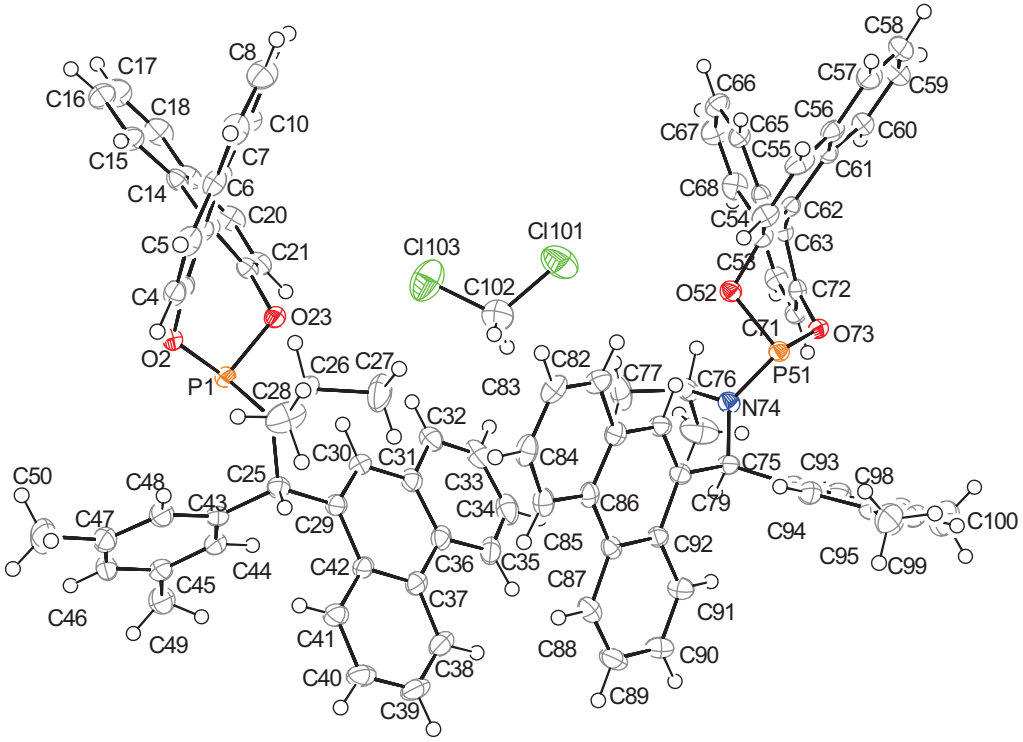
C(69)	30(1)	22(1)	21(1)	1(1)	10(1)	1(1)
C(70)	34(1)	25(1)	27(1)	5(1)	16(1)	1(1)
C(71)	26(1)	21(1)	29(1)	0(1)	13(1)	-2(1)
C(72)	25(1)	16(1)	21(1)	0(1)	8(1)	2(1)
O(73)	18(1)	21(1)	26(1)	-2(1)	5(1)	-1(1)
N(74)	22(1)	24(1)	20(1)	2(1)	6(1)	4(1)
C(75)	18(1)	23(1)	26(1)	3(1)	7(1)	1(1)
C(76)	28(1)	36(1)	21(1)	-2(1)	7(1)	8(1)
C(77)	63(2)	44(2)	30(1)	-15(1)	-1(1)	21(2)
C(78)	41(2)	83(3)	34(1)	13(2)	20(1)	7(2)
C(79)	21(1)	22(1)	23(1)	1(1)	5(1)	3(1)
C(80)	19(1)	26(1)	25(1)	0(1)	6(1)	1(1)
C(81)	26(1)	24(1)	18(1)	-1(1)	6(1)	-1(1)
C(82)	25(1)	31(1)	29(1)	4(1)	5(1)	-3(1)
C(83)	34(1)	27(1)	26(1)	2(1)	5(1)	-10(1)
C(84)	43(1)	19(1)	23(1)	2(1)	6(1)	-2(1)
C(85)	37(1)	22(1)	21(1)	-1(1)	7(1)	4(1)
C(86)	28(1)	23(1)	15(1)	-3(1)	3(1)	1(1)
C(87)	24(1)	24(1)	17(1)	-2(1)	6(1)	4(1)
C(88)	31(1)	28(1)	26(1)	2(1)	10(1)	9(1)
C(89)	24(1)	41(2)	39(1)	1(1)	11(1)	10(1)
C(90)	22(1)	40(2)	38(1)	1(1)	13(1)	-1(1)
C(91)	25(1)	32(1)	32(1)	4(1)	12(1)	1(1)
C(92)	20(1)	23(1)	20(1)	-1(1)	5(1)	2(1)
C(93)	15(1)	24(1)	37(1)	1(1)	5(1)	1(1)
C(94)	24(1)	27(1)	33(1)	-2(1)	6(1)	1(1)
C(95)	20(1)	38(2)	40(1)	-11(1)	2(1)	4(1)
C(96)	21(1)	36(2)	54(2)	-19(1)	0(1)	0(1)
C(97)	24(1)	24(1)	68(2)	-4(1)	6(1)	-1(1)
C(98)	24(1)	26(1)	47(2)	4(1)	8(1)	1(1)
C(99)	43(2)	57(2)	36(2)	-14(2)	2(1)	5(2)
C(100)	61(2)	26(2)	102(3)	-6(2)	18(2)	-6(2)
Cl(101)	49(1)	66(1)	55(1)	8(1)	15(1)	21(1)
C(102)	44(2)	70(3)	87(3)	-30(2)	14(2)	2(2)
Cl(103)	84(1)	56(1)	52(1)	-3(1)	25(1)	-24(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 6791.

	x	y	z	U(eq)
H(41)	4259	3557	7767	31
H(51)	3119	3473	8526	34
H(71)	1521	3854	8732	40
H(81)	-11	4471	8190	44
H(91)	-490	5099	6780	39
H(101)	548	5086	5892	30
H(151)	828	3770	5073	33
H(161)	-560	3484	3774	42
H(171)	-1006	4217	2431	47
H(181)	-47	5204	2404	42
H(201)	1473	5975	3183	36
H(211)	2949	6223	4458	33
H(251)	6924	5248	7927	28
H(261)	4373	5235	7728	34
H(271)	4835	6438	7799	79
H(272)	5917	6272	8538	80
H(273)	4928	6146	8792	80
H(281)	5634	4366	8490	71
H(282)	6390	4998	9019	71
H(283)	5351	4855	9215	70
H(301)	5372	6462	6292	30
H(321)	4870	7616	5532	36
H(331)	5218	8781	5274	42
H(341)	6845	9258	6110	45
H(351)	8117	8568	7129	38
H(381)	9222	7871	7931	39
H(391)	10496	7081	8779	44
H(401)	10127	5862	8841	42
H(411)	8466	5470	8164	34
H(441)	7236	5639	5848	33

H(461)	7785	3632	5220	40
H(481)	6654	3992	7268	36
H(491)	8501	4660	4647	58
H(492)	8268	5424	4887	60
H(493)	7459	5016	4092	59
H(501)	7317	2767	7064	72
H(502)	7637	2613	6200	72
H(503)	6486	2669	6088	73
H(541)	2878	10128	9269	33
H(551)	1602	10517	9776	36
H(571)	177	11347	9637	42
H(581)	-838	12319	8929	50
H(591)	-498	12944	7725	46
H(601)	766	12532	7185	35
H(651)	317	11274	6272	28
H(661)	-906	11349	4780	37
H(671)	-488	11916	3594	46
H(681)	1100	12394	3902	41
H(701)	2872	12658	5018	33
H(711)	4111	12515	6480	29
H(751)	6669	10744	8030	27
H(761)	4112	10875	6658	32
H(771)	4558	9875	5985	74
H(772)	5541	9740	6898	75
H(773)	4429	9660	6934	75
H(781)	6095	10955	6544	76
H(782)	5498	11643	6668	76
H(783)	5040	11157	5751	76
H(801)	5103	9673	8819	29
H(821)	4566	8588	9400	36
H(831)	4858	7421	9953	36
H(841)	6476	6890	10202	37
H(851)	7715	7510	9862	34
H(881)	8866	8129	9697	34
H(891)	10165	8827	9567	40
H(901)	9846	10022	9096	39

H(911)	8209	10506	8736	35
H(941)	6919	10503	10359	35
H(961)	7643	12526	11203	48
H(981)	6674	12062	8457	40
H(991)	7610	11604	12350	73
H(992)	8345	11044	12172	72
H(993)	7227	10826	11998	72
H(1001)	6819	13485	9715	99
H(1002)	7973	13357	9964	99
H(1003)	7230	13260	8947	99
H(1021)	4201	8254	6845	85
H(1022)	4159	7738	7658	85



In the asymmetric unit there are two molecules. The numbering scheme for the second molecule is off-set with 50 compared to the first molecule. One solvent molecule is also found in the asymmetric unit.