

Table S1. Crystal data and structure refinement for 4,5-dicarbomethoxy-1,2,3,5-tetrachlorocyclopentadiene, **7**.

7	
empirical formula	C ₉ H ₆ Cl ₄ O ₄
<i>M_r</i>	319.94
<i>T</i> [K]	300(2)
λ [Å]	0.71073
description	colorless plate
crystal size [mm]	0.06 x 0.28 x 0.30
crystal system	Monoclinic
space group	P2 ₁ /c
<i>a</i> [Å]	8.9176(3)
<i>b</i> [Å]	19.8980(9)
<i>c</i> [Å]	8.0463(4)
α [°]	90.0
β [°]	115.837(2)
γ [°]	90.0
<i>V</i> [Å ³]	1285.03(10)
<i>Z</i>	4
ρ_{calcd} [g cm ⁻³]	1.654
abs. Coeff. [mm ⁻¹]	0.918
<i>F</i> (000)	640
θ range for collection [°]	2.05 to 27.51
limiting indices	-11 < <i>h</i> < 11
	-25 < <i>k</i> < 25
	-10 < <i>l</i> < 10
reflections collected	11297
independent reflections	2870
<i>R</i> (int)	0.0932
refinement method	Full-matrix least-squares on <i>F</i> ²
weighting scheme	$w = 1/[\sigma^2 F_o^2 + (0.0403P((F_o^2 + 2F_c^2)/3))^2 + 1.6544((F_o^2 + 2F_c^2)/3)^2]$
data/restraints/parameters	2870/0/179
goodness-of-fit on <i>F</i> ²	1.043
final <i>R</i> indices [<i>I</i> > 2 σ (<i>I</i>)] ^a	<i>R</i> 1 = 0.0647, <i>wR</i> 2 = 0.1108
<i>R</i> indices (all data) ^a	<i>R</i> 1 = 0.1550, <i>wR</i> 2 = 0.1457
rel. trans. (max., min.)	0.8646, 0.6680
Extinction coeff.	0.0029(10)
Largest diff. peak [eÅ ⁻³]	0.555
Largest diff hole [eÅ ⁻³]	-0.341

$$^a R1 = \Sigma (|| F_o | - | F_c ||) / \Sigma | F_o | ; wR2 = [\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{0.5}$$

Table S2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 7. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cl(1)	4641(2)	5350(1)	6901(2)	65(1)
Cl(2)	1755(2)	4181(1)	4355(2)	77(1)
Cl(3)	-1446(2)	4942(1)	1065(2)	76(1)
Cl(5)	2056(2)	6698(1)	5939(2)	64(1)
O(1)	4440(5)	6922(2)	4413(5)	68(1)
O(2)	3260(4)	6217(2)	2010(4)	54(1)
O(3)	163(5)	7166(2)	1744(6)	90(1)
O(4)	-1907(5)	6445(2)	240(5)	77(1)
C(1)	2792(5)	5483(2)	5013(6)	42(1)
C(2)	1664(6)	5030(2)	4041(7)	47(1)
C(3)	250(5)	5380(3)	2582(6)	47(1)
C(4)	524(5)	6038(2)	2662(6)	44(1)
C(5)	2225(6)	6169(2)	4229(6)	42(1)
C(6)	3454(6)	6503(2)	3587(7)	46(1)
C(7)	4316(10)	6479(4)	1196(10)	69(2)
C(8)	-416(7)	6618(3)	1496(7)	57(1)
C(9)	-2825(11)	7000(4)	-998(11)	96(2)

Table S3. Bond lengths [Å] and angles [deg] for 7.

C(1)-Cl(1)	1.706(5)
C(1)-C(2)	1.323(6)
C(1)-C(5)	1.496(6)
C(2)-Cl(2)	1.705(5)
C(2)-C(3)	1.470(6)
C(3)-Cl(3)	1.712(5)
C(3)-C(4)	1.329(6)
C(4)-C(5)	1.514(6)
C(4)-C(8)	1.493(7)
C(5)-C(6)	1.550(6)
C(5)-Cl(5)	1.790(4)
C(6)-O(2)	1.332(5)
C(6)-O(1)	1.184(5)
C(7)-O(2)	1.458(6)
C(8)-O(4)	1.318(6)
C(8)-O(3)	1.185(6)
C(9)-O(4)	1.474(7)
C(6)-O(2)-C(7)	115.7(4)
C(2)-C(1)-C(5)	110.0(4)
C(2)-C(1)-Cl(1)	127.7(4)
C(5)-C(1)-Cl(1)	122.3(3)
C(8)-O(4)-C(9)	113.6(5)
O(1)-C(6)-O(2)	126.3(4)
O(1)-C(6)-C(5)	125.1(4)
O(2)-C(6)-C(5)	108.5(4)
C(3)-C(4)-C(8)	133.7(5)
C(3)-C(4)-C(5)	107.8(4)
C(8)-C(4)-C(5)	118.3(4)
C(4)-C(3)-C(2)	110.6(4)
C(4)-C(3)-Cl(3)	128.5(4)
C(2)-C(3)-Cl(3)	120.8(4)
O(3)-C(8)-O(4)	126.1(5)
O(3)-C(8)-C(4)	121.4(5)
O(4)-C(8)-C(4)	112.5(5)
C(1)-C(5)-C(4)	103.1(4)
C(1)-C(5)-C(6)	111.9(4)
C(4)-C(5)-C(6)	113.2(4)
C(1)-C(5)-Cl(5)	109.8(3)
C(4)-C(5)-Cl(5)	110.6(3)
C(6)-C(5)-Cl(5)	108.2(3)
C(1)-C(2)-C(3)	108.4(4)
C(1)-C(2)-Cl(2)	127.8(4)
C(3)-C(2)-Cl(2)	123.8(4)

Table S4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for **7**. The anisotropic displacement factor exponent takes the form: $-2p^2 [(ha^*)^2 U_{11} + \dots + 2hka^*b^*U_{12}]$.

	U11	U22	U33	U23	U13	U12
Cl(1)	51(1)	84(1)	52(1)	11(1)	15(1)	8(1)
Cl(2)	96(1)	46(1)	104(1)	3(1)	57(1)	-4(1)
Cl(3)	63(1)	88(1)	70(1)	-20(1)	23(1)	-34(1)
Cl(5)	78(1)	59(1)	65(1)	-16(1)	41(1)	-6(1)
O(1)	75(3)	67(3)	69(3)	-24(2)	38(2)	-36(2)
O(2)	61(2)	60(2)	48(2)	-6(2)	31(2)	-14(2)
O(3)	81(3)	72(3)	99(3)	28(3)	22(3)	-5(3)
O(4)	57(2)	84(3)	70(3)	6(2)	8(2)	7(2)
C(1)	43(3)	49(3)	35(3)	1(2)	17(2)	0(2)
C(2)	57(3)	37(3)	60(3)	-2(2)	36(3)	-3(3)
C(3)	40(3)	62(3)	44(3)	-6(3)	22(2)	-11(3)
C(4)	41(3)	49(3)	44(3)	3(2)	20(2)	-1(2)
C(5)	47(3)	38(3)	42(3)	-6(2)	20(2)	-4(2)
C(6)	47(3)	47(3)	45(3)	1(3)	21(2)	0(3)
C(7)	77(5)	86(5)	54(4)	-4(4)	38(4)	-16(4)
C(8)	47(3)	62(4)	60(3)	1(3)	22(3)	1(3)
C(9)	83(6)	86(6)	79(5)	23(5)	-1(4)	21(5)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **7**.

	x	y	z	U(eq)
H(7A)	4030(67)	6259(28)	23(85)	87(19)
H(7B)	4201(94)	6987(40)	919(101)	147(32)
H(7C)	5431(69)	6409(26)	2057(74)	69(18)
H(9A)	-3697(93)	6731(37)	-2099(104)	137(28)
H(9B)	-1866(82)	7265(36)	-1143(88)	109(25)
H(9C)	-2620(102)	7457(48)	-106(111)	165(34)

Table S6. Crystal data and structure refinement for 4,5,5-tricarbomethoxy-1,2,3-trichlorocyclopentadiene, **8**.

8	
empirical formula	C ₁₁ H ₉ Cl ₃ O ₆
<i>M_r</i>	343.53
<i>T</i> [K]	299(2) K
λ [Å]	0.71073
description	colorless plate
crystal size [mm]	0.10 x 0.18 x 0.30
crystal system	Triclinic
space group	P-1
<i>a</i> [Å]	8.4138(4)
<i>b</i> [Å]	12.0117(5)
<i>c</i> [Å]	14.2489(5)
α [°]	102.368(2)
β [°]	93.306(2)
γ [°]	90.050(2)
<i>V</i> [Å ³]	1404.16(10)
<i>Z</i>	4
ρ_{calcd} [g cm ⁻³]	1.625
abs. Coeff. [mm ⁻¹]	0.673
<i>F</i> (000)	696
θ range for collection [°]	2.42 to 27.53
limiting indices	-8 < <i>h</i> < 10 -15 < <i>k</i> < 13 -11 < <i>l</i> < 18
reflections collected	10349
independent reflections	6326
<i>R</i> (int)	0.0240
refinement method	Full-matrix least-squares on <i>F</i> ²
weighting scheme	$w = 1 / [\sigma^2 F_o^2 + (0.0758P((F_o^2 + 2F_c^2)/3))^2 + 1.7229((F_o^2 + 2F_c^2)/3)]$
data/restraints/parameters	6326 / 0 / 362
goodness-of-fit on <i>F</i> ²	1.046
final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)] ^a	<i>R</i> 1 = 0.0593, <i>wR</i> 2 = 0.1631
<i>R</i> indices (all data) ^a	<i>R</i> 1 = 0.0914, <i>wR</i> 2 = 0.1780
rel. trans. (max., min.)	0.8971, 0.7340
Extinction coeff.	0.010(2)
Largest diff. peak [eÅ ⁻³]	0.602
Largest diff hole [eÅ ⁻³]	-0.294

$$^a R1 = \sum (|F_o| - |F_c|) / \sum |F_o| ; wR2 = [\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{0.5}$$

Table S7. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for **8**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cl(1)	16548(1)	8638(1)	5640(1)	57(1)
Cl(2)	15882(2)	6203(1)	6405(1)	61(1)
Cl(3)	14055(2)	6806(1)	8415(1)	58(1)
Cl(1A)	11861(1)	4132(1)	5593(1)	62(1)
Cl(2A)	11156(2)	6943(1)	6310(1)	67(1)
Cl(3A)	9163(2)	7390(1)	8257(1)	66(1)
O(1)	14029(4)	10846(3)	6406(2)	65(1)
O(2)	12388(3)	9543(2)	6719(2)	47(1)
O(3)	16290(4)	11369(2)	7980(3)	64(1)
O(4)	17683(3)	9802(2)	7953(2)	49(1)
O(5)	13201(4)	9171(3)	9596(2)	71(1)
O(6)	13375(4)	10663(2)	8902(2)	50(1)
O(1A)	11342(4)	2568(3)	7858(3)	66(1)
O(2A)	12718(3)	4173(2)	7948(2)	53(1)
O(3A)	9224(4)	2359(3)	6184(3)	74(1)
O(4A)	7471(3)	3713(2)	6664(2)	49(1)
O(5A)	8087(5)	5656(3)	9396(3)	86(1)
O(6A)	8570(4)	3821(2)	8839(2)	57(1)
C(1)	15651(4)	8507(3)	6644(2)	36(1)
C(2)	15395(4)	7549(3)	6944(3)	37(1)
C(3)	14609(4)	7832(3)	7843(2)	35(1)
C(4)	14377(4)	8963(3)	8107(2)	32(1)
C(5)	15032(4)	9516(3)	7339(2)	31(1)
C(6)	13764(4)	10083(3)	6780(2)	36(1)
C(7)	11148(5)	9875(4)	6090(4)	66(1)
C(8)	16388(4)	10372(3)	7789(3)	36(1)
C(9)	19056(5)	10473(4)	8404(4)	58(1)
C(10)	13583(4)	9585(3)	8952(3)	40(1)
C(11)	12705(6)	11399(4)	9725(3)	58(1)
C(1A)	10835(4)	4769(3)	6546(2)	37(1)
C(2A)	10555(4)	5877(3)	6841(3)	39(1)
C(3A)	9708(4)	6061(3)	7714(3)	39(1)
C(4A)	9442(4)	5074(3)	7966(3)	36(1)
C(5A)	10142(4)	4118(3)	7232(2)	33(1)
C(6A)	11450(4)	3498(3)	7713(3)	38(1)
C(7A)	14058(5)	3737(4)	8439(4)	61(1)
C(8A)	8902(4)	3261(3)	6644(3)	40(1)
C(9A)	6223(5)	3021(4)	6063(4)	64(1)
C(10A)	8622(5)	4900(3)	8803(3)	44(1)
C(11A)	7883(6)	3526(4)	9667(3)	65(1)

Table S8. Bond lengths [Å] and angles [deg] for **8**.

Cl(3)-C(3)	1.696(3)	C(10A)-O(6A)-C(11A)	117.6(3)
Cl(2)-C(2)	1.696(4)	O(3)-C(8)-O(4)	124.7(3)
Cl(1)-C(1)	1.691(4)	O(3)-C(8)-C(5)	126.1(3)
Cl(3A)-C(3A)	1.694(4)	O(4)-C(8)-C(5)	109.2(3)
Cl(1A)-C(1A)	1.694(4)	C(1)-C(2)-C(3)	108.5(3)
Cl(2A)-C(2A)	1.711(4)	C(1)-C(2)-Cl(2)	127.7(3)
O(4)-C(8)	1.323(4)	C(3)-C(2)-Cl(2)	123.7(3)
O(4)-C(9)	1.445(5)	O(1)-C(6)-O(2)	125.2(3)
O(5)-C(10)	1.192(4)	O(1)-C(6)-C(5)	124.2(3)
O(4A)-C(8A)	1.320(4)	O(2)-C(6)-C(5)	110.4(3)
O(4A)-C(9A)	1.455(5)	O(5A)-C(10A)-O(6A)	124.2(4)
C(1A)-C(2A)	1.332(5)	O(5A)-C(10A)-C(4A)	124.4(4)
C(1A)-C(5A)	1.516(5)	O(6A)-C(10A)-C(4A)	111.4(3)
O(5A)-C(10A)	1.207(5)	O(1A)-C(6A)-O(2A)	125.0(3)
O(1A)-C(6A)	1.183(4)	O(1A)-C(6A)-C(5A)	125.7(3)
O(3A)-C(8A)	1.180(5)	O(2A)-C(6A)-C(5A)	109.3(3)
O(3)-C(8)	1.174(4)	C(2)-C(1)-C(5)	110.4(3)
C(10)-O(6)	1.323(4)	C(2)-C(1)-Cl(1)	127.1(3)
C(10)-C(4)	1.470(5)	C(5)-C(1)-Cl(1)	122.5(3)
C(3)-C(4)	1.347(5)	C(3)-C(4)-C(10)	127.9(3)
C(3)-C(2)	1.452(5)	C(3)-C(4)-C(5)	107.7(3)
O(6A)-C(10A)	1.309(5)	C(10)-C(4)-C(5)	124.4(3)
O(6A)-C(11A)	1.452(5)	O(3A)-C(8A)-O(4A)	125.2(4)
C(8)-C(5)	1.549(5)	O(3A)-C(8A)-C(5A)	123.9(4)
C(2)-C(1)	1.333(5)	O(4A)-C(8A)-C(5A)	110.7(3)
C(6)-O(1)	1.181(4)	C(4A)-C(3A)-C(2A)	110.5(3)
C(6)-O(2)	1.316(4)	C(4A)-C(3A)-Cl(3A)	128.9(3)
C(6)-C(5)	1.540(5)	C(2A)-C(3A)-Cl(3A)	120.6(3)
C(10A)-C(4A)	1.465(5)	C(1A)-C(5A)-C(4A)	101.8(3)
C(6A)-O(2A)	1.323(4)	C(1A)-C(5A)-C(6A)	111.1(3)
C(6A)-C(5A)	1.539(5)	C(4A)-C(5A)-C(6A)	110.9(3)
C(1)-C(5)	1.507(5)	C(1A)-C(5A)-C(8A)	107.4(3)
C(4)-C(5)	1.524(4)	C(4A)-C(5A)-C(8A)	114.5(3)
C(8A)-C(5A)	1.543(5)	C(6A)-C(5A)-C(8A)	110.8(3)
C(3A)-C(4A)	1.332(5)	C(3A)-C(4A)-C(10A)	127.2(3)
C(3A)-C(2A)	1.445(5)	C(3A)-C(4A)-C(5A)	108.7(3)
C(5A)-C(4A)	1.521(5)	C(10A)-C(4A)-C(5A)	124.1(3)
O(2)-C(7)	1.448(5)	C(1)-C(5)-C(4)	102.3(3)
O(2A)-C(7A)	1.450(5)	C(1)-C(5)-C(6)	107.3(3)
O(6)-C(11)	1.452(5)	C(4)-C(5)-C(6)	114.4(3)
C(8)-O(4)-C(9)	116.6(3)	C(1)-C(5)-C(8)	111.5(3)
C(8A)-O(4A)-C(9A)	115.8(3)	C(4)-C(5)-C(8)	110.1(3)
C(2A)-C(1A)-C(5A)	109.4(3)	C(6)-C(5)-C(8)	111.0(3)
C(2A)-C(1A)-Cl(1A)	127.6(3)	C(1A)-C(2A)-C(3A)	109.6(3)
C(5A)-C(1A)-Cl(1A)	122.9(3)	C(1A)-C(2A)-Cl(2A)	126.2(3)
O(5)-C(10)-O(6)	125.1(4)	C(3A)-C(2A)-Cl(2A)	124.2(3)
O(5)-C(10)-C(4)	124.3(4)	C(6)-O(2)-C(7)	116.3(3)
O(6)-C(10)-C(4)	110.7(3)	C(6A)-O(2A)-C(7A)	116.8(3)
C(4)-C(3)-C(2)	111.1(3)	C(10)-O(6)-C(11)	116.5(3)
C(4)-C(3)-Cl(3)	127.6(3)		
C(2)-C(3)-Cl(3)	121.2(3)		

Table S9. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for **8**. The anisotropic displacement factor exponent takes the form: $-2p^2 [(ha^*)^2 U_{11} + \dots + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Cl(1)	71(1)	59(1)	42(1)	5(1)	23(1)	-7(1)
Cl(2)	77(1)	33(1)	68(1)	-2(1)	12(1)	9(1)
Cl(3)	77(1)	43(1)	63(1)	28(1)	10(1)	-7(1)
Cl(1A)	59(1)	75(1)	48(1)	3(1)	17(1)	6(1)
Cl(2A)	75(1)	56(1)	77(1)	36(1)	-6(1)	-15(1)
Cl(3A)	82(1)	30(1)	81(1)	-3(1)	5(1)	13(1)
O(1)	60(2)	69(2)	81(2)	50(2)	-13(2)	-14(2)
O(2)	40(2)	44(2)	60(2)	22(1)	-11(1)	-2(1)
O(3)	56(2)	31(2)	98(3)	5(2)	-17(2)	-2(1)
O(4)	35(1)	38(1)	72(2)	8(1)	-8(1)	-3(1)
O(5)	102(3)	63(2)	58(2)	26(2)	41(2)	16(2)
O(6)	68(2)	43(2)	38(1)	5(1)	14(1)	15(1)
O(1A)	55(2)	43(2)	104(3)	32(2)	-13(2)	-3(1)
O(2A)	37(2)	42(2)	80(2)	19(1)	-14(1)	1(1)
O(3A)	59(2)	42(2)	102(3)	-21(2)	-15(2)	8(2)
O(4A)	35(1)	45(2)	63(2)	4(1)	-6(1)	-1(1)
O(5A)	117(3)	55(2)	85(3)	2(2)	63(2)	14(2)
O(6A)	84(2)	45(2)	44(2)	8(1)	20(2)	0(2)
C(1)	36(2)	35(2)	33(2)	4(1)	2(1)	-1(2)
C(2)	39(2)	30(2)	40(2)	5(2)	2(2)	0(2)
C(3)	35(2)	35(2)	37(2)	14(2)	-1(1)	-4(2)
C(4)	29(2)	36(2)	33(2)	9(1)	2(1)	-1(1)
C(5)	34(2)	30(2)	30(2)	8(1)	3(1)	-1(1)
C(6)	40(2)	35(2)	33(2)	10(1)	1(2)	0(2)
C(7)	49(3)	66(3)	86(3)	32(3)	-25(2)	-1(2)
C(8)	34(2)	33(2)	41(2)	9(2)	1(2)	-2(2)
C(9)	37(2)	55(3)	78(3)	8(2)	-10(2)	-8(2)
C(10)	42(2)	43(2)	34(2)	9(2)	4(2)	5(2)
C(11)	69(3)	57(3)	43(2)	-4(2)	11(2)	19(2)
C(1A)	36(2)	41(2)	34(2)	5(2)	1(1)	-1(2)
C(2A)	39(2)	35(2)	45(2)	14(2)	-6(2)	-4(2)
C(3A)	37(2)	29(2)	46(2)	0(2)	-7(2)	3(2)
C(4A)	33(2)	32(2)	40(2)	4(2)	-2(2)	4(1)
C(5A)	32(2)	25(2)	41(2)	5(1)	0(1)	2(1)
C(6A)	36(2)	31(2)	45(2)	6(2)	4(2)	5(2)
C(7A)	41(2)	58(3)	84(3)	19(2)	-18(2)	7(2)
C(8A)	39(2)	31(2)	47(2)	5(2)	-1(2)	-1(2)
C(9A)	46(3)	65(3)	77(3)	12(2)	-15(2)	-17(2)
C(10A)	43(2)	41(2)	44(2)	1(2)	8(2)	1(2)
C(11A)	87(4)	66(3)	47(2)	18(2)	10(2)	-10(3)

Table S10. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **8**.

	x	y	z	U(eq)
H(7A)	10201(5)	9431(4)	6098(4)	99
H(7B)	11495(5)	9744(4)	5446(4)	99
H(7C)	10926(5)	10669(4)	6308(4)	99
H(7AA)	14904(5)	4296(4)	8573(4)	92
H(7AB)	14425(5)	3050(4)	8037(4)	92
H(7AC)	13734(5)	3576(4)	9031(4)	92
H(9A)	19920(5)	9975(4)	8488(4)	87
H(9B)	18796(5)	10913(4)	9020(4)	87
H(9C)	19364(5)	10976(4)	8004(4)	87
H(9AA)	5234(5)	3421(4)	6127(4)	96
H(9AB)	6115(5)	2312(4)	6263(4)	96
H(9AC)	6496(5)	2873(4)	5403(4)	96
H(11A)	7914(6)	2716(4)	9608(3)	98
H(11B)	6799(6)	3773(4)	9697(3)	98
H(11C)	8482(6)	3896(4)	10244(3)	98
H(11D)	12607(6)	12156(4)	9612(3)	87
H(11E)	13393(6)	11415(4)	10290(3)	87
H(11F)	11674(6)	11112(4)	9818(3)	87

Table S11. Crystal data and structure refinement for 7-Carbomethoxy-1,2,3,4,5,6-hexachlorocycloheptatriene, **17**.

17	
empirical formula	C ₉ H ₄ Cl ₆ O ₂
<i>M</i> _r	356.82
<i>T</i> [K]	300(2)
λ [Å]	0.71073
description	colorless plate
crystal size [mm]	0.06 x 0.18 x 0.37
crystal system	Orthorhombic
space group	P2 ₁ 2 ₁ 2 ₁
<i>a</i> [Å]	7.7583(1)
<i>b</i> [Å]	9.2561(1)
<i>c</i> [Å]	18.3732(2)
α [°]	90.0
β [°]	90.0
γ [°]	90.0
<i>V</i> [Å ³]	1319.41(3)
<i>Z</i>	4
ρ_{calcd} [g cm ⁻³]	1.796
abs. Coeff. [mm ⁻¹]	1.285
<i>F</i> (000)	704
θ range for collection [°]	2.22 to 27.66
limiting indices	-10 < <i>h</i> < 10 -12 < <i>k</i> < 10 -23 < <i>l</i> < 24
reflections collected	11778
independent reflections	3059
<i>R</i> (int)	0.0310
refinement method	Full-matrix least-squares on <i>F</i> ²
weighting scheme	$w = 1 / [\sigma^2 F_o^2 + (0.0316 P((F_o^2 + 2F_c^2)/3))^2 + 0.3915((F_o^2 + 2F_c^2)/3)]$
data/restraints/parameters	3059 / 0 / 171
goodness-of-fit on <i>F</i> ²	1.065
final <i>R</i> indices [<i>I</i> > 2 σ (<i>I</i>)] ^a	<i>R</i> 1 = 0.0340, <i>wR</i> 2 = 0.0714
<i>R</i> indices (all data) ^a	<i>R</i> 1 = 0.0452, <i>wR</i> 2 = 0.0770
rel. trans. (max., min.)	0.8372, 0.6210
Extinction coeff.	0.0045(10)
Largest diff. peak [eÅ ⁻³]	0.241
Largest diff hole [eÅ ⁻³]	-0.257

^a*R*1 = $\Sigma (||F_o| - |F_c||) / \Sigma |F_o|$; *wR*2 = $[\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{0.5}$

Table S12. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for **17**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	6595(3)	11027(3)	1981(1)	70(1)
O(2)	6926(3)	9103(2)	1276(1)	59(1)
C(1)	3060(3)	10547(3)	2105(1)	41(1)
C(2)	2730(3)	11693(3)	1694(1)	42(1)
C(3)	3529(4)	11878(3)	985(1)	43(1)
C(4)	3678(4)	10848(3)	483(1)	41(1)
C(5)	3126(3)	9367(3)	586(1)	39(1)
C(6)	3396(3)	8663(3)	1201(1)	41(1)
C(7)	4228(4)	9365(3)	1850(1)	41(1)
C(8)	6062(3)	9963(3)	1709(2)	48(1)
C(9)	8713(5)	9547(7)	1135(3)	85(1)
Cl(1)	2132(1)	10323(1)	2941(1)	68(1)
Cl(2)	1401(1)	13050(1)	1985(1)	73(1)
Cl(3)	4342(1)	13570(1)	821(1)	74(1)
Cl(4)	4633(1)	11206(1)	-338(1)	73(1)
Cl(5)	2162(1)	8537(1)	-147(1)	60(1)
Cl(6)	2716(1)	6928(1)	1318(1)	76(1)

Table S13. Bond lengths [Å] and angles [deg] for **17**

O(1)-C(8)	1.179(4)
O(2)-C(8)	1.310(3)
O(2)-C(9)	1.469(4)
C(1)-Cl(1)	1.708(2)
C(1)-C(2)	1.327(4)
C(1)-C(7)	1.496(4)
C(2)-Cl(2)	1.711(3)
C(2)-C(3)	1.452(4)
C(3)-Cl(3)	1.715(3)
C(3)-C(4)	1.332(4)
C(4)-Cl(4)	1.713(3)
C(4)-C(5)	1.448(4)
C(5)-Cl(5)	1.720(2)
C(5)-C(6)	1.322(4)
C(6)-Cl(6)	1.704(3)
C(6)-C(7)	1.504(4)
C(7)-C(8)	1.548(4)
C(8)-O(2)-C(9)	114.8(3)
C(5)-C(6)-C(7)	122.2(2)
C(5)-C(6)-Cl(6)	121.6(2)
C(7)-C(6)-Cl(6)	116.1(2)
C(6)-C(5)-C(4)	122.1(2)
C(6)-C(5)-Cl(5)	121.1(2)
C(4)-C(5)-Cl(5)	116.7(2)
C(3)-C(4)-C(5)	124.2(2)
C(3)-C(4)-Cl(4)	120.6(2)
C(5)-C(4)-Cl(4)	115.2(2)
C(4)-C(3)-C(2)	125.0(2)
C(4)-C(3)-Cl(3)	120.0(2)
C(2)-C(3)-Cl(3)	115.0(2)
C(1)-C(2)-C(3)	121.5(2)
C(1)-C(2)-Cl(2)	121.7(2)
C(3)-C(2)-Cl(2)	116.8(2)
C(2)-C(1)-C(7)	121.5(2)
C(2)-C(1)-Cl(1)	121.9(2)
C(7)-C(1)-Cl(1)	116.6(2)
C(1)-C(7)-C(6)	107.8(2)
C(1)-C(7)-C(8)	110.3(2)
C(6)-C(7)-C(8)	114.6(2)
O(1)-C(8)-O(2)	125.8(3)
O(1)-C(8)-C(7)	123.4(3)
O(2)-C(8)-C(7)	110.8(2)

Table S14. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for **17**. The anisotropic displacement factor exponent takes the form: $-2p^2 [(ha^*)^2 U_{11} + \dots + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
O(1)	52(1)	82(2)	76(2)	-27(1)	-8(1)	-8(1)
O(2)	43(1)	72(1)	63(1)	-16(1)	6(1)	7(1)
C(1)	39(1)	55(2)	30(1)	-7(1)	-1(1)	1(1)
C(2)	44(1)	45(1)	38(1)	-12(1)	-5(1)	6(1)
C(3)	49(1)	36(1)	44(1)	2(1)	-5(1)	-1(1)
C(4)	44(1)	49(2)	31(1)	3(1)	2(1)	-1(1)
C(5)	40(1)	40(1)	36(1)	-9(1)	0(1)	2(1)
C(6)	45(1)	36(1)	43(1)	-3(1)	1(1)	2(1)
C(7)	46(1)	44(1)	34(1)	6(1)	-1(1)	4(1)
C(8)	42(1)	62(2)	38(1)	4(1)	-6(1)	8(1)
C(9)	44(2)	107(4)	103(4)	-11(3)	19(2)	-5(2)
Cl(1)	72(1)	94(1)	37(1)	-1(1)	15(1)	1(1)
Cl(2)	90(1)	73(1)	56(1)	-21(1)	-6(1)	39(1)
Cl(3)	97(1)	44(1)	83(1)	6(1)	-5(1)	-17(1)
Cl(4)	93(1)	84(1)	43(1)	6(1)	21(1)	-15(1)
Cl(5)	72(1)	63(1)	46(1)	-19(1)	-11(1)	-2(1)
Cl(6)	107(1)	40(1)	81(1)	7(1)	-10(1)	-13(1)

Table S15. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **17**.

	x	y	z	U(eq)
H(7)	4363(36)	8660(31)	2215(15)	48(8)
H(9A)	8752(90)	10181(65)	736(33)	156(27)
H(9B)	9188(73)	8792(57)	1005(30)	122(21)
H(9C)	9128(98)	10274(73)	1685(39)	205(29)

Table S16. Crystal data and structure refinement for (Z)-2-(2-Benzoylphenyl)-1-chloro-1-pentachlorophenyl-2-phenylethene, **23**.

23	
empirical formula	C ₂₇ H ₁₄ Cl ₆ O
<i>M_r</i>	567.08
<i>T</i> [K]	300(2)
λ [Å]	0.71073
description	light yellow plate
crystal size [mm]	0.02 x 0.12 x 0.22
crystal system	Monoclinic
space group	P2 ₁ /c
<i>a</i> [Å]	17.7762(1)
<i>b</i> [Å]	11.2519(3)
<i>c</i> [Å]	12.7982(3)
α [°]	90.0
β [°]	102.965(1)
γ [°]	90.0
<i>V</i> [Å ³]	2494.59(9)
<i>Z</i>	4
ρ_{calcd} [g cm ⁻³]	1.510
abs. Coeff. [mm ⁻¹]	0.709
<i>F</i> (000)	1144
θ range for collection [°]	1.18 to 22.50
limiting indices	-19 < <i>h</i> < 19
	-12 < <i>k</i> < 12
	-14 < <i>l</i> < 13
reflections collected	13848
independent reflections	3241
<i>R</i> (int)	0.0986
refinement method	Full-matrix least-squares on <i>F</i> ²
weighting scheme	$w = 1/[\sigma^2 F_o^2 + (0.0336P((F_o^2 + 2F_c^2)/3))^2 + 1.6288((F_o^2 + 2F_c^2)/3)^2]$
data/restraints/parameters	3220 / 0 / 308
goodness-of-fit on <i>F</i> ²	1.033
final <i>R</i> indices [<i>I</i> > 2 σ (<i>I</i>)] ^a	<i>R</i> 1 = 0.0547, <i>wR</i> 2 = 0.0922
<i>R</i> indices (all data) ^a	<i>R</i> 1 = 0.1068, <i>wR</i> 2 = 0.1116
rel. trans. (max., min.)	0.9423, 0.6368
Extinction coeff.	0.0044(5)
Largest diff. peak [eÅ ⁻³]	0.227
Largest diff hole [eÅ ⁻³]	-0.268

$$^a R1 = \sum (||F_o| - |F_c||) / \sum |F_o|; wR2 = [\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{0.5}$$

Table S17. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for **23**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Cl(1)	3295(1)	2251(1)	6611(1)	54(1)
Cl(4)	4138(1)	-390(1)	7645(1)	62(1)
Cl(5)	5192(1)	-1870(1)	6503(1)	65(1)
Cl(6)	4853(1)	-1940(1)	4017(1)	69(1)
Cl(7)	3406(1)	-682(2)	2679(1)	76(1)
Cl(8)	2337(1)	743(1)	3823(1)	65(1)
O(1)	876(3)	44(4)	8571(4)	94(2)
C(1)	2823(3)	908(4)	6226(4)	39(1)
C(2)	2120(3)	718(4)	6373(4)	38(1)
C(3)	3293(3)	110(4)	5697(4)	38(1)
C(4)	3932(3)	-482(4)	6266(4)	39(1)
C(5)	4410(3)	-1132(4)	5759(4)	41(1)
C(6)	4250(3)	-1187(4)	4647(4)	42(1)
C(7)	3608(3)	-607(5)	4061(4)	45(1)
C(8)	3128(3)	20(4)	4577(4)	39(1)
C(9)	1727(3)	-442(5)	6087(4)	43(1)
C(10)	1040(3)	-501(6)	5337(5)	66(2)
C(11)	648(4)	-1555(7)	5071(6)	84(2)
C(12)	941(4)	-2564(6)	5608(6)	81(2)
C(13)	1618(4)	-2539(5)	6371(5)	71(2)
C(14)	2013(3)	-1486(5)	6599(4)	51(2)
C(15)	1643(3)	1669(5)	6715(4)	44(1)
C(16)	1301(3)	1556(5)	7602(4)	49(2)
C(17)	799(3)	2439(6)	7787(5)	70(2)
C(18)	647(4)	3411(7)	7146(6)	79(2)
C(19)	986(4)	3541(6)	6281(5)	71(2)
C(20)	1470(3)	2681(5)	6068(5)	55(2)
C(21)	1427(4)	528(5)	8347(5)	58(2)
C(22)	2226(3)	176(5)	8907(4)	49(2)
C(23)	2350(4)	-945(6)	9370(5)	66(2)
C(24)	3066(5)	-1262(7)	9967(5)	81(2)
C(25)	3664(4)	-479(8)	10125(5)	76(2)
C(26)	3545(3)	629(6)	9677(4)	62(2)
C(27)	2835(3)	952(5)	9073(4)	50(2)

Table S18. Bond lengths [Å] and angles [deg] for 23.

Cl(8)-C(8)	1.721(5)	C(5)-C(6)-Cl(6)	120.1(4)
Cl(7)-C(7)	1.726(5)	C(4)-C(5)-C(6)	119.8(5)
Cl(6)-C(6)	1.704(5)	C(4)-C(5)-Cl(5)	120.1(4)
Cl(5)-C(5)	1.713(5)	C(6)-C(5)-Cl(5)	120.2(4)
Cl(4)-C(4)	1.724(5)	C(3)-C(4)-C(5)	121.8(4)
Cl(1)-C(1)	1.745(5)	C(3)-C(4)-Cl(4)	118.3(4)
O(1)-C(21)	1.209(6)	C(5)-C(4)-Cl(4)	119.9(4)
C(8)-C(7)	1.384(7)	C(4)-C(3)-C(8)	117.8(4)
C(8)-C(3)	1.401(6)	C(4)-C(3)-C(1)	122.1(4)
C(7)-C(6)	1.381(7)	C(8)-C(3)-C(1)	119.9(4)
C(6)-C(5)	1.388(6)	C(2)-C(1)-C(3)	127.8(5)
C(5)-C(4)	1.388(6)	C(2)-C(1)-Cl(1)	120.7(4)
C(4)-C(3)	1.375(6)	C(3)-C(1)-Cl(1)	111.5(4)
C(3)-C(1)	1.490(6)	C(1)-C(2)-C(9)	120.9(5)
C(1)-C(2)	1.322(6)	C(1)-C(2)-C(15)	123.0(5)
C(2)-C(9)	1.488(7)	C(9)-C(2)-C(15)	115.8(4)
C(2)-C(15)	1.490(7)	C(10)-C(9)-C(14)	117.6(5)
C(9)-C(10)	1.375(7)	C(10)-C(9)-C(2)	120.6(5)
C(9)-C(14)	1.385(7)	C(14)-C(9)-C(2)	121.7(5)
C(10)-C(11)	1.378(8)	C(9)-C(10)-C(11)	122.3(6)
C(11)-C(12)	1.368(8)	C(12)-C(11)-C(10)	118.4(6)
C(12)-C(13)	1.369(8)	C(11)-C(12)-C(13)	121.0(6)
C(13)-C(14)	1.375(7)	C(12)-C(13)-C(14)	119.7(6)
C(15)-C(20)	1.401(7)	C(13)-C(14)-C(9)	120.9(5)
C(15)-C(16)	1.408(7)	C(20)-C(15)-C(16)	118.2(5)
C(16)-C(17)	1.390(7)	C(20)-C(15)-C(2)	118.3(5)
C(16)-C(21)	1.485(8)	C(16)-C(15)-C(2)	123.3(5)
C(17)-C(18)	1.358(8)	C(17)-C(16)-C(15)	118.8(6)
C(18)-C(19)	1.383(8)	C(17)-C(16)-C(21)	117.2(6)
C(19)-C(20)	1.362(7)	C(15)-C(16)-C(21)	123.9(5)
C(21)-C(22)	1.493(8)	C(18)-C(17)-C(16)	121.5(6)
C(22)-C(27)	1.369(7)	C(17)-C(18)-C(19)	120.3(6)
C(22)-C(23)	1.390(7)	C(20)-C(19)-C(18)	119.5(6)
C(23)-C(24)	1.377(8)	C(19)-C(20)-C(15)	121.7(6)
C(24)-C(25)	1.360(9)	O(1)-C(21)-C(16)	119.3(6)
C(25)-C(26)	1.368(8)	O(1)-C(21)-C(22)	120.0(6)
C(26)-C(27)	1.374(7)	C(16)-C(21)-C(22)	120.3(5)
C(7)-C(8)-C(3)	120.9(5)	C(27)-C(22)-C(23)	117.9(6)
C(7)-C(8)-Cl(8)	119.2(4)	C(27)-C(22)-C(21)	122.6(5)
C(3)-C(8)-Cl(8)	119.9(4)	C(23)-C(22)-C(21)	119.2(6)
C(6)-C(7)-C(8)	120.4(4)	C(24)-C(23)-C(22)	120.7(6)
C(6)-C(7)-Cl(7)	119.3(4)	C(25)-C(24)-C(23)	120.6(7)
C(8)-C(7)-Cl(7)	120.3(4)	C(24)-C(25)-C(26)	119.1(7)
C(7)-C(6)-C(5)	119.3(5)	C(25)-C(26)-C(27)	120.9(6)
C(7)-C(6)-Cl(6)	120.6(4)	C(22)-C(27)-C(26)	120.9(6)

Table S19. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for **23**. The anisotropic displacement factor exponent takes the form: $-2p^2 [(ha^*)^2 U_{11} + \dots + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Cl(1)	46(1)	49(1)	64(1)	-7(1)	10(1)	-6(1)
Cl(4)	63(1)	85(1)	33(1)	2(1)	5(1)	22(1)
Cl(5)	50(1)	78(1)	65(1)	6(1)	9(1)	23(1)
Cl(6)	72(1)	76(1)	70(1)	-19(1)	36(1)	5(1)
Cl(7)	88(1)	106(1)	34(1)	-13(1)	12(1)	-4(1)
Cl(8)	60(1)	82(1)	45(1)	9(1)	-7(1)	15(1)
O(1)	58(3)	116(4)	114(4)	11(3)	31(3)	-32(3)
C(1)	38(3)	43(3)	33(3)	-1(2)	3(3)	6(3)
C(2)	35(3)	46(3)	32(3)	-1(2)	2(3)	3(3)
C(3)	39(3)	45(3)	30(3)	2(2)	5(3)	-2(3)
C(4)	39(3)	49(3)	25(3)	-1(3)	3(3)	-3(3)
C(5)	35(3)	46(3)	41(3)	5(3)	8(3)	3(3)
C(6)	45(4)	45(3)	40(3)	-7(3)	16(3)	-7(3)
C(7)	58(4)	48(3)	28(3)	-4(3)	10(3)	-10(3)
C(8)	34(3)	42(3)	38(3)	4(2)	2(3)	-1(3)
C(9)	35(3)	52(4)	41(3)	-8(3)	9(3)	2(3)
C(10)	43(4)	65(4)	85(5)	-11(4)	0(4)	8(3)
C(11)	42(4)	74(5)	122(6)	-29(5)	-8(4)	-3(4)
C(12)	54(5)	57(5)	136(7)	-38(5)	30(5)	-13(4)
C(13)	69(5)	48(4)	95(5)	-13(4)	14(4)	0(4)
C(14)	46(4)	49(4)	55(4)	-10(3)	8(3)	2(3)
C(15)	31(3)	45(4)	49(3)	-11(3)	-4(3)	6(3)
C(16)	30(3)	60(4)	56(4)	-18(3)	7(3)	-3(3)
C(17)	43(4)	91(5)	73(5)	-30(4)	8(3)	9(4)
C(18)	54(4)	86(6)	82(5)	-39(5)	-13(4)	26(4)
C(19)	61(4)	60(4)	77(5)	-7(4)	-16(4)	17(4)
C(20)	50(4)	49(4)	60(4)	-5(3)	-3(3)	9(3)
C(21)	60(5)	61(4)	59(4)	-14(3)	27(4)	-11(4)
C(22)	54(4)	51(4)	45(3)	-4(3)	20(3)	-1(3)
C(23)	90(6)	60(5)	58(4)	3(3)	35(4)	-8(4)
C(24)	111(7)	79(5)	57(5)	19(4)	30(5)	33(5)
C(25)	78(6)	114(6)	39(4)	8(4)	17(4)	30(5)
C(26)	50(4)	86(5)	47(4)	-9(4)	6(3)	5(4)
C(27)	50(4)	56(4)	43(3)	-10(3)	9(3)	3(3)

Table S20. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **23**.

	x	y	z	U(eq)
H(10A)	832(3)	194(6)	4998(5)	80
H(11A)	196(4)	-1579(7)	4539(6)	100
H(12A)	677(4)	-3278(6)	5452(6)	97
H(13A)	1809(4)	-3230(5)	6733(5)	85
H(14A)	2479(3)	-1475(5)	7104(4)	61
H(17A)	563(3)	2361(6)	8362(5)	84
H(18A)	312(4)	3992(7)	7290(6)	94
H(19A)	885(4)	4212(6)	5847(5)	85
H(20A)	1691(3)	2767(5)	5479(5)	66
H(23A)	1945(4)	-1486(6)	9275(5)	80
H(24A)	3141(5)	-2018(7)	10266(5)	97
H(25A)	4147(4)	-694(8)	10530(5)	92
H(26A)	3951(3)	1170(6)	9784(4)	74
H(27A)	2766(3)	1708(5)	8773(4)	60

Table S21. Crystal data and structure refinement for 2,2-Dimethoxy-1,4,5,6,7,8-hexachlorobicyclo[4.2.0]octa-4,7-dien-3-one, **34**.

34	
empirical formula	C ₁₀ H ₆ Cl ₆ O ₃
<i>M_r</i>	386.85
<i>T</i> [K]	300(2)
λ [Å]	0.71073
description	colorless plate
crystal size [mm]	0.04 x 0.20 x 0.24
crystal system	Monoclinic
space group	P2 ₁ /c
<i>a</i> [Å]	16.073(4)
<i>b</i> [Å]	8.186(2)
<i>c</i> [Å]	11.952(3)
α [°]	90.0
β [°]	111.238(10)
γ [°]	90.0
<i>V</i> [Å ³]	1465.8(6)
<i>Z</i>	4
ρ_{calcd} [g cm ⁻³]	1.753
abs. Coeff. [mm ⁻¹]	1.169
<i>F</i> (000)	768
θ range for collection [°]	1.36 to 27.50
limiting indices	-20 < <i>h</i> < 20 -10 < <i>k</i> < 10 -12 < <i>l</i> < 15
reflections collected	12752
independent reflections	3306
<i>R</i> (int)	0.0619
refinement method	Full-matrix least-squares on <i>F</i> ²
weighting scheme	$w = 1 / [\sigma^2 F_o^2 + (0.0295P((F_o^2 + 2F_c^2)/3))^2 + 1.1256((F_o^2 + 2F_c^2)/3)^2]$
data/restraints/parameters	3306 / 0 / 197
goodness-of-fit on <i>F</i> ²	1.049
final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)] ^a	<i>R</i> 1 = 0.0473, <i>wR</i> 2 = 0.0847
<i>R</i> indices (all data) ^a	<i>R</i> 1 = 0.0933, <i>wR</i> 2 = 0.1014
rel. trans. (max., min.)	0.8748, 0.6368
Extinction coeff.	0.0044(7)
Largest diff. peak [eÅ ⁻³]	0.497
Largest diff hole [eÅ ⁻³]	-0.390

$$^a R1 = \sum (|| F_o | - | F_c ||) / \sum | F_o | ; wR2 = [\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{0.5}$$

Table S22. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for **34**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cl(1)	1798(1)	6216(1)	9319(1)	45(1)
Cl(4)	4300(1)	2859(1)	13335(1)	76(1)
Cl(5)	2299(1)	2321(1)	13203(1)	59(1)
Cl(6)	1203(1)	3141(1)	10358(1)	53(1)
Cl(7)	521(1)	5258(1)	12558(1)	61(1)
Cl(8)	957(1)	8959(1)	11115(1)	50(1)
O(1)	4246(2)	5148(3)	11347(3)	62(1)
O(2)	3080(1)	7413(3)	12632(2)	37(1)
O(3)	3370(2)	7892(3)	10883(2)	42(1)
C(1)	2060(2)	6261(4)	10885(3)	28(1)
C(2)	3046(2)	6815(4)	11519(3)	32(1)
C(3)	3643(2)	5281(4)	11703(3)	39(1)
C(4)	3411(2)	3986(4)	12431(3)	42(1)
C(5)	2580(2)	3760(4)	12357(3)	37(1)
C(6)	1817(2)	4632(4)	11445(3)	33(1)
C(7)	1202(2)	5708(4)	11805(3)	34(1)
C(8)	1364(2)	7034(4)	11291(3)	31(1)
C(9)	3955(3)	7842(8)	13459(5)	61(1)
C(10)	2993(4)	9506(5)	10688(5)	64(1)

Table S23. Bond lengths [Å] and angles [deg] for **34**.

Cl(1)-C(1)	1.764(3)	O(2)-C(2)-C(3)	109.9(3)
Cl(4)-C(4)	1.715(3)	O(3)-C(2)-C(1)	116.0(3)
Cl(5)-C(5)	1.716(3)	O(2)-C(2)-C(1)	104.3(2)
Cl(6)-C(6)	1.794(3)	C(3)-C(2)-C(1)	107.6(2)
Cl(7)-C(7)	1.690(3)		
Cl(8)-C(8)	1.690(3)		
O(1)-C(3)	1.197(4)		
O(2)-C(2)	1.400(4)		
O(2)-C(9)	1.440(4)		
O(3)-C(2)	1.383(4)		
O(3)-C(10)	1.437(5)		
C(1)-C(2)	1.555(4)		
C(1)-C(6)	1.603(4)		
C(1)-C(8)	1.511(4)		
C(2)-C(3)	1.547(4)		
C(3)-C(4)	1.501(5)		
C(4)-C(5)	1.319(5)		
C(5)-C(6)	1.495(4)		
C(6)-C(7)	1.499(4)		
C(7)-C(8)	1.319(4)		
C(2)-O(3)-C(10)	117.0(3)		
C(2)-O(2)-C(9)	115.5(3)		
O(1)-C(3)-C(4)	123.0(3)		
O(1)-C(3)-C(2)	124.3(3)		
C(4)-C(3)-C(2)	112.6(3)		
C(5)-C(4)-C(3)	121.2(3)		
C(5)-C(4)-Cl(4)	123.9(3)		
C(3)-C(4)-Cl(4)	114.9(2)		
C(4)-C(5)-C(6)	121.7(3)		
C(4)-C(5)-Cl(5)	122.3(3)		
C(6)-C(5)-Cl(5)	115.8(2)		
C(5)-C(6)-C(7)	121.6(3)		
C(5)-C(6)-C(1)	116.2(2)		
C(7)-C(6)-C(1)	85.3(2)		
C(5)-C(6)-Cl(6)	107.1(2)		
C(7)-C(6)-Cl(6)	111.1(2)		
C(1)-C(6)-Cl(6)	114.6(2)		
C(8)-C(7)-C(6)	95.0(2)		
C(8)-C(7)-Cl(7)	134.6(3)		
C(6)-C(7)-Cl(7)	130.3(2)		
C(7)-C(8)-C(1)	95.7(3)		
C(7)-C(8)-Cl(8)	133.9(3)		
C(1)-C(8)-Cl(8)	130.4(2)		
C(8)-C(1)-C(2)	117.6(2)		
C(8)-C(1)-C(6)	83.8(2)		
C(2)-C(1)-C(6)	113.5(2)		
C(8)-C(1)-Cl(1)	115.4(2)		
C(2)-C(1)-Cl(1)	109.4(2)		
C(6)-C(1)-Cl(1)	115.2(2)		
O(3)-C(2)-O(2)	114.0(2)		
O(3)-C(2)-C(3)	104.9(2)		

Table S24. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for **34**. The anisotropic displacement factor exponent takes the form: $-2p^2 [(\text{ha}^*)^2 U_{11} + \dots + 2\text{hka}^*\text{b}^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Cl(4)	54(1)	69(1)	90(1)	31(1)	8(1)	24(1)
Cl(5)	72(1)	46(1)	56(1)	19(1)	22(1)	-10(1)
Cl(6)	61(1)	39(1)	49(1)	-9(1)	10(1)	-15(1)
Cl(7)	49(1)	78(1)	68(1)	1(1)	37(1)	-12(1)
Cl(8)	52(1)	38(1)	65(1)	-1(1)	25(1)	13(1)
Cl(1)	60(1)	44(1)	29(1)	1(1)	14(1)	1(1)
O(1)	48(2)	62(2)	91(2)	7(2)	42(2)	12(1)
O(3)	46(1)	39(1)	49(2)	6(1)	29(1)	-5(1)
O(2)	34(1)	43(1)	35(1)	-8(1)	14(1)	-9(1)
C(3)	29(2)	42(2)	45(2)	1(2)	13(2)	1(2)
C(4)	41(2)	35(2)	46(2)	6(2)	13(2)	7(2)
C(5)	45(2)	28(2)	35(2)	4(1)	12(2)	-3(2)
C(6)	37(2)	28(2)	31(2)	-2(1)	10(2)	-7(1)
C(7)	25(2)	41(2)	37(2)	-5(2)	13(2)	-6(1)
C(8)	28(2)	31(2)	33(2)	-4(1)	10(1)	0(1)
C(1)	33(2)	27(2)	26(2)	0(1)	12(1)	0(1)
C(2)	34(2)	31(2)	35(2)	-1(1)	19(2)	-2(1)
C(9)	43(2)	86(4)	49(3)	-21(3)	12(2)	-24(3)
C(10)	82(4)	37(2)	83(4)	16(2)	41(3)	-1(2)

Table S25. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **34**.

	x	y	z	U(eq)
H(9A)	3915(29)	8380(58)	14115(43)	85(16)
H(9B)	4293(38)	6885(72)	13763(49)	119(23)
H(9C)	4236(32)	8449(59)	13102(41)	87(17)
H(10A)	2918(30)	9957(58)	11416(42)	90(17)
H(10B)	2416(34)	9494(59)	10108(43)	94(18)
H(10C)	3393(30)	10186(60)	10492(39)	87(15)

Table S26. Summary of Crystal Data and Structure Refinement.

	7	8	17	23	34
empirical formula	C ₉ H ₆ Cl ₄ O ₄	C ₁₁ H ₆ Cl ₃ O ₆	C ₉ H ₄ Cl ₆ O ₂	C ₂₇ H ₁₄ Cl ₆ O	C ₁₀ H ₆ Cl ₆ O ₃
<i>M_r</i>	319.94	343.53	356.82	567.08	386.85
<i>T</i> [K]	300(2)	299(2)	300(2)	300(2)	300(2)
λ [Å]	0.71073	0.71073	0.71073	0.71073	0.71073
description	colorless plate	colorless plate	colorless plate	light yellow plate	colorless plate
crystal size [mm]	0.06 x 0.28 x 0.30	0.10 x 0.18 x 0.30	0.06 x 0.18 x 0.37	0.02 x 0.12 x 0.22	0.04 x 0.20 x 0.24
crystal system	Monoclinic	Triclinic	Orthorhombic	Monoclinic	Monoclinic
space group	P2 ₁ /c	P $\bar{1}$	P2 ₁ 2 ₁ 2 ₁	P2 ₁ /c	P2 ₁ /c
<i>a</i> [Å]	8.9176(3)	8.4138(4)	7.7583(1)	17.7762(1)	11.952(3)
<i>b</i> [Å]	19.8980(9)	12.0117(5)	9.2561(1)	11.2519(3)	16.073(4)
<i>c</i> [Å]	8.0463(4)	14.2489(5)	18.3732(2)	12.7982(3)	8.186(2)
α [°]	90.0	102.368(2)	90.0	90.0	90.0
β [°]	115.837(2)	93.306(2)	90.0	102.965(1)	111.238(10)
γ [°]	90.0	90.050(2)	90.0	90.0	90.0
<i>V</i> [Å ³], <i>Z</i>	1285.03(10), 4	1404.16(10), 4	1319.41(3), 4	2494.59(9), 4	1465.8(6), 4
ρ_{calc} [g cm ⁻³]	1.654	1.625	1.796	1.510	1.753
abs. coeff. [mm ⁻¹]	0.918	0.673	1.285	0.709	1.169
θ range/index ranges [°]	2.05 to 27.51	2.42 to 27.53	2.22 to 27.66	1.18 to 22.50	1.36 to 27.50
limiting indices	-11 < <i>h</i> < 11 -25 < <i>k</i> < 25 10 < <i>l</i> < 10	-8 < <i>h</i> < 10 -15 < <i>k</i> < 13 -11 < <i>l</i> < 18	-10 < <i>h</i> < 10 -12 < <i>k</i> < 10 -23 < <i>l</i> < 24	-19 < <i>h</i> < 19 -12 < <i>k</i> < 12 -14 < <i>l</i> < 13	-20 < <i>h</i> < 20 -10 < <i>k</i> < 10 -12 < <i>l</i> < 15
reflections collected	11297	10349	11778	13848	12752
independent reflections	2870	6326	3059	3241	3306
<i>R</i> (int)	0.0932	0.0240	0.0310	0.0986	0.0619
goodness-of-fit on <i>F</i> ²	1.043	1.046	1.065	1.033	1.049
final <i>R</i> indices [<i>I</i> > 2 σ (<i>I</i>)] ^a	<i>R</i> 1 = 0.0647 <i>wR</i> 2 = 0.1108	<i>R</i> 1 = 0.0393 <i>wR</i> 2 = 0.1631	<i>R</i> 1 = 0.0340 <i>wR</i> 2 = 0.0714	<i>R</i> 1 = 0.0547 <i>wR</i> 2 = 0.0922	<i>R</i> 1 = 0.0473 <i>wR</i> 2 = 0.0847
<i>R</i> indices (all data) ^a	<i>R</i> 1 = 0.1550 <i>wR</i> 2 = 0.1457	<i>R</i> 1 = 0.0914 <i>wR</i> 2 = 0.1780	<i>R</i> 1 = 0.0452 <i>wR</i> 2 = 0.0770	<i>R</i> 1 = 0.1068 <i>wR</i> 2 = 0.1116	<i>R</i> 1 = 0.0933 <i>wR</i> 2 = 0.1014
rel. trans. (max., min.)	0.8646, 0.6680	0.8971, 0.7340	0.8372, 0.6210	0.9423, 0.6368	0.8748, 0.6368

$$^a R1 = \Sigma (|F_o| - |F_c|) / \Sigma |F_o|; wR2 = [\Sigma (w(F_o^2 - F_c^2)^2) / \Sigma (w(F_o^2)^2)]^{0.5}$$