

Electronic Supplementary information for the paper

**Low melting molecular complexes. Part 2. The structures of molecular complexes of tri- and di-chloromethanes with small ketones and 1,4-dioxane<sup>i</sup>**

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Table S1 Bond Lengths for **1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C11	C1S	1.7604(16)	C1	C4	1.511(2)
C12	C1S	1.7615(15)	C1	C2	1.511(2)
C13	C1S	1.7531(16)	C3	C4	1.528(3)
C1	O1	1.196(2)	C3	C2	1.538(3)

Table S2 Bond Angles for **1**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	C1	C4	133.77(16)	C11	C1S	C12	110.40(8)
O1	C1	C2	133.83(15)	C4	C3	C2	90.62(14)
C4	C1	C2	92.34(14)	C1	C4	C3	88.43(14)
C13	C1S	C11	111.25(9)	C1	C2	C3	88.03(13)
C13	C1S	C12	110.29(9)				

Table S3 Bond Lengths for **2**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C11	C1S	1.752(3)	C1	C4	1.5156(18)
C12	C1S	1.756(2)	C2	C3	1.5471(19)
O1	C1	1.2036(16)	C3	C4	1.535(2)
C1	C2	1.505(2)			

Table S4 Bond Angles for **2**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C11	C1S	C12	111.66(13)	C1	C4	C3	87.92(11)
O1	C1	C2	133.66(12)	C2	C1	C4	92.70(11)
O1	C1	C4	133.49(14)	C4	C3	C2	90.32(11)
C1	C2	C3	87.86(11)				

Table S5 Bond Lengths for **3**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.2160(17)	C4	C5	1.519(2)
C1	C6	1.497(2)	C5	C6	1.529(2)
C1	C2	1.497(2)	C11	C1S	1.759(2)
C2	C3	1.527(2)	C12	C1S	1.7624(18)
C3	C4	1.506(3)			

Table S6 Bond Angles for **3**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	C1	C6	122.67(15)	C3	C4	C5	111.37(14)
O1	C1	C2	121.93(17)	C4	C5	C6	111.39(13)
C6	C1	C2	115.39(14)	C1	C6	C5	111.69(14)
C1	C2	C3	112.05(14)	C11	C1S	C12	111.08(10)
C4	C3	C2	111.75(17)				

Table S7 Bond Lengths for **4**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C11	C1S	1.764(7)	C1	C2	1.57(2)
C12	C1S	1.739(6)	C1	C3	1.510(18)
C13	C1S	1.752(7)	C3	C4	1.616(19)
C14	C2S	1.752(7)	O1A	C1A	1.233(14)
C15	C2S	1.749(7)	C1A	C2A	1.44(2)

Cl6	C2S	1.776(7)	C1A	C3A	1.430(19)
O1	C1	1.194(14)	C3A	C4A	1.42(3)

Table S8 Bond Angles for 4.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl2	C1S	C11	110.6(3)	O1	C1	C3	123.2(12)
Cl2	C1S	C13	112.1(4)	C1	C3	C4	112.0(10)
Cl3	C1S	C11	110.4(3)	C3	C1	C2	116.9(11)
Cl4	C2S	Cl6	109.7(4)	O1A	C1A	C2A	124.5(13)
Cl5	C2S	Cl4	111.1(4)	O1A	C1A	C3A	123.1(13)
Cl5	C2S	Cl6	109.8(4)	C1A	C3A	C4A	115.5(15)
O1	C1	C2	119.4(13)	C3A	C1A	C2A	112.5(13)

Table S9 Bond Lengths for 5.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C1S	1.7595(17)	C1	C2	1.494(3)
Cl2	C1S	1.7629(18)	C2	C3	1.485(2)
O1	C2	1.2127(18)	C3	C4	1.502(3)

Table S10 Bond Angles for 5.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl1	C1S	Cl2	110.71(10)	C2	C3	C4	114.91(16)
O1	C2	C1	122.01(16)	C3	C2	C1	116.44(16)
O1	C2	C3	121.54(17)				

Table S11 Bond Lengths for 6.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C1S	1.7629(11)	O1	C1	1.2148(15)
Cl2	C1S	1.7619(12)	C1	C2	1.491(2)
Cl3	C1S	1.7591(12)	C1	C3	1.501(2)

Table S12 Bond Angles for 6.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C12	C1S	C11	110.18(6)	O1	C1	C2	121.92(14)
C13	C1S	C11	110.52(7)	O1	C1	C3	120.80(15)
C13	C1S	C12	110.17(6)	C2	C1	C3	117.28(13)

Table S13 Bond Lengths for **7**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C11	C1S	1.765(2)	C1	C2	1.489(3)
C12	C1S	1.758(2)	C1	C3	1.488(2)
O1	C1	1.207(2)			

Table S14 Bond Angles for **7**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C12	C1S	C11	111.22(10)	O1	C1	C3	121.89(17)
O1	C1	C2	120.85(17)	C3	C1	C2	117.26(19)

Table S15 Bond Lengths for **8**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C11	C1S	1.751(2)	O1	C2	1.429(2)
C12	C1S	1.757(2)	C1	C2	1.498(3)
C13	C1S	1.758(2)	C2	C1	1.498(3)
O1	C1	1.429(3)			

<sup>1</sup>-X,1-Y,1-Z

Table S16 Bond Angles for **8**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	O1	C2	109.31(15)	C12	C1S	C13	110.32(13)
C11	C1S	C12	111.19(10)	O1	C1	C2	110.81(16)
C11	C1S	C13	110.66(11)	O1	C2	C1	110.65(18)

<sup>1</sup>-X,1-Y,1-Z

Table S17 Bond Lengths for **9**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C2	1.424(2)	C2	C1	1.492(3)
O1	C1	1.426(2)	C11	C1S	1.763(2)
C1	C2 <sup>1</sup>	1.492(3)	C12	C1S	1.750(2)

<sup>1</sup>-X,1-Y,-Z

Table S18 Bond Angles for **9**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	O1	C1	109.75(14)	O1	C2	C1	110.40(16)
O1	C1	C2 <sup>1</sup>	110.73(15)	C12	C1S	C11	111.32(11)

<sup>1</sup>-X,1-Y,-Z

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<sup>i</sup> Part 1 see D.S.Yufit and J.A.K.Howard, CrystEngComm, 2010, **12**, 737-741