Electronic Supplementary Material (ESI) for Chemical Communications

SUPPORTING INFORMATION

Reduction of 2,2,2-Trichloro-1-Aryl-Ethanones by RMgX: Mechanistic Investigations and the Synthesis of Substituted α,α-Dichloro-Ketones

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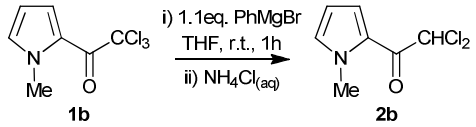
Solvent and concentration effects, Table S1

Table S1 Solvent and Concentration Effects



1b **2b**

Entry	Solvent	Total Rxn. Volume/mL[b]	Isolated % Yield (**2b**)	% Conversion[a]
1	THF	1.55	94	>95
2	THF	3.10	-	>95
3	THF	5.55	-	>95
4	THF	20.55	-	67%
5	Et_2O	1.55	95	>95
6	Hexane	1.55	94	>95

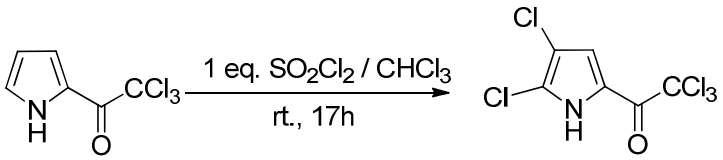
[a] Conversion estimated by ^{1}H NMR of crude reaction mixture. [b] All reactions contain ~0.55 mL of THF from the solution of PhMgBr used.

Experimental information

^{1}H and ^{13}C NMR spectra were recorded directly with a Jeol Lambda 500 MHz, Jeol ECS-400 MHz or Bruker Avance 300 MHz. EPR spectra were collected with a Bruker MicroEMX EPR spectrometer working at X-band (9.4 GHz) microwave frequency. HRMS data were provided by the EPSRC National Mass Spectrometry Service (University of Swansea). X-ray diffraction data was obtained on an Oxford Diffraction Gemini. IR spectra were obtained as neat samples using a Varian 800 FT-IR Scimitar Series spectrometer scanning from 4000-600 cm^{-1}.THF and Et_2O were distilled from sodium/benzophenone and used directly. Compounds **1a** and **1b** were obtained commercially and used as supplied.

Experimental procedures:

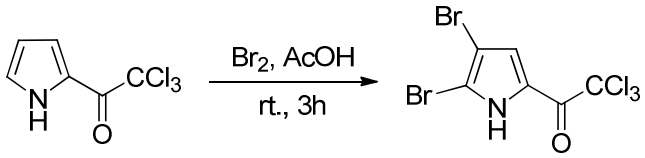
2,2,2-Trichloro-1-(4,5-dichloro-1*H*-pyrrol-2-yl)ethanone (1c)



To a solution of 2-(trichloroacetyl) pyrrole (0.85 g, 4 mmol) in chloroform (10 mL) at room temperature was added sulfuryl chloride (1.08 g, 8 mmol). The mixture was stirred for 17 hours in the dark. The reaction was quenched by the addition of 2M sodium bicarbonate solution (15 mL) and extracted with dichloromethane (3 × 15 mL). The combined organic layers were collected, dried over magnesium sulphate ($MgSO_4$), filtered and concentrated under reduced pressure to give the crude product as a yellow solid. The crude material was purified by column chromatography (SiO_2) (petrol / ethyl acetate, 9:1) to give 2,2,2-trichloro-1-(4,5-dichloro-1*H*-pyrrol-2-yl)ethanone (**1c**) as a white crystalline solid (0.964 g, 86% yield).

Mp: 128-130˚C (lit: 129-131˚C)[1]; R_f = 0.45 (petrol / ethyl acetate, 9:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H 9.58 (br s, 1H), 7.32 (d, J = 3.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ_C 173.3, 124.6, 122.6, 119.9, 116.0, 94.8; IR(neat): υ_{max}/cm^{-1} 3267, 3140, 1652; Anal. Calcd for $C_6H_2Cl_5NO$: C, 25.61; H, 0.72; N, 4.98. Found: C, 25.72; H, 0.73; N, 4.93; HRMS(APCI): calcd for $C_6H_2Cl_5NO$ $[M+H]^+$: 281.8622; observed: 281.8627.

2,2,2-Trichloro-1-(4,5-dibromo-1*H*-pyrrol-2-yl)ethanone (1d)

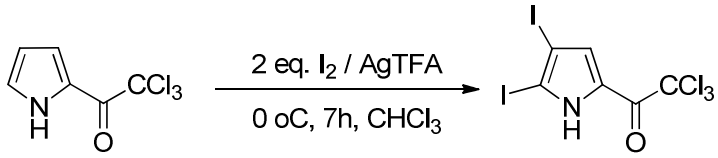


To a stirred solution of 2-(trichloroacetyl)pyrrole (1.06 g, 5 mmol) in AcOH (2.5 mL), was added Br_2 (1.60 g, 10 mmol) in AcOH (22.5 mL) dropwise over 15 minutes (slight temp increase). The solution turned brown/dark brown and was left for 2 hours with stirring. The solvent was removed under reduced pressure by azeotropic distillation with toluene (3 x 50 mL), the reaction mixture was quenched with $K_2CO_{3\ (aq)}$ (60 mL) and then extracted with ether (2 x 30 mL). The combined organics were washed with saturated NaCl solution (30 mL), dried over Na_2SO_4 and filtered. The solvent was removed under reduced pressure to obtain the crude product as brown oil. The crude material was purified by dissolving in the minimum amount of hot toluene (30 mL) followed by a hot filtration, and the solution was

then allowed to cool to give needle like crystals that were collected by filtration and washed with pentane to give 2,2,2-trichloro-1-(4,5-dibromo-1*H*-pyrrol-2-yl)ethanone (**1d**) as light brown crystals (0.93 g, 50 %).

Mp: 136-139 ˚C (lit. 136-138˚C)[1]; R_f = 0.53 (Toluene); ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 9.90 (1H, s), 7.37 (d, *J* = 2.9 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.8, 124.0, 122.8, 112.5, 102.4, 93.9, 77.3, 77.1, 76.9, 76.5; IR(neat): υ_{max}/cm^{-1} 3278, 1653; MS (ESI): m/z 366 (68%), 368 (97), 370 (100), 372 (82), 374 (33, $[M-H]^-$).

2,2,2-Trichloro-1-(4,5-diiodo-1*H*-pyrrol-2-yl)ethanone (1e)



To a mixture of 2-(trichloroacetyl) pyrrole (0.85 g, 4 mmol) and silver trifluoroacetate (1.77 g, 8 mmol) in chloroform (10 mL) at 0˚C (ice-bath) under a nitrogen atmosphere, was added iodine (2.03 g, 8 mmol) in chloroform (10 mL) dropwise over 10 minutes. The reaction was warmed to room temperature and stirred for 7 h, in the dark, before the addition of aqueous sodium sulphite (15 mL) and brine (15 mL). The reaction mixture was extracted with ethyl acetate (3 × 15 mL), and the combined organic extracts were dried over magnesium sulphate ($MgSO_4$). The crude material was purified by silica gel column chromatography (petrol / ethyl acetate, 9:1) to give 2,2,2-trichloro-1-(4,5-diiodo-1*H*-pyrrol-2-yl)ethanone (**1e**) a yellow crystalline solid (1.48 g, 80% yield).

Mp: 176-178 ˚C (lit. 176-177˚C)[1]; Rf = 0.32 (petrol / ethyl acetate, 9:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 9.60 (s, 1H), 7.37 (d, *J* = 2.8 Hz); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 171.4, 129.1, 128.0, 93.7, 90.2, 79.0; IR(neat): υ_{max}/cm^{-1} 3286, 3129, 1649; Anal. Calcd for $C_6H_2Cl_3I_2NO$: C, 15.52; H, 0.43; N, 3.02. Found: C, 15.63; H, 0.49; N, 3.00; HRMS (APCI) calcd for $C_6H_2Cl_3I_2NO$ $[M+H]^+$: 463.7364; observed: 463.7368.

2,2,2-Trichloro-1-(*p*-tolyl)ethanone (1f)

To a round bottom flask was added sequentially $AlCl_3$ (8.82 g, 66 mmol) and DCM (30 mL). The reaction mixture was cooled to 0 ^{o}C, toluene (6.4 mL, 60 mmol) and then 2,2,2-trichloroacetylchloride (7.4 mL, 66 mmol) were added. The solution was stirred for 1 hour

under nitrogen atmosphere. The reaction was quenched with 30 mL of saturated $Na_2CO_{3(aq)}$, washed with 30 mL of brine then dried over $MgSO_4$. The solvent was removed under reduce pressure to give an oil. The crude product was purified by reduced pressure distillation (0.02 torr, b.p. = 115-116 ^oC) to give 2,2,2-trichloro-1-(*p*-tolyl)ethanone (**1f**) as a yellow oil (9.23 g, 65%).

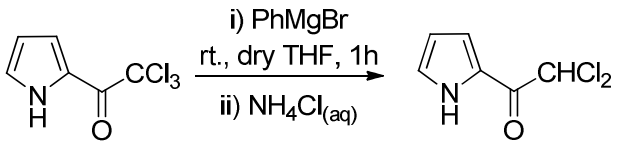
R_f : 0.46 (UV active, petrol 40/60 : ether = 90: 1); ^1H NMR (300 MHz, $CDCl_3$): δ_H 8.19 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 180.6, 145.6, 131.8, 129.3, 126.2, 95.9, 21.5; IR(neat): ν_{max}/cm^{-1} 1705, 1605, 842, 745, 657; HRMS (APCI): calcd for $C_9H_8OCl_3$ $[M+H]^+$: 236.9641, found 236.9637.

1-(4-(*tert*-Butyl)phenyl)-2,2,2-trichloroethanone (1g)

To a round bottom flask was added sequentially DCM (10 mL), *t*-butyl benzene (7.74 mL, 50 mmol) and $AlCl_3$ (6.68 g, 50.1 mmol). The reaction was cooled to -30 ^oC, and a solution of 2,2,2-trichloroacetylchloride (5.58 mL, 50.1 mmol) in DCM (10 mL) was added over 30 minutes. The solution was stirred for 4 days at -30 ^oC and was then quenched with ice (50 g) and diluted with DCM (50 mL). The organic layer was washed with 2M $NaOH_{(aq)}$ (5 x 50 mL), brine (5 x 50 mL) and dried over $MgSO_4$. The solvent was removed under reduce pressure to give an oil residue. The crude product was purified by distillation under reduced pressure (0.02 torr, b.p. = 76-77 ^oC) to give 1-(4-(*tert*-butyl)phenyl)-2,2,2-trichloroethanone (**1g**) as a colourless oil (4.00 g, 45%).

R_f : 0.32 (UV active, petrol 40/60 : ether = 7: 3); ^1H NMR (300 MHz, $CDCl_3$): δ_H 8.24 (d, *J* = 8.7 Hz, 2H), 7.53 (d, *J* = 8.7 Hz, 2H), 1.38 (s, 9H), ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 180.7, 158.5, 131.8, 126.2, 125.6, 95.8, 35.4, 31.1; IR(neat): ν_{max}/cm^{-1} 2971, 1710, 1603, 1231, 854, 784, 700; HRMS (APCI): calcd for $C_{12}H_{13}OCl_3$ $[M+H]^+$: 279.0110, found 279.0104.

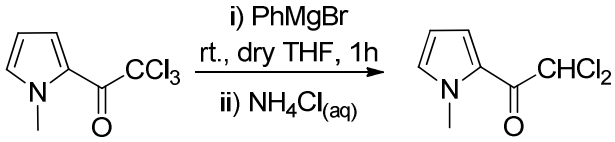
2,2-Dichloro-1-(1*H*-pyrrol-2-yl)ethanone (2a)



Under an atmosphere of nitrogen, PhMgBr (2M, 1.1 mL, 2.2 mmol) was added to a 25 mL round bottomed flask. 2,2,2-Trichloroacetyl pyrrole (**1a**) (0.212 g, 1.0 mmol) was dissolved in dry THF (1 mL), added dropwise over 10 minutes to the PhMgBr solution and then allowed to stir for an hour at room temperature. The mixture was quenched by the addition of saturated $NH_4Cl_{(aq)}$ (20 mL), and the product was extracted using ethyl acetate (3 x 15 mL). The combined organic extracts were dried over magnesium sulphate $MgSO_4$, filtered and the solvent removed under reduced pressure to give the crude product as a yellow oil. The crude product was purified by column chromatography (SiO_2) (petrol / diethyl ether, 7:3), to give 2,2-dichloro-1-(1*H*-pyrrol-2-yl)ethanone (**2a**) as white solid (0.160 g, 90% yield).

Mp: 87-89 ˚C (lit: 89-90˚C)[1]; Rf = 0.34 (petrol / diethyl ether, 7:3); ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.41 (s, 1H), 7.14-7.09 (m, 2H), 6.41 (s, 1H), 6.32 (app. dt, *J* = 4.0, 2.5 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 177.0, 127.8, 126.1, 119.1, 111.9, 67.3; IR(neat): υ_{max}/cm^{-1} 3287, 3138, 1667; Anal. Calcd for $C_6H_5Cl_2NO$: C, 40.48; H, 2.83; N, 7.87;. Found: C, 40.57; H, 2.81; N, 7.84; HRMS (APCI) calcd for $C_6H_5Cl_2NO$ $[M+H]^+$: 177.9821; observed: 177.9821.

2,2-Dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)ethanone (2b)

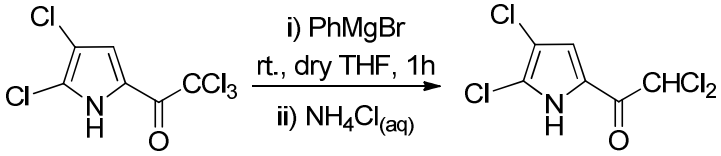


Under an atmosphere of nitrogen, PhMgBr (2M, 0.55 mL, 1.1 mmol) was added to a 25 mL round bottomed flask. 2,2,2-Trichloro-1-(1-methyl-*1H*-pyrrol-2-yl)ethanone (**1b**) (0.226 g, 1.0 mmol) was dissolved in dry THF (1 mL), added to the dropwise over 10 minutes to the PhMgBr solution and allowed to stir for an hour at room temperature. The mixture was quenched by the addition of saturated $NH_4Cl_{(aq)}$ (20 mL) and the product was extracted using ethyl acetate (3 x 15 mL). The combined organic extracts were dried over magnesium sulphate $MgSO_4$, filtered and the solvent removed under reduced pressure to give the crude product as a yellow oil. The crude product was purified by column chromatography (SiO_2) (petrol / diethyl ether, 9:1) to give 2,2-dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)ethanone (**2b**) as a white crystalline solid (0.181 g, 94% yield).

Mp: 67-68˚C (lit. 65-66 ˚C);[2] R_f = 0.37 (petrol / diethyl ether, 9:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.05 (dd, *J* = 4.4, 1.6 Hz, 1H), 6.90 (br s, 1H), 6.54 (s, 1H), 6.12 (dd, *J* = 4.4, 2.5 Hz, 1H), 3.87 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 176.6, 134.2, 125.2, 121.4, 109.4, 68.1, 38.0; IR(neat): υ_{max}/cm^{-1} 3117, 3022, 1656; HRMS (NSI) calcd for $C_7H_7Cl_2NO$

$[M+H]^+$: 191.9977, observed: 191.9978; Anal: Calcd for $C_7H_7Cl_2NO$: C, 43.78; H 3.67; N, 7.29, Found; C, 43.82; H, 3.75; N, 7.23.

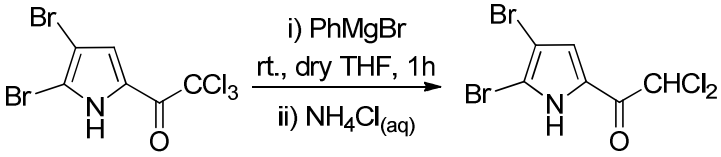
2,2-Dichloro-1-(4,5-dichloro-1*H*-pyrrol-2-yl)ethanone (2c)



Under nitrogen, PhMgBr (2M, 1.1 mL, 2.2 mmol) was added to a 25 mL round bottomed flask. 2,2,2-Trichloro-1-(4,5-dichloro-*1H*-pyrrol-2-yl)ethanone (**1c**) (0.282 g, 1.0 mmol) was dissolved in dry THF (1 mL) and added to the PhMgBr solution dropwise over 10 minutes and allowed to stir for an hour at room temperature. The mixture was quenched by adding to NH_4Cl (20 mL), and the product was extracted using ethyl acetate (3 x 15 mL). The combined organic extracts were dried over magnesium sulphate $MgSO_4$, filtered and the solvent removed under reduced pressure to give yellow orange crystals. The crude product was purified by column chromatography (SiO_2) (petrol / diethyl ether, 7:3) to give 2,2-dichloro-1-(4,5-dichloro-1*H*-pyrrol-2-yl)ethanone (**2c**) as a pink crystalline solid (0.172 g, 70% yield).

Mp. 104-106˚C (lit. 104-107˚C)[1]; R_f = 0.5 (petrol / diethyl ether, 7:3); ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 10.07 (s, 1H), 7.10 (d, J = 3.0 Hz, 1H), 6.28 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 176.4, 124.2, 123.0, 118.7, 113.2, 66.8; IR(neat): υ_{max}/cm^{-1} 3247, 3123, 1650; Anal. Calcd for $C_6H_3Cl_4NO$: C, 29.19; H, 1.22; N, 5.67. Found: C, 29.31; H, 1.23; N, 5.58; HRMS (APCI) calcd for $C_6H_3Cl_4NO$ $[M+H]^+$: 247.9012; observed: 247.9014.

2,2-Dichloro-1-(4,5-dibromo-1*H*-pyrrol-2-yl)ethanone (2d)

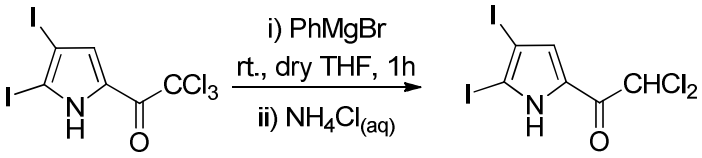


Under nitrogen, PhMgBr (2M, 0.55 mL, 1.1 mmol) was added to a 25 mL round bottomed flask. 2,2,2-Trichloro-1-(4,5-dibromo-*1H*-pyrrol-2-yl)ethanone (**1d**) (0.185 g, 0.5 mmol) was dissolved in dry THF (1 mL), added to the PhMgBr solution dropwise over 10 minutes and allowed to stir for an hour at room temperature. The mixture was quenched by adding to NH_4Cl (20 mL), and the product was extracted using ethyl acetate (3 x 15 mL). The combined organic extracts were dried over magnesium sulphate $MgSO_4$, filtered and the

solvent removed under reduced pressure to give yellow-orange crystals. The crude product was purified by column chromatography (SiO_2) (petrol / diethyl ether, 9:1) to give 2,2-dichloro-1-(4,5-dibromo-1*H*-pyrrol-2-yl)ethanone (**2d**) as a pink crystalline solid (0.175 g, 95% yield).

Mp. 127-128˚C (lit. 127-129 ˚C)[1]; R_f = 0.25 (petrol / diethyl ether, 9:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 9.86 (s, 1H), 7.22 (d, J = 2.9 Hz, 1H), 6.35 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 176.0, 126.6, 121.2, 113.4, 102.3, 66.8; IR(neat): υ_{max}/cm^{-1} 3252, 2989, 1646; HRMS (APCI) calcd for $C_6H_3Br_2Cl_2NO$ $[M+H]^+$: 335.8009; observed: 335.8014.

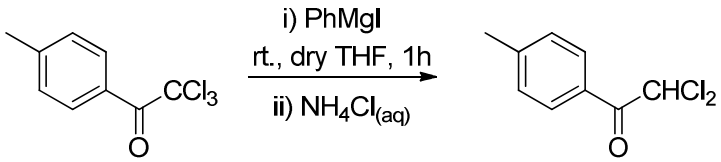
2,2-Dichloro-1-(4,5-diiodo-1*H*-pyrrol-2-yl)ethanone (2e)



Under nitrogen, PhMgBr (2M, 0.275 mL, 0.55 mmol) was added to a 25 mL round bottomed flask. 2,2,2-Trichloro-1-(4,5-diiodo-*1H*-pyrrol-2-yl)ethanone (**1e**) (0.116 g, 0.25 mmol) was dissolved in dry THF (1 mL) and added to the PhMgBr solution dropwise over 10 minutes and allowed to stir for an hour at room temperature. The reaction was quenched by adding saturated $NH_4Cl_{(aq)}$ (20 mL), and the product was extracted using ethyl acetate (3 x 15 mL). The combined organic extracts were dried over magnesium sulphate $MgSO_4$, filtered and the solvent removed under reduced pressure to give yellow-orange crystals. The crude product was purified by column chromatography (SiO_2) (petrol / diethyl ether, 9:1) to give 2,2-dichloro-1-(4,5-diiodo-1*H*-pyrrol-2-yl)ethanone (**2e**) as a yellow crystalline solid (0.108 g, 93% yield).

Mp. 138-140 ˚C; R_f = 0.19 (petrol / diethyl ether, 9:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 9.61 (s, 1H), 7.23 (d, J = 2.7 Hz, 1H), 6.33 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 175.3, 131.8, 126.1, 90.3, 78.7, 66.6; IR(neat): υ_{max}/cm^{-1} 3260, 2942, 1629; HRMS (APCI) calcd for $C_6H_3Cl_2I_2NO$ $[M+H]^+$: 429.7754, observed: 429.7745; Anal. Calcd for $C_6H_3Cl_2I_2NO$: C, 16.77; H 0.70; N, 3.26. Found: C, 16.84; H, 0.60; N, 3.19.

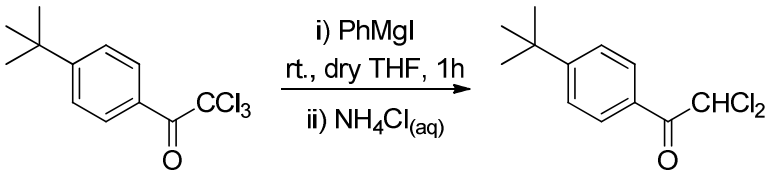
2,2-Dichloro-1-(*p*-tolyl)ethanone (2f)



Under nitrogen, PhMgI (0.38M, 2.9 mL, 1.1 mmol) was added to a 25 mL round bottomed flask. 2,2,2-Trichloro-1-(*p*-tolyl) ethanone (0.237 g, 1.0 mmol) was dissolved in dry THF (1 mL) and then added to the PhMgI solution dropwise over 10 minutes and allowed to stir for a further one hour. The mixture was quenched by adding to saturated $NH_4Cl_{(aq)}$ (20 mL), and the product was extracted using ethyl acetate (3 x 15 mL). The combined organic extracts were dried over $MgSO_4$, filtered and the solvent removed under reduced pressure. The crude product was purified by column chromatography (SiO_2) (petrol / diethyl ether 9.9:0.1) to give 2,2-Dichloro-1-(*p*-tolyl)ethanone (**2f**) as a white crystaline solid (0.195 g, 96% yield).

Mp: 58-59˚C; R_f = 0.38 (petrol / diethyl ether, 9.5:0.5); ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.89 (d, *J* = 8.1 Hz, 1H), 7.22 (d, *J* = 8.1 Hz, 2H), 6.61 (s, 1H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 185.7, 146.0, 129.9, 129.7, 128.8, 67.9, 21.9; IR(neat): υ_{max}/cm^{-1} 3017, 1689; HRMS (APCI) calcd for $C_9H_8Cl_2O$ $[M+H]^+$: 203.0025; observed: 203.0027.

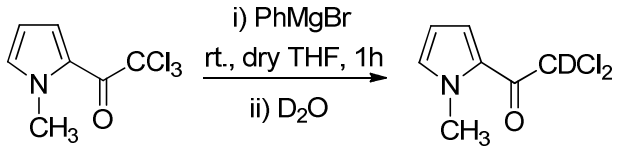
1-(4(*t*-Butyl)phenyl)-2,2-dichloroethanone (2g)



Under nitrogen, PhMgI (0.38M, 2.9 mL, 1.1 mmol) was added to a 25 mL round bottomed flask. 1-(4-(*tert*-Butyl)phenyl)-2,2,2-trichloroethanone (0.279 g, 1.0 mmol) was dissolved in dry THF (1 mL) and then added to the PhMgI solution dropwise over 10 minutes and allowed to stir for a further one hour. The mixture was quenched by adding to saturated $NH_4Cl_{(aq)}$ (20 mL), and the product was extracted using ethyl acetate (3 x 15 mL). The combined organic extracts were dried over $MgSO_4$, filtered and the solvent removed under reduced pressure. The crude was purified by column chromatography (SiO_2) (petrol / diethyl ether 9.9:0.1) to give 1-(4(*t*-butyl)phenyl)-2,2-dichloroethanone (**2g**) as a white crystaline solid (0.239 g, 98% yield).

Mp: 63-64˚C; R_f : 0.43 (UV active, petrol 40/60 : ether = 50: 1); ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 8.05 (d, *J* = 8.5 Hz, 2H), 7.55 (d, *J* = 8.5 Hz, 2H), 6.70 (s, 1H), 1.37 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$): δ_C 185.5, 158.6, 129.7, 128.8, 125.8, 67.8, 35.3, 30.9; IR(neat): ν_{max}/cm^{-1} 2964.6, 2869.9, 1703.6, 852.9, 701.3; HRMS (APCI): calcd. for $C_{12}H_{14}OCl_2$ $[M+H]^+$ 245.0500, found 245.0493.

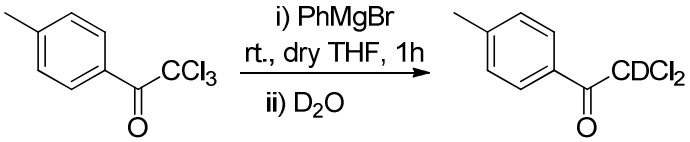
2,2-Dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)ethanone ((2-*d*)-2b)



PhMgBr (2M, 0.55 mL, 1.1 mmol) was added to a 25 mL round bottomed flask under an atmosphere of nitrogen. The 2,2,2-trichloro-1-(1-methyl-*1H*-pyrrol-2-yl) ethanone (0.226 g, 1.0 mmol) was dissolved in dry THF (1 mL), added to the PhMgBr solution dropwise over 10 minutes and allowed to stir for an hour. The mixture was quenched by adding D_2O (0.18 mL, 10 mmol) and then saturated $NH_4Cl_{(aq)}$ (20 mL). The product was extracted using ethyl acetate (3 x 15 mL), the combined organic extracts were dried over magnesium sulphate $MgSO_4$, filtered and the solvent removed under reduced pressure to give a yellow oil. The crude product was purified by column chromatography (SiO_2) (petrol / diethyl ether, 7:3) to give 2-deutero-2,2-dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)ethanone (**(2-*d*)-2b**) as a white crystalline solid (0.166 g, 86% yield, 89% deuterium incorporation by ^{1}H NMR).

Mp: 68-70˚C; R_f= 0.31 (petrol / diethyl ether, 9:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.07 (dd, J = 4.3, 1.6 Hz, 1H), 6.92 – 6.91 (m, 1H), 6.16 (dd, J = 4.3, 2.4 Hz, 1H), 3.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 177.0, 134.0, 125.7, 121.5, 109.6, 68.2 ($J_{C\text{-}D}$ = 27.0 Hz), 38.0; IR(neat): υ_{max}/cm^{-1} 3117, 1650; Anal. Calcd for $C_7H_6DCl_2NO$: C, 43.55; H 4.18; N, 7.26. Found: C, 43.46; H, 4.09; N, 7.19; HRMS (APCI): calcd. for $C_7H_6DCl_2NO$ $[M+H]^+$: 193.0040; observed: 193.0038.

2-Deutero-2,2-dichloro-1-(*p*-tolyl)ethanone ((2-*d*)-2f)

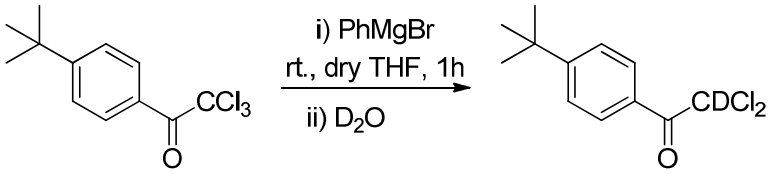


Under nitrogen, PhMgBr (2M, 0.55 mL, 1.1 mmol) was added to a 25 mL round bottomed flask. 2,2,2-Trichloro-1-(*p*-tolyl) ethanone (0.237 g, 1.0 mmol) was dissolved in dry THF (1 mL) and then added to the PhMgBr solution, dropwise over 10 minutes and allowed to stir for a further one hour. The mixture was quenched by adding D_2O (1 mL), and after 10 min. NH_4Cl (20 mL) was added. The product was extracted using ethyl acetate (3 x 15 mL). The combined organic extracts were dried over $MgSO_4$, filtered and the solvent removed under reduced pressure. The crude product was purified by silica gel column chromatography

(petrol / diethyl ether 9.5:0.5) to give 2-deutero-2,2-dichloro-1-(*p*-tolyl)ethanone ((2-*d*)-**2f**) as an oil (0.102 g, 50% yield, >95% deuterium incorporation by ^{1}H NMR).

R_f = 0.30 (petrol / diethyl ether, 49/1); 1H NMR (300 MHz, $CDCl_3$): δ_H 8.19 (d, J = 8.4 Hz, 2H), 7.31 (d, J = 8.4 Hz, 2H), 2.46(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 185.7, 146.0, 129.9, 129.7, 128.8, 67.6 ($J_{C\text{-}D}$ = 27.1 Hz), 21.9; IR(neat): υ_{max}/cm^{-1} 2924, 1690; MS (ESI): m/z 226.0 $[M+Na]^+$.

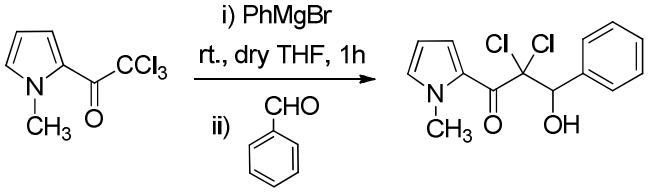
1-(4-(*tert*-Butyl)phenyl)-2-deutero-2,2-dichloroethanone ((2-*d*)-2g)



To a 25 mL round bottom flask was added PhMgBr (0.55 mL, 1.1 mmol) and under nitrogen. Into that flask was added 2,2,2-trichloro-1-(4-(*t*-butyl)phenyl)ethenone (0.279 g, 1 mmol) in THF (1 mL) and the reaction was stirred for 1 hour. The reaction was quenched with D_2O (0.02 mL) and extracted with ethylacetate (3x15 mL). The combined organic layers were dried over $MgSO_4$ and the solvent was removed under reduced pressure to give an oil. The crude product purified by silica gel column chromatography (40/60 petrol : ether, 70 : 1) to give 1-(4-(*tert*-butyl)phenyl)-2-deutero-2,2-dichloroethanone (**(2-*d*)-2f**) as a colourless oil (0.238 g, 96%, 93% deuterium incorporation by ^{1}H NMR).

R_f : 0.33 (UV active, petrol 40/60 : ether = 70: 1); ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 8.05 (d, J = 8.8 Hz, 2H), 7.55 (d, J = 8.8 Hz, 2H), 1.37 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) : δ_C 185.5, 158.6, 129.7, 128.8, 125.8, 67.6 ($J_{C\text{-}D}$ = 27.0 Hz), 35.3, 30.9; IR(neat): ν_{max}/cm^{-1} 2964.8, 2870.1, 1699.3, 1603.5, 1256.3, 916.8, 767.5, 695.8; HRMS(APCI): calcd for $C_{12}H_{13}DOCl_2$ $[M+H]^+$: 246.0558, found 246.0557.

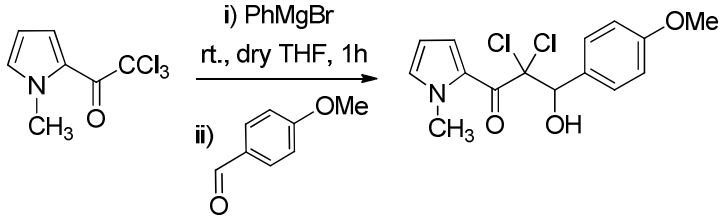
2,2-Dichloro-3-hydroxy-1-(1-methyl-1*H*-pyrrol-2-yl)-3-phenylpropan-1-one (3a)



PhMgBr (2M, 0.55 mL, 1.1 mmol) was added to a 25 mL round bottomed flask under nitrogen. 2,2,2-Trichloro-1-(1-methyl-*1H*-pyrrol-2-yl)ethanone (0.226 g, 1.0 mmol) was dissolved in dry THF (1 mL) and then added to the PhMgBr solution, dropwise over 10

minutes and allowed to stir for a further one hour. The reaction mixture was added to benzaldehyde (0.10 mL, 1.0 mmol) in THF (1 mL) and left to stir for 1h. The reaction was quenched by addition to saturated $NH_4Cl_{(aq)}$ (20 mL), and the product was extracted with EtOAc (3 x 15 mL). The combined organic extracts were dried over $MgSO_4$, filtered and the solvent removed under reduced pressure to give dark oil. The crude product was purified by column chromatography (SiO_2) (petrol / diethyl ether, 8:2) to give 2,2-dichloro-3-hydroxy-1-(1-methyl-1*H*-pyrrol-2-yl)-3-phenylpropan-1-one (**3a**) as white powder (0.24 g, 81% yield). Mp: 91-93 ˚C; R_f = 0.38 (petrol / diethyl ether, 7:3); ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.67 (dd, *J* = 4.4, 1.6 Hz, 1H), 7.65-7.63 (m, 2H), 7.44-7.37 (m, 2H), 6.96 (app t, *J* = 2.0 Hz, 1H), 6.25 (dd, *J* = 4.4, 2.4 Hz, 1H), 5.57 (d, *J* = 3.8 Hz, 1H), 4.16 (d, *J* = 3.8 Hz, 1H), 3.98 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 182.0, 136.0, 133.5, 129.9, 128.8, 127.5, 125.1, 124.7, 108.9, 87.0, 78.3, 38.7; IR(neat): υ_{max}/cm^{-1} 3525, 1627; Anal. Calcd for $C_{14}H_{13}Cl_2NO_2$: C, 56.39; H 4.39; N, 4.70. Found: C, 56.42; H, 4.40; N, 4.80; HRMS (NSI): calcd. for $C_{14}H_{13}Cl_2NO_2$ $[M+Na]^+$: 320.0216; observed: 320.0216.

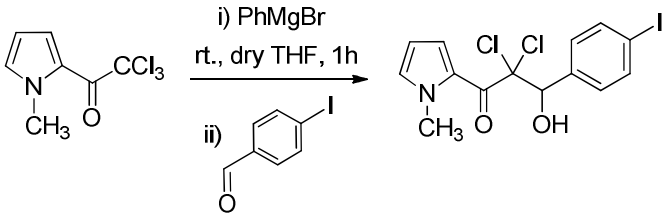
2,2-Dichloro-3-hydroxy-3-(4-methoxyphenyl)-1-(1-methyl-1*H*-pyrrol-2-yl)propan-1-one (3b)



PhMgBr (2M, 0.55 mL, 1.1 mmol) was added to a 25 mL round bottomed flask under nitrogen. 2,2,2-Trichloro-1-(1-methyl-*1H*-pyrrol-2-yl) ethanone (0.226 g, 1.0 mmol) was dissolved in dry THF (1 mL) and then added to the PhMgBr solution, dropwise over 10 minutes and allowed to stir for a further two hour. The reaction mixture was added to a solution of *p*-methoxy benzaldehyde (0.136 g, 1.0 mmol) in 1 mL of THF and left to stir for 3h. The reaction mixture was quenched by the addition of saturated $NH_4Cl_{(aq)}$ (20 mL), and the product was extracted using ethyl acetate (3 x 15 mL). The combined organic extracts were dried over $MgSO_4$, filtered and the solvent removed under reduced pressure to give dark oil. The crude product was purified by silica gel column chromatography (petrol / diethyl ether, 8:2) to give 2,2-dichloro-3-hydroxy-3-(4-methoxyphenyl)-1-(1-methyl-1*H*-pyrrol-2-yl)propan-1-one (**3b**) as a pink solid, (0.280 g, 85% yield).

Mp: 125-127 ˚C; R_f = 0.17 (petrol / diethyl ether, 8:2); ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.66 (dd, *J* = 4.4, 1.6 Hz, 1H), 7.55 (d, *J* = 8.7, 2H), 6.97-6.90 (m, 3H), 6.24 (dd, *J* = 4.4, 2.4 Hz, 1H), 5.52 (d, *J* = 3.6 Hz, 1H), 4.16 (d, *J* = 3.6 Hz, 1H), 3.96 (s, 3H), 3.85 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 182.0, 160.0, 133.4, 131.0, 128.2, 125.2, 124.7, 112.9, 108.9, 87.6, 77.9, 55.3, 38.7; IR(neat): υ_{max}/cm^{-1} 3505, 1618; HRMS (NSI): calcd for $C_{15}H_{15}Cl_2NO_3$ $[M+Na]^+$: 350.0321; observed: 350.0323.

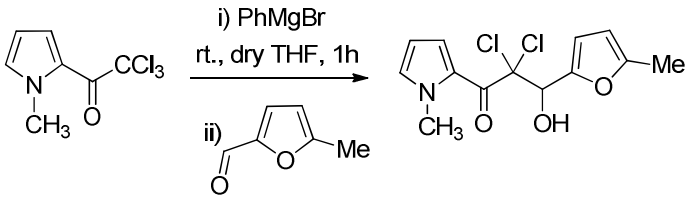
2,2-Dichloro-3-hydroxy-3-(4-iodophenyl)-1-(1-methyl-1*H*-pyrrol-2-yl)propan-1-one (3c)



Under nitrogen, PhMgBr (2M, 0.55 mL, 1.1 mmol) was added to a 25 mL round bottomed flask. 2,2,2-Trichloro-1-(1-methyl-*1H*-pyrrol-2-yl)ethanone (0.226 g, 1.0 mmol) was dissolved in dry THF (1 mL) and then added to the PhMgBr solution, dropwise over 10 minutes and the reaction was allowed to stir for a further one hour. The mixture was added to a solution of *p*-iodobenzaldehyde (0.232 g, 1.0 mmol) in THF (1 mL) and left to stir for 1h. The mixture was quenched by adding to NH_4Cl (20 mL), and the product was extracted using ethyl acetate (3 x 15 mL). The combined organic extracts were dried over $MgSO_4$, filtered and the solvent removed under reduced pressure to give yellow oil which was purified by silica gel column chromatography (petrol / diethyl ether, 7:3) to give 2,2-Dichloro-3-hydroxy-3-(4-iodophenyl)-1-(1-methyl-1*H*-pyrrol-2-yl)propan-1-one (**3c**) as a white solid (0.399 g, 94% yield).

Mp: 117-118˚C. R_f = 0.31 (petrol 7/ diethyl ether 3); ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.61 (d, *J* = 8.3 Hz, 2H), 7.52 (dd, *J* = 4.4, 1.6 Hz, 1H), 7.24 (d, *J* = 8.3 Hz, 2H), 6.82 (app t, *J* = 2.0 Hz, 1H), 6.11 (dd, *J* = 4.4, 2.4 Hz, 1H), 5.37 (d, *J* = 3.7 Hz, 1H), 4.10 (d, *J* = 3.7 Hz, 1H), 3.83 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 181.8, 136.6, 135.7, 133.7, 131.9, 124.9, 124.9, 109.1, 95.1, 86.4, 77.8, 38.8;. IR(neat): υ_{max}/cm^{-1} 3475, 3104, 1629;Anal. Calcd for $C_{14}H_{12}Cl_2INO_2$: C, 39.65; H 2.85; N, 3.30. Found: C, 39.73; H, 2.80; N, 3.27; HRMS (NSI): calcd for $C_{14}H_{12}Cl_2INO_2$ $[M+H]^+$: 423.9363; observed: 423.9360.

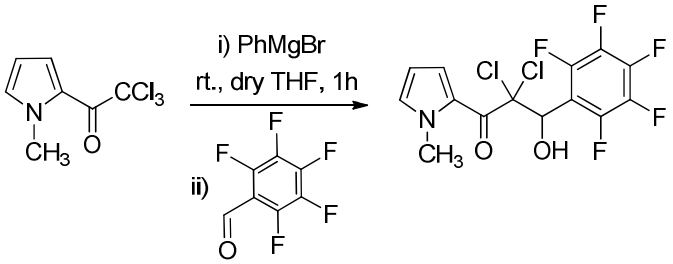
2,2-Dichloro-3-hydroxy-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(5-methylfuran-2-yl)propan-1-one (3d)



Under nitrogen, PhMgBr (2M, 0.55 mL, 1.1 mmol) was added to a 25 mL round bottomed flask. 2,2,2-Trichloro-1-(1-methyl-*1H*-pyrrol-2-yl)ethanone (0.226 g, 1.0 mmol) was dissolved in dry THF (1 mL) and then added to the PhMgBr solution, dropwise over 10 minutes and allowed to stir for a further one hour. The mixture was added to 5-methylfuran-2-carbaldehyde (0.11 g, 1.0 mmol / 1 mL dry THF) and left to stir for 1h. The mixture was quenched by adding to NH_4Cl (20 mL), and the product was extracted using ethyl acetate (3 x 15 mL). The combined organic extracts were dried over $MgSO_4$, filtered and the solvent removed under reduced pressure. The crude product was purified by silica gel column chromatography (petrol / diethyl ether, 6:4) to give 2,2-dichloro-3-hydroxy-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(5-methylfuran-2-yl)propan-1-one (**3d**) as a dark brown solid, (0.210 g, 70% yield).

Mp: 82-84 ˚C; R_f = 0.19 (petrol / diethyl ether, 8:2); ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.65 (dd, *J* = 4.4, 1.6 Hz, 1H), 6.94 (app t, *J* = 2.0 Hz, 1H), 6.48 (d, *J* = 3.1 Hz, 1H), 6.24 (dd, *J* = 4.4, 2.4 Hz, 1H), 6.02 (dt, *J* = 3.1, 1.0 Hz, 1H), 5.54 (d, *J* = 5.8 Hz, 1H), 3.96 (s, 3H), 3.90 (d, *J* = 5.8 Hz, 1H), 2.34 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 181.1, 152.4, 148.4, 133.4, 124.9, 124.3, 111.3, 108.9, 106.6, 86.4, 74.0, 38.6, 13.7; IR(neat): υ_{max}/cm^{-1} 3107, 2921, 1624; HRMS (NSI) calcd for $C_{14}H_{11}O_4N_2Cl_2$ $[M+Na]^+$: 324.0165, observed: 324.0168; Anal. Calcd for $C_{13}H_{13}Cl_2NO_3$: C, 51.68; H 4.34; N, 4.64. Found: C, 51.59; H, 4.46; N, 4.78.

2,2-Dichloro-3-hydroxy-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(perfluorophenyl)propan-1-one (3e)

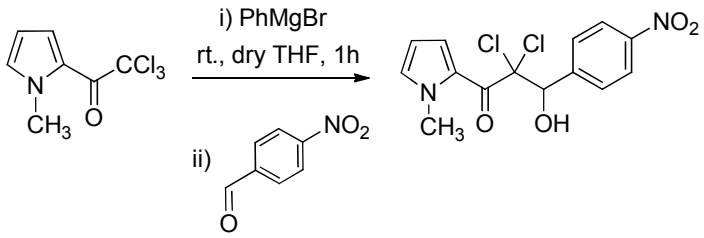


Under nitrogen, PhMgBr (2M, 0.55 mL, 1.1 mmol) was added to a 25 mL round bottomed flask. 2,2,2-Trichloro-1-(1-methyl-*1H*-pyrrol-2-yl) ethanone (0.226 g, 1.0 mmol) was dissolved in dry THF (1 mL) and then added to the PhMgBr solution dropwise over 10 minutes and allowed to stir for a further one hour. The mixture was added to pentafluoro benzaldehyde (0.196 g, 1.0 mmol / 1 mL dry THF) and left to stir for 1h. The mixture was quenched by adding to NH_4Cl (20 mL), and the product was extracted using ethyl acetate (3 x 15 mL). The combined organic extracts were dried over $MgSO_4$, filtered and the solvent removed under reduced pressure to give yellow oil. The crude product was purified by silica gel column chromatography (petrol / diethyl ether, 7:3) to give 2,2-dichloro-3-hydroxy-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(perfluorophenyl)propan-1-one (**3e**) as a white solid (0.270 g, 70% yield).

Mp: 98-99°C; R_f = 0.30 (petrol 7/ diethyl ether 3); ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.56 (dd, *J* = 4.4, 1.6 Hz, 1H), 6.89 (app t, *J* = 2.0 Hz, 1H), 6.16 (dd, *J* = 4.4, 2.4 Hz, 1H), 5.99 (d, *J* = 6.2 Hz, 1H), 4.04 (d, *J* = 6.2 Hz, 1H), 3.89 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 180.3, 133.9, 124.6, 124.4, 109.1, 85.8, 73.4, 38.7; ^{19}F NMR (376 MHz, $CDCl_3$): δ_F -134.5 (d, *J* = 20.8 Hz), -151.3 (t, *J* = 21.0 Hz), -161.7 (app t, *J* = 21.0 Hz); IR(neat): υ_{max}/cm^{-1} 3371, 2963, 1656; Anal. Calcd for $C_{14}H_8Cl_2F_5NO_2$: C, 43.32; H 2.08; N, 3.61. Found: C, 43.38; H, 1.99; N, 3.56; HRMS (NIS): calcd for $C_{14}H_8Cl_2F_5NO_2$ $[M+Na]^+$:409.9744; observed: 409.9747.

NB: some ^{13}C signals not observed due to F coupling

2,2-Dichloro-3-hydroxy-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(4-nitrophenyl)propan-1-one (3f)

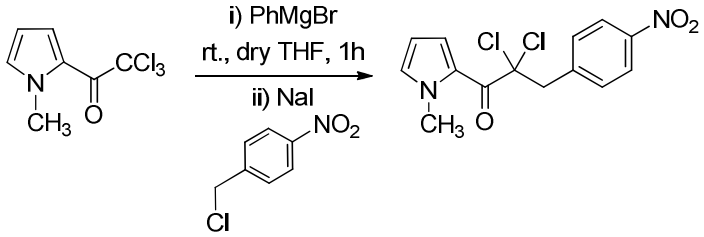


Under nitrogen, PhMgBr (2M, 0.55 mL, 1.1 mmol) was added to a 25 mL round bottomed flask. 2,2,2-Trichloro-1-(1-methyl-*1H*-pyrrol-2-yl) ethanone (0.226 g, 1.0 mmol) was dissolved in dry THF (1 mL) and then added to the PhMgBr solution dropwise over 10 minutes and allowed to stir for a further one hour. The reaction mixture was added to aolution of *p*-nitrobenzalaldehyde (0.15 g, 1.0 mmol) in THF (1 mL) and left to stir for 1h. The reaction mixture was quenched by adding to NH_4Cl (20 mL), and the product was extracted using ethyl acetate (3 x 15 mL). The combined organic extracts were dried over $MgSO_4$, filtered and the solvent removed under reduced pressure. The crude product was purified by

silica gel column chromatography (petrol / diethyl ether, 5:5) to give 2,2-dichloro-3-hydroxy-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(4-nitrophenyl)propan-1-one (**3f**) as brown solid (0.33 g, 96% yield).

Mp: 170-173 ˚C; R_f = 0.4 (petrol / diethyl ether 5:5); ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 8.18 (d, *J* = 8.8 Hz, 2H), 7.74 (d, *J* = 8.8 Hz, 2H), 7.55 (dd, *J* = 4.4, 1.6 Hz, 1H), 6.90 (t, *J* = 2.0 Hz, 1H), 6.16 (dd, *J* = 4.5, 2.4 Hz, 1H), 5.55 (d, *J* = 3.4 Hz, 1H), 4.21 (d, *J* = 3.5 Hz, 1H), 3.91 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 181.5, 148.1, 142.8, 133.9, 130.9, 125.0, 124.6, 122.4, 109.1, 85.4, 38.7; IR(neat): υ_{max}/cm^{-1} 3499, 3132, 1644; HRMS (APCI) calcd for $C_{14}H_{12}Cl_2N_2O_4$ $[M+H]^+$: 341.0090; observed: 341.0090; Anal. Calcd for $C_{14}H_{12}Cl_2N_2O_4$: C, 49.00; H 3.52; N, 8.16. Found: C, 49.09; H, 3.43; N, 8.10.

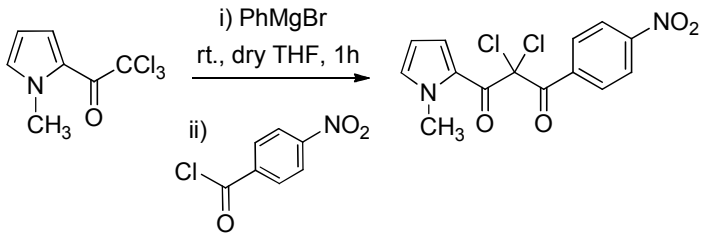
2,2-Dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(4-nitrophenyl)propan-1-one (3g)



Under nitrogen, PhMgBr (2M, 0.55 mL, 1.1 mmol) was added to a 25 mL round bottomed flask. 2,2,2-Trichloro-1-(1-methyl-*1H*-pyrrol-2-yl) ethanone (0.226 g, 1.0 mmol) was dissolved in dry THF (1 mL) and then added to the PhMgBr solution dropwise over 10 minutes and allowed to stir for a further two hours. The reaction mixture was added to a solution of 4-nitrobenzyl chloride (0.171 g, 1.0 mmol) and NaI (0.015 g) in THF (1 mL) and left to stir for 24h. The mixture was quenched by adding to NH_4Cl (20 mL), and the product was extracted using ethyl acetate (3 x 15 mL). The combined organic extracts were dried over $MgSO_4$, filtered and the solvent removed under reduced pressure to give brown solid. The crude product was purified by silica gel column chromatography (petrol / diethyl ether, 4:1) to give 2,2-dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(4-nitrophenyl)propan-1-one (**3g**) as a white solid (0.120 g, 37%).

Mp: 140-142 ˚C; R_f= 0.46 (petrol / diethyl ether, 4:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 8.22 (d, *J* = 8.6 Hz, 2H), 7.64 (d, *J* = 8.6 Hz, 2H), 7.61-7.60 (m, 1H), 6.95 (s, 1H), 6.23 (dd, *J* = 4.4, 2.4 Hz, 1H), 3.97 (s, 3H), 3.86 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 179.4, 147.6, 141.8, 133.1, 133.0, 123.6, 123.0, 108.7, 85.5, 48.8, 38.6; IR(neat): υ_{max}/cm^{-1} 1640; HRMS(APCI): calcd for $C_{14}H_{12}Cl_2N_2O_3$ $[M+H]^+$: 327.0298; observed: 327.0295; Anal. Calcd for $C_{14}H_{12}Cl_2N_2O_3$: C, 51.40; H 3.70; N, 8.56. Found: C, 51.49; H, 3.72; N, 8.58.

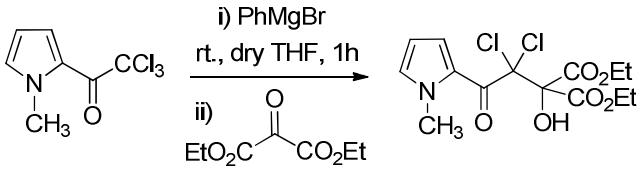
2,2-Dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(4-nitrophenyl)propane-1,3-dione (3h)



Under nitrogen, PhMgBr (2M, 0.55 mL, 1.1 mmol) was added to a 25 mL round bottomed flask. 2,2,2-Trichloro-1-(1-methyl-*1H*-pyrrol-2-yl) ethanone (0.226 g, 1.0 mmol) was dissolved in dry THF (1 mL) and then added to the PhMgBr solution dropwise over 10 minutes and allowed to stir for a further two hours. The reaction mixture was added to 4-nitrobenzoyl chloride (0.186 g, 1.0 mmol) in THF (1 mL) and left to stir for 1h. The mixture was quenched by adding to NH_4Cl (20 mL), and the product was extracted using ethyl acetate (3 x 15 mL). The combined organic extracts were dried over $MgSO_4$, filtered and the solvent removed under reduced pressure to give brown solid. The crude product was purified by silica gel column chromatography (petrol / diethyl ether, 9:1) to give 2,2-dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(4-nitrophenyl)propane-1,3-dione (**3h**) as a yellow solid, (0.325 g, 95% yield).

Mp: 160-162 ˚C; R_f = 0.14(petrol / diethyl ether, 9:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 8.24 (m, 2H), 8.14 (m, 2H), 7.12 (dd, *J* = 4.3, 1.6 Hz, 1H), 6.93 (t, *J* = 2.0 Hz, 1H), 6.14 (dd, *J* = 4.4, 2.4 Hz, 1H), 3.94 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 184.0, 175.4, 150.4, 137.0, 134.2, 131.4, 124.8, 123.7, 123.5, 109.9, 87.7, 38.5; IR(neat): υ_{max}/cm^{-1} 3121, 1660; HRMS (APCI) calcd for $C_{14}H_{11}O_4N_2Cl_2$ $[M+H]^+$: 341.0090; observed: 341.0090; Anal. Calcd for $C_{14}H_{10}Cl_2N_2O_4$: C, 49.29; H 2.95; N, 8.21. Found: C, 49.35; H, 2.92; N, 8.15.

Diethyl 2-(1,1-dichloro-2-(1-methyl-1*H*-pyrrol-2-yl)-2-oxoethyl)-2-hydroxymalonate (3i)

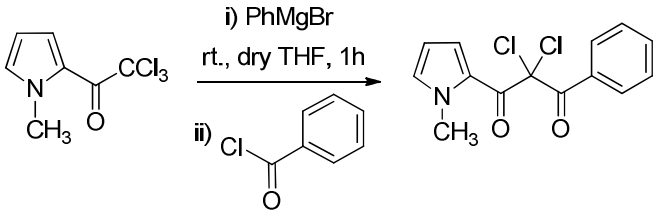


Under nitrogen, PhMgBr (2M, 0.55 mL, 1.1 mmol) was added to a 25 mL round bottomed flask. 2,2,2-Trichloro-1-(1-methyl-*1H*-pyrrol-2-yl) ethanone (0.226 g, 1.0 mmol) was dissolved in dry THF (1 mL) and then added to the PhMgBr solution dropwise over 10 minutes and allowed to stir for a further two hours. The mixture was added to diethyl

ketomalonate (0.174 g, 1.0 mmol) in THF (1 mL) and left to stir for two hours. The mixture was quenched by adding to NH_4Cl (20 mL), and the product was extracted using ethyl acetate (3 x 15 mL). The combined organic extracts were dried over $MgSO_4$, filtered and the solvent removed under reduced pressure to give a brown solid. The crude product was purified by silica gel column chromatography (petrol / diethyl ether, 9:1 then with 6.4) to give diethyl 2-(1,1-dichloro-2-(1-methyl-1*H*-pyrrol-2-yl)-2-oxoethyl)-2-hydroxymalonate (**3i**) was obtained as a yellow oil, (0.310 g, 79% yield)

R_f = 0.28 (petrol / diethyl ether 6.4); ^{1}H NMR (300 MHz, $CDCl_3$): δ_H 7.66 (dd, *J* = 4.4, 1.6 Hz, 1H), 6.92 (app t, *J* = 2.0 Hz, 1H), 6.21 (dd, *J* = 4.4, 2.4 Hz, 1H), 4.66 (s, 1H), 4.36 (q, *J* = 7.1 Hz, 4H), 3.88 (s, 3H), 1.33 (t, *J* = 7.1 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 178.8, 166.8, 133.3, 124.2, 123.9, 108.8, 85.0, 82.7, 63.2, 38.5, 14.0; IR(neat): υ_{max}/cm^{-1} 3454, 1738, 1646; HRMS (NSI): calcd for $C_{14}H_{17}Cl_2NO_6$ [M+H] : 366.0506; observed: 366.0512; Anal. Calcd for $C_{14}H_{17}Cl_2NO_6$: C, 45.92; H 4.68; N, 3.82. Found: C, 46.02; H, 4.59; N, 3.75.

2,2-Dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)-3-phenylpropane-1,3-dione (3j)



Under nitrogen, PhMgBr (2M, 2.2 mL, 4.4 mmol) was added to a 50 mL round bottomed flask. 2,2,2-Trichloro-1-(1-methyl-*1H*-pyrrol-2-yl) ethanone (0.904 g, 4 mmol) was dissolved in dry THF (4 mL) and then added to the PhMgBr solution dropwise over 10 minutes and allowed to stir for a further two hour. The mixture was added to benzoyl chloride (0.464 mL, 4.0 mmol) in THF (4 mL) and left to stir for 1h. The mixture was quenched by adding to saturated $NH_4Cl_{(aq)}$ (50 mL), and the product was extracted using ethyl acetate (3 x 25 mL). The combined organic extracts were dried over $MgSO_4$, filtered and the solvent removed under reduced pressure to give brown solid crude. The crude product was purified by column chromatography (SiO_2) (petrol / diethyl ether, 5:1) to give 2,2-Dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)-3-phenylpropane-1,3-dione (**3j**) as white-yellow solid (0.590 g, 50% yield).

Mp. 67-68 ˚C; R_f = 0.26 (petrol / diethyl ether, 5:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.98 (d, *J* = 7.4 Hz, 2H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.46 – 7.32 (m, 2H), 7.03 (dd, *J* = 4.5, 1.6 Hz, 1H), 6.86 (app t, *J* = 2.0 Hz, 1H), 6.09 (dd, *J* = 4.5, 2.4 Hz, 1H), 3.94 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 185.1, 175.6, 134.0, 133.6, 132.0, 130.4, 128.7, 125.1, 123.0, 109.6, 88.9,

36.4; IR(neat): υ_{max}/cm^{-1} 2951, 1699, 1659; HRMS (APCI): calcd for $C_{14}H_{11}Cl_2NO_2$ $[M+H]^+$: 296.0240; observed: 296.0244.

References:

1) Bailey, D. M.; Johnson R. E. *J. Med. Chem.,* **1973***, 16,* 1300.
2) Taylor, J. E.; Jones, M. D.; Williams, J. M. J.; Bull, S. D. *Org. Lett.,* **2010**, *12*, 5740.

Structural diagrams, data and notes for single crystal X-ray structures:

2,2,2-Trichloro-1-(4,5-dibromo-1*H*-pyrrol-2-yl)ethanone (1d)

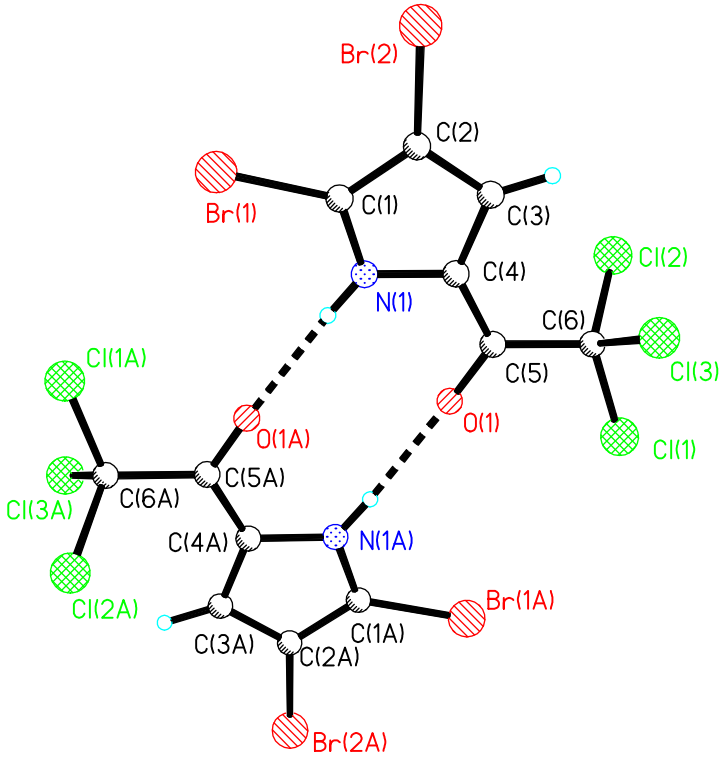


Table 1. Crystal data and structure refinement for mjh4.

Identification code	mjh4	
Chemical formula (moiety)	$C_6H_2Br_2Cl_3NO$	
Chemical formula (total)	$C_6H_2Br_2Cl_3NO$	
Formula weight	370.26	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, $P2_1/c$	
Unit cell parameters	a = 9.971(3) Å	α = 90°
	b = 16.520(4) Å	β = 102.18(2)°
	c = 6.6012(16) Å	γ = 90°
Cell volume	1062.9(5) $Å^3$	
Z	4	
Calculated density	2.314 g/cm^3	
Absorption coefficient μ	8.338 mm^{-1}	
F(000)	696	
Crystal colour and size	colourless, 0.54 × 0.50 × 0.40 mm^3	
Reflections for cell refinement	75 (θ range 2.5 to 27.5°)	
Data collection method	Nonius KappaCCD diffractometer	
	ϕ and ω scans	
θ range for data collection	4.0 to 27.6°	
Index ranges	h −12 to 12, k −21 to 21, l −8 to 8	

Completeness to θ = 26.0°	99.7 %
Reflections collected	21651
Independent reflections	2433 (R_{int} = 0.0536)
Reflections with $F^2>2\sigma$	1990
Absorption correction	semi-empirical from equivalents
Min. and max. transmission	0.0936 and 0.1352
Structure solution	direct methods
Refinement method	Full-matrix least-squares on F^2
Weighting parameters a, b	0.0038, 1.7240
Data / restraints / parameters	2433 / 0 / 123
Final R indices [$F^2>2\sigma$]	R1 = 0.0249, wR2 = 0.0446
R indices (all data)	R1 = 0.0406, wR2 = 0.0502
Goodness-of-fit on F^2	1.138
Extinction coefficient	0.0022(2)
Largest and mean shift/su	0.001 and 0.000
Largest diff. peak and hole	0.70 and −0.87 e $Å^{-3}$

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for mjh4. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Br(1)	0.64716(3)	0.32144(2)	–0.14075(6)	0.03433(11)
Br(2)	0.44528(3)	0.385688(19)	0.23119(5)	0.02711(9)
Cl(1)	1.04425(9)	0.70121(5)	0.44769(13)	0.0371(2)
Cl(2)	0.74819(8)	0.70224(4)	0.33381(11)	0.03015(18)
Cl(3)	0.89093(7)	0.59499(4)	0.65733(10)	0.02130(15)
O(1)	0.9867(2)	0.57714(12)	0.1472(3)	0.0232(4)
N(1)	0.7910(2)	0.45663(14)	0.0594(4)	0.0179(5)
C(1)	0.6820(3)	0.40742(17)	0.0461(4)	0.0196(6)
C(2)	0.6073(3)	0.43312(17)	0.1882(4)	0.0200(6)
C(3)	0.6739(3)	0.50035(17)	0.2917(4)	0.0195(6)
C(4)	0.7898(3)	0.51446(16)	0.2104(4)	0.0168(5)
C(5)	0.8968(3)	0.57472(16)	0.2467(4)	0.0161(5)
C(6)	0.8963(3)	0.64093(16)	0.4155(4)	0.0181(6)

Table 3. Bond lengths [Å] and angles [°] for mjh4.

Br(1)–C(1)	1.865(3)	Br(2)–C(2)	1.870(3)
Cl(1)–C(6)	1.755(3)	Cl(2)–C(6)	1.778(3)
Cl(3)–C(6)	1.778(3)	O(1)–C(5)	1.218(3)
N(1)–H(1)	0.80(3)	N(1)–C(1)	1.344(3)
N(1)–C(4)	1.382(3)	C(1)–C(2)	1.382(4)
C(2)–C(3)	1.397(4)	C(3)–H(3A)	0.9500
C(3)–C(4)	1.393(4)	C(4)–C(5)	1.442(4)
C(5)–C(6)	1.563(4)		

H(1)–N(1)–C(1)	125(2)	H(1)–N(1)–C(4)	126(2)
C(1)–N(1)–C(4)	109.6(2)	Br(1)–C(1)–N(1)	122.6(2)
Br(1)–C(1)–C(2)	129.1(2)	N(1)–C(1)–C(2)	108.3(2)
Br(2)–C(2)–C(1)	125.5(2)	Br(2)–C(2)–C(3)	126.6(2)
C(1)–C(2)–C(3)	107.9(2)	C(2)–C(3)–H(3A)	126.5
C(2)–C(3)–C(4)	107.0(2)	H(3A)–C(3)–C(4)	126.5
N(1)–C(4)–C(3)	107.2(2)	N(1)–C(4)–C(5)	118.6(2)
C(3)–C(4)–C(5)	134.2(2)	O(1)–C(5)–C(4)	122.4(2)
O(1)–C(5)–C(6)	118.4(2)	C(4)–C(5)–C(6)	119.2(2)
Cl(1)–C(6)–Cl(2)	109.66(15)	Cl(1)–C(6)–Cl(3)	108.51(15)
Cl(1)–C(6)–C(5)	110.74(18)	Cl(2)–C(6)–Cl(3)	109.57(14)
Cl(2)–C(6)–C(5)	108.05(18)	Cl(3)–C(6)–C(5)	110.30(18)

Table 4. Anisotropic displacement parameters ($Å^2$) for mjh4. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	0.02473(17)	0.03287(18)	0.0449(2)	–0.02196(15)	0.00635(14)	–0.00270(13)
Br(2)	0.01790(15)	0.03020(17)	0.03518(18)	–0.00326(13)	0.01002(12)	–0.00740(12)
Cl(1)	0.0435(5)	0.0392(5)	0.0335(4)	–0.0129(3)	0.0190(4)	–0.0261(4)
Cl(2)	0.0435(4)	0.0217(4)	0.0244(4)	0.0012(3)	0.0051(3)	0.0151(3)
Cl(3)	0.0221(3)	0.0267(4)	0.0155(3)	0.0045(3)	0.0046(3)	0.0013(3)
O(1)	0.0251(11)	0.0222(10)	0.0269(11)	–0.0025(8)	0.0155(9)	–0.0022(8)
N(1)	0.0133(11)	0.0208(12)	0.0215(12)	–0.0050(10)	0.0081(10)	0.0006(9)
C(1)	0.0170(13)	0.0195(14)	0.0218(14)	–0.0054(11)	0.0027(11)	–0.0001(11)
C(2)	0.0148(13)	0.0220(14)	0.0238(15)	–0.0011(11)	0.0057(11)	–0.0020(11)
C(3)	0.0185(13)	0.0204(14)	0.0212(14)	–0.0035(11)	0.0081(11)	0.0001(11)
C(4)	0.0168(13)	0.0170(13)	0.0181(13)	–0.0011(10)	0.0068(11)	0.0004(10)
C(5)	0.0172(13)	0.0157(13)	0.0161(13)	0.0034(10)	0.0050(11)	0.0045(10)
C(6)	0.0220(14)	0.0160(13)	0.0174(14)	0.0001(10)	0.0073(11)	–0.0021(11)

Table 5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for mjh4.

	x	y	z	U
H(1)	0.850(3)	0.4507(18)	–0.004(5)	0.020(8)
H(3A)	0.6456	0.5307	0.3976	0.023

Table 6. Torsion angles [°] for mjh4.

C(4)–N(1)–C(1)–Br(1)	179.90(19)	C(4)–N(1)–C(1)–C(2)	0.5(3)
Br(1)–C(1)–C(2)–Br(2)	0.2(4)	Br(1)–C(1)–C(2)–C(3)	–179.6(2)
N(1)–C(1)–C(2)–Br(2)	179.6(2)	N(1)–C(1)–C(2)–C(3)	–0.2(3)
Br(2)–C(2)–C(3)–C(4)	–180.0(2)	C(1)–C(2)–C(3)–C(4)	–0.2(3)
C(1)–N(1)–C(4)–C(3)	–0.6(3)	C(1)–N(1)–C(4)–C(5)	–178.7(2)
C(2)–C(3)–C(4)–N(1)	0.5(3)	C(2)–C(3)–C(4)–C(5)	178.1(3)
N(1)–C(4)–C(5)–O(1)	1.1(4)	N(1)–C(4)–C(5)–C(6)	179.5(2)
C(3)–C(4)–C(5)–O(1)	–176.3(3)	C(3)–C(4)–C(5)–C(6)	2.1(5)
O(1)–C(5)–C(6)–Cl(1)	–7.0(3)	O(1)–C(5)–C(6)–Cl(2)	113.1(2)
O(1)–C(5)–C(6)–Cl(3)	–127.1(2)	C(4)–C(5)–C(6)–Cl(1)	174.6(2)
C(4)–C(5)–C(6)–Cl(2)	–65.3(3)	C(4)–C(5)–C(6)–Cl(3)	54.4(3)

Table 7. Hydrogen bonds for mjh4 [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
N(1)–H(1)...O(1A)	0.80(3)	2.10(3)	2.892(3)	173(3)

Symmetry operations for equivalent atoms
A –x+2,–y+1,–z

2,2-Dichloro-3-hydroxy-1-(1-methyl-1*H*-pyrrol-2-yl)-3-phenylpropan-1-one (3a)

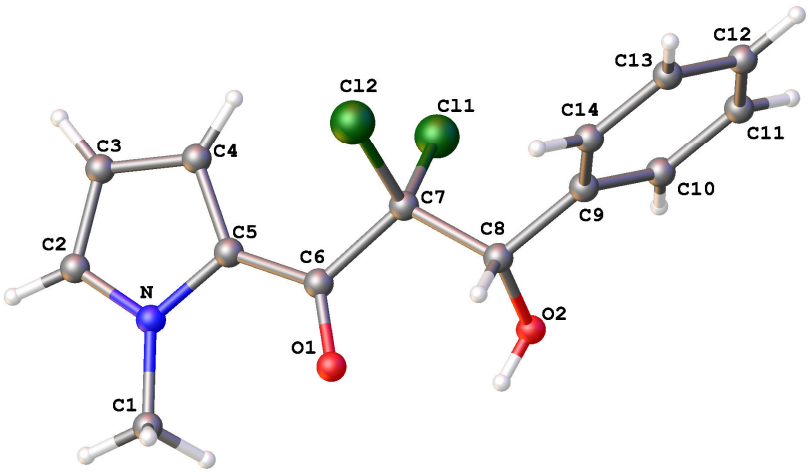


Table 1. Crystal data and structure refinement for mjh78.

Identification code	mjh78	
Chemical formula (moiety)	$C_{14}H_{13}Cl_2NO_2$	
Chemical formula (total)	$C_{14}H_{13}Cl_2NO_2$	
Formula weight	298.15	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	orthorhombic, Pbcn	
Unit cell parameters	a = 21.1956(11) Å	α = 90°
	b = 7.5271(4) Å	β = 90°
	c = 17.1302(14) Å	γ = 90°
Cell volume	2733.0(3) $Å^3$	
Z	8	
Calculated density	1.449 g/cm^3	
Absorption coefficient μ	0.471 mm^{-1}	
F(000)	1232	
Reflections for cell refinement	3920 (θ range 2.9 to 28.6°)	
Data collection method	Xcalibur, Atlas, Gemini ultra	
	thick-slice ω scans	
θ range for data collection	2.9 to 28.6°	
Index ranges	h –27 to 24, k –8 to 10, l –20 to 13	
Completeness to θ = 28.6°	84.7 %	
Reflections collected	9986	
Independent reflections	2977 (R_{int} = 0.0337)	
Reflections with $F^2>2\sigma$	2347	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.88578 and 1.00000	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0457, 1.9659	
Data / restraints / parameters	2977 / 0 / 177	
Final R indices [$F^2>2\sigma$]	R1 = 0.0429, wR2 = 0.0981	
R indices (all data)	R1 = 0.0606, wR2 = 0.1091	
Goodness-of-fit on F^2	1.046	
Largest and mean shift/su	0.000 and 0.000	
Largest diff. peak and hole	0.49 and –0.24 e $Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for mjh78. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cl(1)	0.36856(3)	0.33388(7)	0.15066(3)	0.03307(17)
Cl(2)	0.30354(2)	0.11348(8)	0.03655(3)	0.03294(16)
O(1)	0.45936(9)	0.1490(3)	–0.01866(11)	0.0487(5)
O(2)	0.47200(8)	0.0518(3)	0.13511(10)	0.0372(4)
N	0.43398(10)	0.4797(3)	–0.09231(12)	0.0378(5)
C(1)	0.48997(13)	0.4064(4)	–0.12988(16)	0.0473(7)
C(2)	0.40511(15)	0.6303(4)	–0.11512(18)	0.0509(7)
C(3)	0.35388(14)	0.6628(4)	–0.06903(17)	0.0503(7)
C(4)	0.35088(12)	0.5266(3)	–0.01479(15)	0.0387(6)
C(5)	0.40089(11)	0.4117(3)	–0.02887(13)	0.0324(5)
C(6)	0.41768(10)	0.2452(3)	0.00608(13)	0.0308(5)
C(7)	0.37911(10)	0.1717(3)	0.07638(12)	0.0266(5)
C(8)	0.41036(10)	0.0035(3)	0.11089(13)	0.0283(5)
C(9)	0.37512(10)	–0.0771(3)	0.17880(13)	0.0276(5)
C(10)	0.39203(11)	–0.0343(3)	0.25466(14)	0.0327(5)
C(11)	0.35973(12)	–0.1084(3)	0.31687(15)	0.0398(6)
C(12)	0.31104(12)	–0.2261(4)	0.30432(15)	0.0414(6)
C(13)	0.29436(12)	–0.2718(3)	0.22899(16)	0.0410(6)
C(14)	0.32644(12)	–0.1966(3)	0.16699(14)	0.0337(5)

Table 3. Bond lengths [Å] and angles [°] for mjh78.

Cl(1)–C(7)	1.777(2)	Cl(2)–C(7)	1.795(2)
O(1)–C(6)	1.218(3)	O(2)–H(2)	0.82(4)
O(2)–C(8)	1.418(3)	N–C(1)	1.458(3)
N–C(2)	1.346(3)	N–C(5)	1.391(3)
C(1)–H(1A)	0.980	C(1)–H(1B)	0.980
C(1)–H(1C)	0.980	C(2)–H(2A)	0.950
C(2)–C(3)	1.365(4)	C(3)–H(3)	0.950
C(3)–C(4)	1.385(4)	C(4)–H(4)	0.950
C(4)–C(5)	1.389(3)	C(5)–C(6)	1.434(3)
C(6)–C(7)	1.557(3)	C(7)–C(8)	1.546(3)
C(8)–H(8)	1.000	C(8)–C(9)	1.510(3)
C(9)–C(10)	1.386(3)	C(9)–C(14)	1.384(3)
C(10)–H(10)	0.950	C(10)–C(11)	1.384(3)
C(11)–H(11)	0.950	C(11)–C(12)	1.377(4)
C(12)–H(12)	0.950	C(12)–C(13)	1.382(4)
C(13)–H(13)	0.950	C(13)–C(14)	1.382(3)
C(14)–H(14)	0.950		

H(2)–O(2)–C(8)	108(2)	C(1)–N–C(2)	124.1(2)
C(1)–N–C(5)	128.0(2)	C(2)–N–C(5)	107.9(2)
N–C(1)–H(1A)	109.5	N–C(1)–H(1B)	109.5
N–C(1)–H(1C)	109.5	H(1A)–C(1)–H(1B)	109.5
H(1A)–C(1)–H(1C)	109.5	H(1B)–C(1)–H(1C)	109.5
N–C(2)–H(2A)	124.9	N–C(2)–C(3)	110.2(2)
H(2A)–C(2)–C(3)	124.9	C(2)–C(3)–H(3)	126.5
C(2)–C(3)–C(4)	106.9(2)	H(3)–C(3)–C(4)	126.5
C(3)–C(4)–H(4)	126.0	C(3)–C(4)–C(5)	108.0(2)
H(4)–C(4)–C(5)	126.0	N–C(5)–C(4)	107.0(2)
N–C(5)–C(6)	121.5(2)	C(4)–C(5)–C(6)	131.4(2)
O(1)–C(6)–C(5)	123.6(2)	O(1)–C(6)–C(7)	116.0(2)
C(5)–C(6)–C(7)	120.21(19)	Cl(1)–C(7)–Cl(2)	109.11(11)
Cl(1)–C(7)–C(6)	112.08(15)	Cl(1)–C(7)–C(8)	110.03(15)
Cl(2)–C(7)–C(6)	105.14(14)	Cl(2)–C(7)–C(8)	109.12(15)
C(6)–C(7)–C(8)	111.20(17)	O(2)–C(8)–C(7)	107.25(18)
O(2)–C(8)–H(8)	108.5	O(2)–C(8)–C(9)	109.48(18)
C(7)–C(8)–H(8)	108.5	C(7)–C(8)–C(9)	114.33(17)
H(8)–C(8)–C(9)	108.5	C(8)–C(9)–C(10)	120.1(2)
C(8)–C(9)–C(14)	121.2(2)	C(10)–C(9)–C(14)	118.7(2)
C(9)–C(10)–H(10)	120.0	C(9)–C(10)–C(11)	120.0(2)
H(10)–C(10)–C(11)	120.0	C(10)–C(11)–H(11)	119.7
C(10)–C(11)–C(12)	120.6(2)	H(11)–C(11)–C(12)	119.7
C(11)–C(12)–H(12)	120.1	C(11)–C(12)–C(13)	119.9(2)
H(12)–C(12)–C(13)	120.1	C(12)–C(13)–H(13)	120.3
C(12)–C(13)–C(14)	119.3(2)	H(13)–C(13)–C(14)	120.3
C(9)–C(14)–C(13)	121.4(2)	C(9)–C(14)–H(14)	119.3
C(13)–C(14)–H(14)	119.3		

Table 4. Anisotropic displacement parameters ($Å^2$) for mjh78. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	0.0394(3)	0.0304(3)	0.0294(3)	–0.0066(2)	0.0073(2)	0.0006(2)
Cl(2)	0.0271(3)	0.0385(3)	0.0332(3)	–0.0005(2)	–0.0036(2)	0.0012(2)
O(1)	0.0467(10)	0.0614(12)	0.0380(10)	0.0139(9)	0.0190(8)	0.0270(10)
O(2)	0.0278(8)	0.0564(11)	0.0273(9)	–0.0015(8)	0.0012(7)	0.0052(8)
N	0.0433(11)	0.0370(11)	0.0331(12)	–0.0001(9)	0.0051(9)	–0.0074(10)
C(1)	0.0472(15)	0.0536(16)	0.0410(16)	0.0030(13)	0.0136(12)	–0.0138(13)
C(2)	0.071(2)	0.0363(14)	0.0453(17)	0.0085(12)	0.0005(14)	–0.0091(14)
C(3)	0.0643(18)	0.0344(14)	0.0524(18)	0.0055(12)	–0.0016(14)	0.0099(13)
C(4)	0.0434(14)	0.0372(13)	0.0356(14)	–0.0019(11)	0.0000(11)	0.0050(12)
C(5)	0.0344(12)	0.0343(13)	0.0284(12)	–0.0006(10)	0.0018(9)	–0.0033(10)
C(6)	0.0289(11)	0.0383(13)	0.0252(12)	–0.0001(9)	0.0025(9)	0.0025(10)
C(7)	0.0242(10)	0.0328(12)	0.0228(11)	–0.0052(9)	0.0029(8)	0.0016(9)
C(8)	0.0281(11)	0.0338(12)	0.0230(12)	–0.0041(9)	–0.0009(9)	0.0059(10)
C(9)	0.0315(11)	0.0292(11)	0.0221(11)	–0.0030(9)	–0.0003(9)	0.0079(10)
C(10)	0.0385(12)	0.0323(12)	0.0274(12)	–0.0047(10)	–0.0027(10)	0.0019(11)
C(11)	0.0531(15)	0.0429(14)	0.0233(12)	0.0020(10)	0.0000(11)	0.0044(13)
C(12)	0.0496(15)	0.0410(14)	0.0337(14)	0.0115(11)	0.0072(11)	0.0031(13)
C(13)	0.0432(14)	0.0330(13)	0.0469(16)	0.0067(11)	–0.0031(12)	–0.0051(11)
C(14)	0.0427(13)	0.0285(12)	0.0298(13)	–0.0037(9)	–0.0047(10)	0.0001(11)

Table 5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for mjh78.

	x	y	z	U
H(2)	0.4960(16)	0.038(4)	0.098(2)	0.072(11)
H(1A)	0.5054	0.4901	–0.1693	0.071
H(1B)	0.4793	0.2934	–0.1550	0.071
H(1C)	0.5229	0.3866	–0.0906	0.071
H(2A)	0.4185	0.7033	–0.1572	0.061
H(3)	0.3256	0.7604	–0.0733	0.060
H(4)	0.3200	0.5139	0.0251	0.046
H(8)	0.4139	–0.0877	0.0687	0.034
H(10)	0.4258	0.0459	0.2640	0.039
H(11)	0.3713	–0.0778	0.3687	0.048
H(12)	0.2890	–0.2758	0.3474	0.050
H(13)	0.2612	–0.3541	0.2199	0.049
H(14)	0.3148	–0.2276	0.1152	0.040

Table 6. Torsion angles [°] for mjh78.

C(1)–N–C(2)–C(3)	179.4(2)	C(5)–N–C(2)–C(3)	–0.4(3)
N–C(2)–C(3)–C(4)	0.3(3)	C(2)–C(3)–C(4)–C(5)	0.0(3)
C(3)–C(4)–C(5)–N	–0.2(3)	C(3)–C(4)–C(5)–C(6)	–175.4(3)
C(1)–N–C(5)–C(4)	–179.5(2)	C(1)–N–C(5)–C(6)	–3.7(4)
C(2)–N–C(5)–C(4)	0.4(3)	C(2)–N–C(5)–C(6)	176.1(2)
N–C(5)–C(6)–O(1)	–3.3(4)	N–C(5)–C(6)–C(7)	–179.2(2)
C(4)–C(5)–C(6)–O(1)	171.3(3)	C(4)–C(5)–C(6)–C(7)	–4.6(4)
O(1)–C(6)–C(7)–Cl(1)	134.5(2)	O(1)–C(6)–C(7)–Cl(2)	–107.1(2)
O(1)–C(6)–C(7)–C(8)	10.9(3)	C(5)–C(6)–C(7)–Cl(1)	–49.3(3)
C(5)–C(6)–C(7)–Cl(2)	69.1(2)	C(5)–C(6)–C(7)–C(8)	–173.0(2)
Cl(1)–C(7)–C(8)–O(2)	–65.58(19)	Cl(1)–C(7)–C(8)–C(9)	56.0(2)
Cl(2)–C(7)–C(8)–O(2)	174.74(14)	Cl(2)–C(7)–C(8)–C(9)	–63.7(2)
C(6)–C(7)–C(8)–O(2)	59.2(2)	C(6)–C(7)–C(8)–C(9)	–179.21(18)
O(2)–C(8)–C(9)–C(10)	25.1(3)	O(2)–C(8)–C(9)–C(14)	–153.8(2)
C(7)–C(8)–C(9)–C(10)	–95.3(2)	C(7)–C(8)–C(9)–C(14)	85.9(3)
C(8)–C(9)–C(10)–C(11)	–180.0(2)	C(14)–C(9)–C(10)–C(11)	–1.1(3)
C(9)–C(10)–C(11)–C(12)	0.6(4)	C(10)–C(11)–C(12)–C(13)	0.4(4)
C(11)–C(12)–C(13)–C(14)	–0.8(4)	C(12)–C(13)–C(14)–C(9)	0.3(4)
C(8)–C(9)–C(14)–C(13)	179.5(2)	C(10)–C(9)–C(14)–C(13)	0.6(3)

Table 7. Hydrogen bonds for mjh78 [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
O(2)–H(2)...O(1A)	0.82(4)	2.17(3)	2.895(2)	147(3)
O(2)–H(2)...O(1)	0.82(4)	2.30(4)	2.747(3)	115(3)

Symmetry operations for equivalent atoms
A −x+1,−y,−z

2,2-Dichloro-3-hydroxy-3-(4-methoxyphenyl)-1-(1-methyl-1*H*-pyrrol-2-yl)propan-1-one (3b)

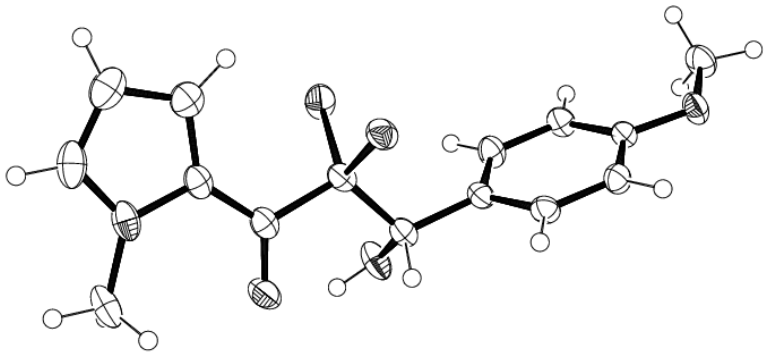


Table 1. Crystal data and structure refinement for mjh76.

Identification code	mjh76	
Chemical formula (moiety)	$C_{15}H_{15}Cl_2NO_3$	
Chemical formula (total)	$C_{15}H_{15}Cl_2NO_3$	
Formula weight	328.18	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, $P12_1/n1$	
Unit cell parameters	a = 8.9648(6) Å	α = 90°
	b = 12.0920(7) Å	β = 106.344(8)°
	c = 14.0270(11) Å	γ = 90°
Cell volume	1459.11(17) $Å^3$	
Z	4	
Calculated density	1.494 g/cm^3	
Absorption coefficient μ	0.454 mm^{-1}	
F(000)	680	
Crystal colour and size	colourless, 0.40 × 0.30 × 0.30 mm^3	
Reflections for cell refinement	3062 (θ range 2.9 to 28.4°)	
Data collection method	Xcalibur, Atlas, Gemini ultra	
	thick-slice ω scans	
θ range for data collection	2.9 to 28.4°	
Index ranges	h −11 to 10, k −15 to 13, l −18 to 18	
Completeness to θ = 25.0°	99.9 %	
Reflections collected	9278	
Independent reflections	3145 (R_{int} = 0.0284)	
Reflections with $F^2>2\sigma$	2539	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.8394 and 0.8759	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0342, 0.6168	
Data / restraints / parameters	3145 / 0 / 196	
Final R indices [$F^2>2\sigma$]	R1 = 0.0369, wR2 = 0.0784	
R indices (all data)	R1 = 0.0509, wR2 = 0.0868	
Goodness-of-fit on F^2	1.041	
Largest and mean shift/su	0.000 and 0.000	
Largest diff. peak and hole	0.32 and −0.21 e $Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for mjh76. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cl(2)	0.04358(5)	0.17039(4)	0.09179(3)	0.02894(13)
O(4)	0.68450(14)	0.04804(10)	0.40294(10)	0.0291(3)
Cl(1)	−0.05052(6)	−0.04115(4)	0.15533(4)	0.03477(15)
C(7)	−0.0514(2)	0.10504(14)	0.17291(14)	0.0240(4)
O(1)	−0.26157(15)	0.19557(12)	0.21180(10)	0.0338(3)
O(2)	−0.02943(17)	0.08008(13)	0.34767(11)	0.0364(4)
C(11)	0.4199(2)	−0.02164(15)	0.36889(14)	0.0260(4)
N	−0.47373(18)	0.17147(13)	0.01733(12)	0.0309(4)
C(14)	0.3175(2)	0.19123(15)	0.31509(14)	0.0254(4)
C(12)	0.5268(2)	0.06214(15)	0.37217(13)	0.0230(4)
C(6)	−0.2227(2)	0.14796(15)	0.14549(14)	0.0254(4)
C(9)	0.2086(2)	0.10787(15)	0.31024(13)	0.0235(4)
C(10)	0.2625(2)	0.00213(16)	0.33824(14)	0.0277(4)
C(15)	0.7405(2)	−0.06237(16)	0.42445(16)	0.0336(5)
C(8)	0.0376(2)	0.13513(16)	0.28105(14)	0.0253(4)
C(13)	0.4749(2)	0.16867(15)	0.34557(14)	0.0267(4)
C(4)	−0.2981(2)	0.07495(16)	−0.03360(15)	0.0325(5)
C(3)	−0.4345(3)	0.07963(18)	−0.11077(16)	0.0391(5)
C(5)	−0.3217(2)	0.13179(15)	0.04724(14)	0.0267(4)
C(1)	−0.5563(2)	0.23437(19)	0.07529(17)	0.0400(5)
C(2)	−0.5389(2)	0.13963(18)	−0.07703(16)	0.0384(5)

Table 3. Bond lengths [Å] and angles [°] for mjh76.

Cl(2)–C(7)	1.7856(18)	O(4)–C(12)	1.368(2)
O(4)–C(15)	1.428(2)	Cl(1)–C(7)	1.7852(18)
C(7)–C(6)	1.564(2)	C(7)–C(8)	1.545(3)
O(1)–C(6)	1.225(2)	O(2)–C(8)	1.412(2)
O(2)–H(2)	0.85(3)	C(11)–H(11A)	0.950
C(11)–C(12)	1.387(2)	C(11)–C(10)	1.385(3)
N–C(5)	1.393(2)	N–C(1)	1.458(3)
N–C(2)	1.344(3)	C(14)–H(14A)	0.950
C(14)–C(9)	1.392(3)	C(14)–C(13)	1.381(3)
C(12)–C(13)	1.385(2)	C(6)–C(5)	1.427(3)
C(9)–C(10)	1.384(3)	C(9)–C(8)	1.508(2)
C(10)–H(10A)	0.950	C(15)–H(15A)	0.980
C(15)–H(15B)	0.980	C(15)–H(15C)	0.980
C(8)–H(8A)	1.000	C(13)–H(13A)	0.950
C(4)–H(4A)	0.950	C(4)–C(3)	1.388(3)
C(4)–C(5)	1.392(3)	C(3)–H(3A)	0.950
C(3)–C(2)	1.369(3)	C(1)–H(1A)	0.980
C(1)–H(1B)	0.980	C(1)–H(1C)	0.980
C(2)–H(2A)	0.950		

C(12)–O(4)–C(15)	117.00(14)	Cl(2)–C(7)–Cl(1)	109.20(10)
Cl(2)–C(7)–C(6)	107.93(12)	Cl(2)–C(7)–C(8)	108.34(12)
Cl(1)–C(7)–C(6)	109.68(12)	Cl(1)–C(7)–C(8)	110.34(12)
C(6)–C(7)–C(8)	111.29(15)	C(8)–O(2)–H(2)	108.6(18)
H(11A)–C(11)–C(12)	120.2	H(11A)–C(11)–C(10)	120.2
C(12)–C(11)–C(10)	119.56(17)	C(5)–N–C(1)	128.22(17)
C(5)–N–C(2)	108.37(17)	C(1)–N–C(2)	123.39(17)
H(14A)–C(14)–C(9)	119.6	H(14A)–C(14)–C(13)	119.6
C(9)–C(14)–C(13)	120.89(16)	O(4)–C(12)–C(11)	124.26(16)
O(4)–C(12)–C(13)	116.12(16)	C(11)–C(12)–C(13)	119.59(16)
C(7)–C(6)–O(1)	116.03(16)	C(7)–C(6)–C(5)	119.55(16)
O(1)–C(6)–C(5)	124.41(17)	C(14)–C(9)–C(10)	118.14(16)
C(14)–C(9)–C(8)	120.05(16)	C(10)–C(9)–C(8)	121.71(16)
C(11)–C(10)–C(9)	121.56(17)	C(11)–C(10)–H(10A)	119.2
C(9)–C(10)–H(10A)	119.2	O(4)–C(15)–H(15A)	109.5
O(4)–C(15)–H(15B)	109.5	O(4)–C(15)–H(15C)	109.5
H(15A)–C(15)–H(15B)	109.5	H(15A)–C(15)–H(15C)	109.5
H(15B)–C(15)–H(15C)	109.5	C(7)–C(8)–O(2)	109.92(15)
C(7)–C(8)–C(9)	114.79(15)	C(7)–C(8)–H(8A)	108.0
O(2)–C(8)–C(9)	107.86(15)	O(2)–C(8)–H(8A)	108.0
C(9)–C(8)–H(8A)	108.0	C(14)–C(13)–C(12)	120.25(17)
C(14)–C(13)–H(13A)	119.9	C(12)–C(13)–H(13A)	119.9
H(4A)–C(4)–C(3)	125.9	H(4A)–C(4)–C(5)	125.9
C(3)–C(4)–C(5)	108.21(19)	C(4)–C(3)–H(3A)	126.6
C(4)–C(3)–C(2)	106.85(19)	H(3A)–C(3)–C(2)	126.6
N–C(5)–C(6)	122.24(17)	N–C(5)–C(4)	106.55(17)
C(6)–C(5)–C(4)	131.17(18)	N–C(1)–H(1A)	109.5
N–C(1)–H(1B)	109.5	N–C(1)–H(1C)	109.5
H(1A)–C(1)–H(1B)	109.5	H(1A)–C(1)–H(1C)	109.5
H(1B)–C(1)–H(1C)	109.5	N–C(2)–C(3)	110.03(18)
N–C(2)–H(2A)	125.0	C(3)–C(2)–H(2A)	125.0

Table 4. Anisotropic displacement parameters ($Å^2$) for mjh76. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(2)	0.0271(2)	0.0297(3)	0.0338(3)	–0.0009(2)	0.0146(2)	–0.00252(19)
O(4)	0.0194(6)	0.0265(7)	0.0413(8)	0.0020(6)	0.0081(6)	0.0023(5)
Cl(1)	0.0291(3)	0.0181(2)	0.0528(3)	–0.0019(2)	0.0045(2)	0.00063(18)
C(7)	0.0232(9)	0.0165(8)	0.0354(10)	0.0019(8)	0.0131(8)	–0.0008(7)
O(1)	0.0278(7)	0.0401(8)	0.0355(7)	–0.0001(6)	0.0122(6)	0.0090(6)
O(2)	0.0231(7)	0.0507(9)	0.0387(8)	0.0132(7)	0.0139(6)	0.0052(7)
C(11)	0.0253(9)	0.0206(9)	0.0327(10)	0.0048(8)	0.0091(8)	0.0026(7)
N	0.0208(8)	0.0349(9)	0.0373(9)	0.0109(8)	0.0084(7)	–0.0020(7)
C(14)	0.0261(9)	0.0192(9)	0.0321(10)	–0.0003(8)	0.0100(8)	0.0020(7)
C(12)	0.0200(9)	0.0259(9)	0.0242(9)	–0.0009(8)	0.0080(7)	0.0008(7)
C(6)	0.0227(9)	0.0221(9)	0.0332(10)	0.0048(8)	0.0107(8)	–0.0003(7)
C(9)	0.0210(9)	0.0261(9)	0.0252(9)	–0.0003(8)	0.0094(8)	0.0013(7)
C(10)	0.0240(9)	0.0244(9)	0.0358(10)	0.0043(8)	0.0103(8)	–0.0021(8)
C(15)	0.0264(10)	0.0306(10)	0.0428(11)	0.0035(9)	0.0080(9)	0.0084(8)
C(8)	0.0217(9)	0.0254(9)	0.0310(10)	0.0022(8)	0.0108(8)	0.0016(7)
C(13)	0.0238(9)	0.0219(9)	0.0353(10)	–0.0012(8)	0.0096(8)	–0.0038(7)
C(4)	0.0334(11)	0.0273(10)	0.0376(11)	0.0016(9)	0.0111(9)	–0.0042(8)
C(3)	0.0440(13)	0.0375(12)	0.0333(11)	0.0029(9)	0.0070(10)	–0.0124(10)
C(5)	0.0221(9)	0.0231(9)	0.0360(10)	0.0053(8)	0.0100(8)	–0.0021(7)
C(1)	0.0205(10)	0.0520(13)	0.0492(13)	0.0104(11)	0.0124(9)	0.0068(9)
C(2)	0.0272(11)	0.0447(12)	0.0387(12)	0.0137(10)	0.0020(9)	–0.0095(9)

Table 5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for mjh76.

	x	y	z	U
H(11A)	0.4544	–0.0949	0.3875	0.031
H(14A)	0.2832	0.2647	0.2972	0.030
H(10A)	0.1897	–0.0555	0.3364	0.033
H(15A)	0.8541	–0.0614	0.4499	0.050
H(15B)	0.7097	–0.1069	0.3637	0.050
H(15C)	0.6961	–0.0946	0.4745	0.050
H(8A)	0.0266	0.2165	0.2897	0.030
H(13A)	0.5478	0.2264	0.3483	0.032
H(4A)	–0.2047	0.0391	–0.0356	0.039
H(3A)	–0.4522	0.0474	–0.1748	0.047
H(1A)	–0.6562	0.2596	0.0318	0.060
H(1B)	–0.4938	0.2985	0.1053	0.060
H(1C)	–0.5745	0.1872	0.1278	0.060
H(2A)	–0.6422	0.1563	–0.1148	0.046
H(2)	–0.122(3)	0.103(2)	0.3381(19)	0.056(8)

Table 6. Torsion angles [°] for mjh76.

C(15)–O(4)–C(12)–C(11)	5.7(3)	C(15)–O(4)–C(12)–C(13)	–175.98(17)
C(10)–C(11)–C(12)–O(4)	178.77(17)	C(10)–C(11)–C(12)–C(13)	0.5(3)
Cl(2)–C(7)–C(6)–O(1)	–120.13(16)	Cl(2)–C(7)–C(6)–C(5)	58.86(19)
Cl(1)–C(7)–C(6)–O(1)	120.99(16)	Cl(1)–C(7)–C(6)–C(5)	–60.01(19)
C(8)–C(7)–C(6)–O(1)	–1.4(2)	C(8)–C(7)–C(6)–C(5)	177.61(15)
C(13)–C(14)–C(9)–C(10)	1.0(3)	C(13)–C(14)–C(9)–C(8)	177.34(17)
C(14)–C(9)–C(10)–C(11)	–1.0(3)	C(8)–C(9)–C(10)–C(11)	–177.32(17)
C(12)–C(11)–C(10)–C(9)	0.3(3)	C(14)–C(9)–C(8)–C(7)	102.5(2)
C(14)–C(9)–C(8)–O(2)	–134.64(17)	C(10)–C(9)–C(8)–C(7)	–81.3(2)
C(10)–C(9)–C(8)–O(2)	41.6(2)	Cl(2)–C(7)–C(8)–O(2)	–176.91(12)
Cl(2)–C(7)–C(8)–C(9)	–55.12(18)	Cl(1)–C(7)–C(8)–O(2)	–57.41(17)
Cl(1)–C(7)–C(8)–C(9)	64.38(17)	C(6)–C(7)–C(8)–O(2)	64.58(19)
C(6)–C(7)–C(8)–C(9)	–173.63(14)	C(9)–C(14)–C(13)–C(12)	–0.2(3)
O(4)–C(12)–C(13)–C(14)	–178.94(16)	C(11)–C(12)–C(13)–C(14)	–0.6(3)
C(5)–C(4)–C(3)–C(2)	0.6(2)	C(3)–C(4)–C(5)–N	–0.5(2)
C(3)–C(4)–C(5)–C(6)	176.98(19)	C(1)–N–C(5)–C(6)	0.9(3)
C(1)–N–C(5)–C(4)	178.64(18)	C(2)–N–C(5)–C(6)	–177.50(17)
C(2)–N–C(5)–C(4)	0.3(2)	C(7)–C(6)–C(5)–N	–177.72(16)
C(7)–C(6)–C(5)–C(4)	5.1(3)	O(1)–C(6)–C(5)–N	1.2(3)
O(1)–C(6)–C(5)–C(4)	–175.96(19)	C(5)–N–C(2)–C(3)	0.1(2)
C(1)–N–C(2)–C(3)	–178.39(18)	C(4)–C(3)–C(2)–N	–0.4(2)

Table 7. Hydrogen bonds for mjh76 [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
O(2)–H(2)...O(1)	0.85(3)	2.17(3)	2.772(2)	128(2)
O(2)–H(2)...O(4A)	0.85(3)	2.28(3)	2.9064(19)	131(2)

Symmetry operations for equivalent atoms
A x−1,y,z

2,2-Dichloro-3-hydroxy-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(4-nitrophenyl) propan-1-one (3f)

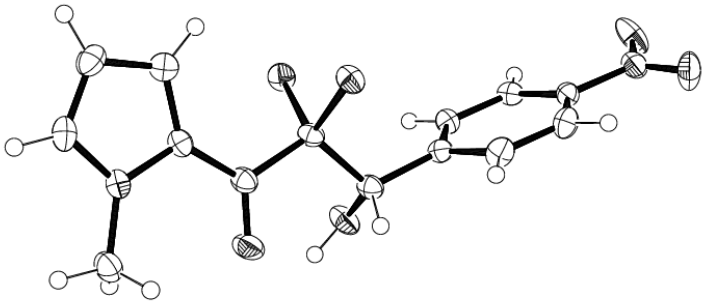


Table 1. Crystal data and structure refinement for mjh75.

Identification code	mjh75	
Chemical formula (moiety)	$C_{14}H_{12}Cl_2N_2O_4$	
Chemical formula (total)	$C_{14}H_{12}Cl_2N_2O_4$	
Formula weight	343.16	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, $P12_1/c1$	
Unit cell parameters	a = 8.4490(5) Å	α = 90°
	b = 21.9722(12) Å	β = 112.479(7)°
	c = 8.5158(6) Å	γ = 90°
Cell volume	1460.78(16) $Å^3$	
Z	4	
Calculated density	1.560 g/cm^3	
Absorption coefficient μ	0.464 mm^{-1}	
F(000)	704	
Reflections for cell refinement	3678 (θ range 3.0 to 28.5°)	
Data collection method	Xcalibur, Atlas, Gemini ultra thick-slice ω scans	
θ range for data collection	3.0 to 28.6°	
Index ranges	h −11 to 11, k −26 to 23, l −11 to 10	
Completeness to θ = 25.0°	98.3 %	
Reflections collected	9235	
Independent reflections	3125 (R_{int} = 0.0288)	
Reflections with $F^2>2\sigma$	2589	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.98895 and 1.00000	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0233, 0.7057	
Data / restraints / parameters	3125 / 0 / 205	
Final R indices [$F^2>2\sigma$]	R1 = 0.0335, wR2 = 0.0681	
R indices (all data)	R1 = 0.0467, wR2 = 0.0753	
Goodness-of-fit on F^2	1.067	
Extinction coefficient	0.0018(7)	
Largest and mean shift/su	0.001 and 0.000	
Largest diff. peak and hole	0.31 and −0.24 e $Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for mjh75. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cl(1)	0.12458(5)	0.38070(2)	0.49321(5)	0.02499(13)
Cl(2)	0.02398(5)	0.46383(2)	0.70320(6)	0.02658(13)
N(1)	0.60443(17)	0.43446(7)	0.93114(19)	0.0223(3)
N(2)	−0.64083(19)	0.28722(8)	0.2368(2)	0.0283(4)
O(1)	0.34572(15)	0.35509(7)	0.94600(18)	0.0377(4)
O(2)	−0.00284(16)	0.35250(7)	0.89104(17)	0.0319(3)
O(3)	−0.75967(15)	0.32090(7)	0.22784(17)	0.0395(4)
O(4)	−0.65717(18)	0.24318(7)	0.1451(2)	0.0431(4)
C(1)	0.6877(2)	0.39261(9)	1.0719(3)	0.0302(5)
C(2)	0.6880(2)	0.47930(9)	0.8871(2)	0.0275(4)
C(3)	0.5774(2)	0.50956(9)	0.7476(2)	0.0294(4)
C(4)	0.4180(2)	0.48215(8)	0.7032(2)	0.0266(4)
C(5)	0.4343(2)	0.43518(8)	0.8173(2)	0.0218(4)
C(6)	0.3114(2)	0.39267(8)	0.8331(2)	0.0238(4)
C(7)	0.1232(2)	0.39235(8)	0.6998(2)	0.0212(4)
C(8)	0.0217(2)	0.33990(8)	0.7396(2)	0.0230(4)
C(9)	−0.1520(2)	0.32816(8)	0.6021(2)	0.0208(4)
C(10)	−0.1721(2)	0.28208(8)	0.4850(2)	0.0277(4)
C(11)	−0.3321(2)	0.26844(8)	0.3632(3)	0.0279(4)
C(12)	−0.4702(2)	0.30159(8)	0.3637(2)	0.0221(4)
C(13)	−0.4550(2)	0.34719(8)	0.4790(2)	0.0221(4)
C(14)	−0.2944(2)	0.36049(8)	0.5989(2)	0.0217(4)

Table 3. Bond lengths [Å] and angles [°] for mjh75.

Cl(1)–C(7)	1.7824(18)	Cl(2)–C(7)	1.7859(18)
N(1)–C(1)	1.460(2)	N(1)–C(2)	1.346(2)
N(1)–C(5)	1.393(2)	N(2)–O(3)	1.226(2)
N(2)–O(4)	1.218(2)	N(2)–C(12)	1.468(2)
O(1)–C(6)	1.215(2)	O(2)–H(2)	0.88(3)
O(2)–C(8)	1.409(2)	C(1)–H(1A)	0.980
C(1)–H(1B)	0.980	C(1)–H(1C)	0.980
C(2)–H(2A)	0.950	C(2)–C(3)	1.370(3)
C(3)–H(3A)	0.950	C(3)–C(4)	1.389(2)
C(4)–H(4A)	0.950	C(4)–C(5)	1.387(3)
C(5)–C(6)	1.441(2)	C(6)–C(7)	1.560(2)
C(7)–C(8)	1.550(2)	C(8)–H(8A)	1.000
C(8)–C(9)	1.509(2)	C(9)–C(10)	1.385(3)
C(9)–C(14)	1.388(2)	C(10)–H(10A)	0.950
C(10)–C(11)	1.386(2)	C(11)–H(11A)	0.950
C(11)–C(12)	1.377(2)	C(12)–C(13)	1.374(3)
C(13)–H(13A)	0.950	C(13)–C(14)	1.382(2)
C(14)–H(14A)	0.950		

C(1)–N(1)–C(2)	123.39(14)	C(1)–N(1)–C(5)	128.57(15)
C(2)–N(1)–C(5)	108.01(15)	O(3)–N(2)–O(4)	123.40(16)
O(3)–N(2)–C(12)	117.77(16)	O(4)–N(2)–C(12)	118.82(16)
H(2)–O(2)–C(8)	110.2(17)	N(1)–C(1)–H(1A)	109.5
N(1)–C(1)–H(1B)	109.5	N(1)–C(1)–H(1C)	109.5
H(1A)–C(1)–H(1B)	109.5	H(1A)–C(1)–H(1C)	109.5
H(1B)–C(1)–H(1C)	109.5	N(1)–C(2)–H(2A)	125.0
N(1)–C(2)–C(3)	109.91(15)	H(2A)–C(2)–C(3)	125.0
C(2)–C(3)–H(3A)	126.5	C(2)–C(3)–C(4)	107.09(17)
H(3A)–C(3)–C(4)	126.5	C(3)–C(4)–H(4A)	126.1
C(3)–C(4)–C(5)	107.81(16)	H(4A)–C(4)–C(5)	126.1
N(1)–C(5)–C(4)	107.17(15)	N(1)–C(5)–C(6)	121.09(16)
C(4)–C(5)–C(6)	131.73(16)	O(1)–C(6)–C(5)	123.48(16)
O(1)–C(6)–C(7)	116.17(15)	C(5)–C(6)–C(7)	120.34(15)
Cl(1)–C(7)–Cl(2)	108.81(9)	Cl(1)–C(7)–C(6)	109.24(12)
Cl(1)–C(7)–C(8)	108.80(12)	Cl(2)–C(7)–C(6)	109.77(12)
Cl(2)–C(7)–C(8)	110.36(12)	C(6)–C(7)–C(8)	109.84(14)
O(2)–C(8)–C(7)	109.96(15)	O(2)–C(8)–H(8A)	108.2
O(2)–C(8)–C(9)	107.69(14)	C(7)–C(8)–H(8A)	108.2
C(7)–C(8)–C(9)	114.38(15)	H(8A)–C(8)–C(9)	108.2
C(8)–C(9)–C(10)	119.90(15)	C(8)–C(9)–C(14)	120.39(16)
C(10)–C(9)–C(14)	119.57(15)	C(9)–C(10)–H(10A)	119.6
C(9)–C(10)–C(11)	120.83(16)	H(10A)–C(10)–C(11)	119.6
C(10)–C(11)–H(11A)	121.0	C(10)–C(11)–C(12)	117.95(17)
H(11A)–C(11)–C(12)	121.0	N(2)–C(12)–C(11)	118.59(16)
N(2)–C(12)–C(13)	118.72(16)	C(11)–C(12)–C(13)	122.69(16)
C(12)–C(13)–H(13A)	120.7	C(12)–C(13)–C(14)	118.64(16)
H(13A)–C(13)–C(14)	120.7	C(9)–C(14)–C(13)	120.32(17)
C(9)–C(14)–H(14A)	119.8	C(13)–C(14)–H(14A)	119.8

Table 4. Anisotropic displacement parameters ($Å^2$) for mjh75. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	0.0217(2)	0.0332(3)	0.0209(2)	–0.00057(18)	0.00909(17)	0.00017(17)
Cl(2)	0.0231(2)	0.0264(3)	0.0297(3)	–0.00104(18)	0.00946(18)	0.00372(17)
N(1)	0.0196(7)	0.0255(8)	0.0215(8)	–0.0040(6)	0.0075(6)	–0.0018(6)
N(2)	0.0245(8)	0.0381(10)	0.0214(8)	0.0020(7)	0.0079(7)	–0.0083(7)
O(1)	0.0215(6)	0.0504(9)	0.0336(8)	0.0195(7)	0.0020(6)	–0.0051(6)
O(2)	0.0204(6)	0.0524(9)	0.0215(7)	0.0050(6)	0.0065(6)	–0.0021(6)
O(3)	0.0201(6)	0.0709(11)	0.0235(8)	–0.0067(7)	0.0037(6)	0.0057(7)
O(4)	0.0399(8)	0.0380(9)	0.0439(9)	–0.0153(7)	0.0075(7)	–0.0144(7)
C(1)	0.0220(9)	0.0355(11)	0.0288(11)	0.0008(8)	0.0048(8)	–0.0001(8)
C(2)	0.0234(9)	0.0313(11)	0.0295(10)	–0.0087(8)	0.0120(8)	–0.0076(8)
C(3)	0.0341(10)	0.0271(11)	0.0318(11)	–0.0016(8)	0.0179(9)	–0.0058(8)
C(4)	0.0266(9)	0.0268(10)	0.0272(10)	0.0000(8)	0.0113(8)	0.0017(7)
C(5)	0.0185(8)	0.0262(10)	0.0205(9)	–0.0023(7)	0.0075(7)	0.0005(7)
C(6)	0.0190(8)	0.0291(10)	0.0225(10)	0.0021(8)	0.0072(7)	0.0013(7)
C(7)	0.0186(8)	0.0257(10)	0.0195(9)	0.0027(7)	0.0076(7)	0.0031(7)
C(8)	0.0174(8)	0.0278(10)	0.0234(10)	0.0036(7)	0.0073(7)	0.0018(7)
C(9)	0.0180(8)	0.0215(9)	0.0237(9)	0.0033(7)	0.0088(7)	0.0008(7)
C(10)	0.0223(9)	0.0242(10)	0.0385(12)	–0.0013(8)	0.0137(8)	0.0029(7)
C(11)	0.0300(9)	0.0239(10)	0.0323(11)	–0.0068(8)	0.0149(8)	–0.0037(8)
C(12)	0.0202(8)	0.0254(10)	0.0201(9)	0.0015(7)	0.0068(7)	–0.0052(7)
C(13)	0.0184(8)	0.0265(10)	0.0234(9)	0.0038(7)	0.0101(7)	0.0024(7)
C(14)	0.0212(8)	0.0242(10)	0.0203(9)	–0.0014(7)	0.0087(7)	0.0004(7)

Table 5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for mjh75.

	x	y	z	U
H(2)	0.092(3)	0.3453(11)	0.980(3)	0.054(7)
H(1A)	0.8104	0.4019	1.1237	0.045
H(1B)	0.6717	0.3507	1.0294	0.045
H(1C)	0.6368	0.3972	1.1572	0.045
H(2A)	0.8060	0.4886	0.9442	0.033
H(3A)	0.6046	0.5430	0.6917	0.035
H(4A)	0.3161	0.4935	0.6112	0.032
H(8A)	0.0911	0.3018	0.7570	0.028
H(10A)	−0.0749	0.2596	0.4881	0.033
H(11A)	−0.3460	0.2372	0.2819	0.033
H(13A)	−0.5529	0.3691	0.4763	0.027
H(14A)	−0.2814	0.3919	0.6796	0.026

Table 6. Torsion angles [°] for mjh75.

C(1)–N(1)–C(2)–C(3)	178.11(17)	C(5)–N(1)–C(2)–C(3)	0.1(2)
N(1)–C(2)–C(3)–C(4)	0.0(2)	C(2)–C(3)–C(4)–C(5)	−0.1(2)
C(3)–C(4)–C(5)–N(1)	0.2(2)	C(3)–C(4)–C(5)–C(6)	178.97(19)
C(1)–N(1)–C(5)–C(4)	−178.03(17)	C(1)–N(1)–C(5)–C(6)	3.0(3)
C(2)–N(1)–C(5)–C(4)	−0.2(2)	C(2)–N(1)–C(5)–C(6)	−179.13(16)
N(1)–C(5)–C(6)–O(1)	1.6(3)	N(1)–C(5)–C(6)–C(7)	−177.39(15)
C(4)–C(5)–C(6)–O(1)	−177.1(2)	C(4)–C(5)–C(6)–C(7)	4.0(3)
O(1)–C(6)–C(7)–Cl(1)	−121.94(17)	O(1)–C(6)–C(7)–Cl(2)	118.83(17)
O(1)–C(6)–C(7)–C(8)	−2.7(2)	C(5)–C(6)–C(7)–Cl(1)	57.1(2)
C(5)–C(6)–C(7)–Cl(2)	−62.13(19)	C(5)–C(6)–C(7)–C(8)	176.35(16)
Cl(1)–C(7)–C(8)–O(2)	−171.48(11)	Cl(1)–C(7)–C(8)–C(9)	−50.18(18)
Cl(2)–C(7)–C(8)–O(2)	−52.17(16)	Cl(2)–C(7)–C(8)–C(9)	69.13(18)
C(6)–C(7)–C(8)–O(2)	69.00(18)	C(6)–C(7)–C(8)–C(9)	−169.70(14)
O(2)–C(8)–C(9)–C(10)	−139.77(17)	O(2)–C(8)–C(9)–C(14)	35.9(2)
C(7)–C(8)–C(9)–C(10)	97.7(2)	C(7)–C(8)–C(9)–C(14)	−86.7(2)
C(8)–C(9)–C(10)–C(11)	176.59(17)	C(14)–C(9)–C(10)–C(11)	0.9(3)
C(9)–C(10)–C(11)–C(12)	−0.7(3)	C(10)–C(11)–C(12)–N(2)	−179.32(16)
C(10)–C(11)–C(12)–C(13)	0.2(3)	O(3)–N(2)–C(12)–C(11)	−172.91(17)
O(3)–N(2)–C(12)–C(13)	7.6(2)	O(4)–N(2)–C(12)–C(11)	6.4(3)
O(4)–N(2)–C(12)–C(13)	−173.10(17)	N(2)–C(12)–C(13)–C(14)	179.73(15)
C(11)–C(12)–C(13)–C(14)	0.2(3)	C(12)–C(13)–C(14)–C(9)	−0.1(3)
C(8)–C(9)–C(14)–C(13)	−176.15(16)	C(10)–C(9)–C(14)–C(13)	−0.5(3)

Table 7. Hydrogen bonds for mjh75 [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
O(2)–H(2)...O(3A)	0.88(3)	2.07(3)	2.9023(19)	157(2)
O(2)–H(2)...O(1)	0.88(3)	2.28(2)	2.8002(18)	118(2)

Symmetry operations for equivalent atoms
A x+1,y,z+1

2,2-Dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(4-nitrophenyl)propan-1-one (3g)

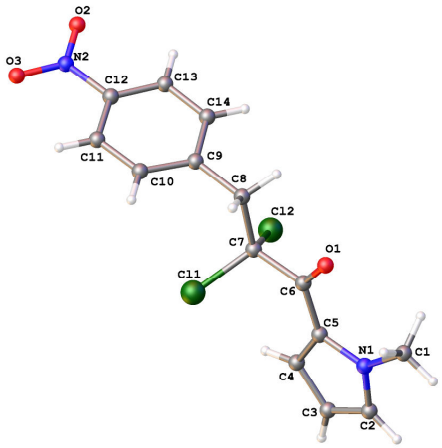


Table 1. Crystal data and structure refinement for **3g** - 2,2-dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(4-nitrophenyl)propan-1-one (mjh79).

Identification code	mjh79	
Chemical formula (moiety)	$C_{14}H_{12}Cl_2N_2O_3$	
Chemical formula (total)	$C_{14}H_{12}Cl_2N_2O_3$	
Formula weight	327.16	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, $P\bar{1}$	
Unit cell parameters	a = 8.8490(11) Å	α = 88.060(6)°
	b = 8.8572(6) Å	β = 72.636(10)°
	c = 9.6786(9) Å	γ = 80.267(8)°
Cell volume	713.48(12) $Å^3$	
Z	2	
Calculated density	1.523 g/cm^3	
Absorption coefficient μ	0.466 mm^{-1}	
F(000)	336	
Crystal colour and size	colourless, 0.30 × 0.30 × 0.10 mm^3	
Reflections for cell refinement	2302 (θ range 3.1 to 28.7°)	
Data collection method	Xcalibur, Atlas, Gemini ultra	
	thick-slice ω scans	
θ range for data collection	3.1 to 28.7°	
Index ranges	h −9 to 10, k −11 to 10, l −10 to 12	
Completeness to θ = 25.0°	99.8 %	
Reflections collected	5166	
Independent reflections	2967 (R_{int} = 0.0211)	
Reflections with $F^2>2\sigma$	2526	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.8729 and 0.9549	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0249, 0.3136	
Data / restraints / parameters	2967 / 0 / 210	
Final R indices [$F^2>2\sigma$]	R1 = 0.0331, wR2 = 0.0711	
R indices (all data)	R1 = 0.0422, wR2 = 0.0768	
Goodness-of-fit on F^2	1.055	
Largest and mean shift/su	0.001 and 0.000	
Largest diff. peak and hole	0.34 and −0.29 e $Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for mjh79. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cl(1)	−0.05490(5)	0.28680(5)	0.99107(5)	0.02487(12)
Cl(2)	0.18045(5)	0.07567(4)	0.77599(5)	0.02435(12)
N(1)	0.40970(17)	0.19442(16)	1.10096(15)	0.0206(3)
N(2)	−0.3412(2)	0.29794(19)	0.45195(18)	0.0327(4)
O(1)	0.34112(16)	0.39016(14)	0.87719(14)	0.0294(3)
O(2)	−0.297(2)	0.239(2)	0.340(3)	0.056(4)
O(3)	−0.4839(8)	0.358(4)	0.5092(14)	0.057(4)
O(2A)	−0.2938(12)	0.2536(15)	0.3226(13)	0.035(2)
O(3A)	−0.4757(18)	0.283(4)	0.5301(13)	0.051(4)
C(1)	0.5315(2)	0.2937(2)	1.0627(2)	0.0287(4)
C(2)	0.4025(2)	0.0883(2)	1.20500(19)	0.0270(4)
C(3)	0.2797(2)	0.0092(2)	1.2112(2)	0.0289(4)
C(4)	0.2095(2)	0.06849(19)	1.10611(19)	0.0245(4)
C(5)	0.2905(2)	0.18525(18)	1.03724(18)	0.0194(3)
C(6)	0.2659(2)	0.28678(18)	0.92238(18)	0.0193(4)
C(7)	0.1339(2)	0.26537(18)	0.85226(18)	0.0191(3)
C(8)	0.1240(2)	0.38215(19)	0.73397(19)	0.0218(4)
C(9)	0.0013(2)	0.36383(18)	0.65867(18)	0.0204(4)
C(10)	−0.1588(2)	0.4327(2)	0.71373(19)	0.0252(4)
C(11)	−0.2725(2)	0.4114(2)	0.64752(19)	0.0272(4)
C(12)	−0.2221(2)	0.3236(2)	0.52235(19)	0.0236(4)
C(13)	−0.0645(2)	0.2571(2)	0.46146(19)	0.0253(4)
C(14)	0.0467(2)	0.2772(2)	0.53085(19)	0.0250(4)

Table 3. Bond lengths [Å] and angles [°] for mjh79.

Cl(1)–C(7)	1.7893(17)	Cl(2)–C(7)	1.7906(16)
N(1)–C(1)	1.460(2)	N(1)–C(2)	1.349(2)
N(1)–C(5)	1.386(2)	N(2)–O(2)	1.149(18)
N(2)–O(3)	1.249(8)	N(2)–O(2A)	1.249(11)
N(2)–O(3A)	1.231(9)	N(2)–C(12)	1.465(2)
O(1)–C(6)	1.216(2)	C(1)–H(1A)	0.980
C(1)–H(1B)	0.980	C(1)–H(1C)	0.980
C(2)–H(2A)	0.950	C(2)–C(3)	1.375(3)
C(3)–H(3A)	0.950	C(3)–C(4)	1.388(3)
C(4)–H(4A)	0.950	C(4)–C(5)	1.395(2)
C(5)–C(6)	1.450(2)	C(6)–C(7)	1.555(2)
C(7)–C(8)	1.529(2)	C(8)–H(8A)	0.990
C(8)–H(8B)	0.990	C(8)–C(9)	1.509(2)
C(9)–C(10)	1.393(2)	C(9)–C(14)	1.394(2)
C(10)–H(10A)	0.950	C(10)–C(11)	1.384(3)
C(11)–H(11A)	0.950	C(11)–C(12)	1.377(3)
C(12)–C(13)	1.376(3)	C(13)–H(13A)	0.950
C(13)–C(14)	1.383(3)	C(14)–H(14A)	0.950

C(1)–N(1)–C(2)	123.13(15)	C(1)–N(1)–C(5)	128.16(14)
C(2)–N(1)–C(5)	108.64(14)	O(2)–N(2)–O(3)	122.9(10)
O(2)–N(2)–O(2A)	8.7(16)	O(2)–N(2)–O(3A)	117.5(13)
O(2)–N(2)–C(12)	118.8(9)	O(3)–N(2)–O(2A)	120.8(7)
O(3)–N(2)–O(3A)	32.1(4)	O(3)–N(2)–C(12)	117.8(5)
O(2A)–N(2)–O(3A)	120.9(6)	O(2A)–N(2)–C(12)	118.8(5)
O(3A)–N(2)–C(12)	117.7(6)	N(1)–C(1)–H(1A)	109.5
N(1)–C(1)–H(1B)	109.5	N(1)–C(1)–H(1C)	109.5
H(1A)–C(1)–H(1B)	109.5	H(1A)–C(1)–H(1C)	109.5
H(1B)–C(1)–H(1C)	109.5	N(1)–C(2)–H(2A)	125.3
N(1)–C(2)–C(3)	109.35(17)	H(2A)–C(2)–C(3)	125.3
C(2)–C(3)–H(3A)	126.3	C(2)–C(3)–C(4)	107.30(16)
H(3A)–C(3)–C(4)	126.3	C(3)–C(4)–H(4A)	126.1
C(3)–C(4)–C(5)	107.72(16)	H(4A)–C(4)–C(5)	126.1
N(1)–C(5)–C(4)	106.98(15)	N(1)–C(5)–C(6)	121.81(14)
C(4)–C(5)–C(6)	131.20(16)	O(1)–C(6)–C(5)	124.24(16)
O(1)–C(6)–C(7)	116.97(15)	C(5)–C(6)–C(7)	118.78(14)
Cl(1)–C(7)–Cl(2)	109.31(8)	Cl(1)–C(7)–C(6)	108.36(11)
Cl(1)–C(7)–C(8)	109.56(12)	Cl(2)–C(7)–C(6)	108.29(11)
Cl(2)–C(7)–C(8)	109.51(12)	C(6)–C(7)–C(8)	111.76(13)
C(7)–C(8)–H(8A)	108.7	C(7)–C(8)–H(8B)	108.7
C(7)–C(8)–C(9)	114.16(14)	H(8A)–C(8)–H(8B)	107.6
H(8A)–C(8)–C(9)	108.7	H(8B)–C(8)–C(9)	108.7
C(8)–C(9)–C(10)	121.38(15)	C(8)–C(9)–C(14)	120.23(16)
C(10)–C(9)–C(14)	118.39(16)	C(9)–C(10)–H(10A)	119.3
C(9)–C(10)–C(11)	121.36(16)	H(10A)–C(10)–C(11)	119.3
C(10)–C(11)–H(11A)	121.0	C(10)–C(11)–C(12)	118.04(17)
H(11A)–C(11)–C(12)	121.0	N(2)–C(12)–C(11)	118.79(17)
N(2)–C(12)–C(13)	118.51(16)	C(11)–C(12)–C(13)	122.69(17)
C(12)–C(13)–H(13A)	120.8	C(12)–C(13)–C(14)	118.39(16)
H(13A)–C(13)–C(14)	120.8	C(9)–C(14)–C(13)	121.08(17)
C(9)–C(14)–H(14A)	119.5	C(13)–C(14)–H(14A)	119.5

Table 4. Anisotropic displacement parameters ($Å^2$) for mjh79. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	0.0147(2)	0.0333(2)	0.0261(2)	–0.00174(17)	–0.00435(17)	–0.00508(16)
Cl(2)	0.0248(2)	0.0218(2)	0.0294(2)	–0.00541(16)	–0.01165(18)	–0.00398(16)
N(1)	0.0149(7)	0.0255(7)	0.0224(8)	–0.0010(6)	–0.0072(6)	–0.0029(6)
N(2)	0.0324(10)	0.0426(10)	0.0297(10)	–0.0005(8)	–0.0170(8)	–0.0104(8)
O(1)	0.0270(7)	0.0308(7)	0.0389(8)	0.0091(6)	–0.0174(6)	–0.0165(6)
O(2)	0.074(8)	0.052(6)	0.050(7)	–0.035(6)	–0.046(6)	0.024(5)
O(3)	0.0224(18)	0.110(11)	0.042(3)	–0.018(4)	–0.0135(17)	–0.007(3)
O(2A)	0.036(4)	0.050(3)	0.025(3)	0.000(3)	–0.017(2)	–0.012(3)
O(3A)	0.027(3)	0.089(11)	0.043(3)	–0.005(5)	–0.013(2)	–0.024(4)
C(1)	0.0210(10)	0.0408(11)	0.0310(10)	0.0023(8)	–0.0137(8)	–0.0130(8)
C(2)	0.0230(10)	0.0339(10)	0.0235(10)	0.0002(7)	–0.0092(8)	0.0012(8)
C(3)	0.0303(11)	0.0265(9)	0.0273(10)	0.0050(7)	–0.0061(8)	–0.0032(8)
C(4)	0.0216(10)	0.0248(9)	0.0279(10)	–0.0009(7)	–0.0067(8)	–0.0072(7)
C(5)	0.0157(9)	0.0218(8)	0.0215(9)	–0.0034(6)	–0.0061(7)	–0.0034(6)
C(6)	0.0146(8)	0.0209(8)	0.0230(9)	–0.0037(7)	–0.0054(7)	–0.0042(6)
C(7)	0.0138(8)	0.0211(8)	0.0226(9)	–0.0035(6)	–0.0045(7)	–0.0046(6)
C(8)	0.0194(9)	0.0243(9)	0.0239(9)	0.0014(7)	–0.0082(7)	–0.0066(7)
C(9)	0.0201(9)	0.0216(8)	0.0217(9)	0.0034(7)	–0.0086(7)	–0.0060(7)
C(10)	0.0235(10)	0.0298(9)	0.0233(9)	–0.0056(7)	–0.0101(8)	–0.0004(7)
C(11)	0.0191(10)	0.0375(10)	0.0241(10)	–0.0029(8)	–0.0068(8)	–0.0006(7)
C(12)	0.0234(10)	0.0292(9)	0.0221(9)	0.0029(7)	–0.0108(7)	–0.0082(7)
C(13)	0.0298(10)	0.0276(9)	0.0186(9)	–0.0027(7)	–0.0084(8)	–0.0025(7)
C(14)	0.0209(9)	0.0307(10)	0.0212(9)	0.0004(7)	–0.0049(7)	–0.0007(7)

Table 5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for mjh79.

	x	y	z	U
H(1A)	0.6046	0.2685	1.1219	0.043
H(1B)	0.4792	0.4009	1.0804	0.043
H(1C)	0.5923	0.2783	0.9600	0.043
H(2A)	0.4715	0.0708	1.2646	0.032
H(3A)	0.2487	–0.0711	1.2755	0.035
H(4A)	0.1220	0.0355	1.0849	0.029
H(8A)	0.0978	0.4864	0.7776	0.026
H(8B)	0.2309	0.3731	0.6608	0.026
H(10A)	–0.1905	0.4956	0.7985	0.030
H(11A)	–0.3820	0.4560	0.6873	0.033
H(13A)	–0.0329	0.1989	0.3739	0.030
H(14A)	0.1558	0.2312	0.4908	0.030

Table 6. Torsion angles [°] for mjh79.

C(1)–N(1)–C(2)–C(3)	−177.42(16)	C(5)–N(1)–C(2)–C(3)	−0.2(2)
N(1)–C(2)–C(3)–C(4)	0.4(2)	C(2)–C(3)–C(4)–C(5)	−0.5(2)
C(1)–N(1)–C(5)–C(4)	176.92(16)	C(1)–N(1)–C(5)–C(6)	−3.8(3)
C(2)–N(1)–C(5)–C(4)	−0.17(19)	C(2)–N(1)–C(5)–C(6)	179.08(15)
C(3)–C(4)–C(5)–N(1)	0.43(19)	C(3)–C(4)–C(5)–C(6)	−178.71(17)
N(1)–C(5)–C(6)–O(1)	−3.1(3)	N(1)–C(5)–C(6)–C(7)	177.70(14)
C(4)–C(5)–C(6)–O(1)	175.93(18)	C(4)–C(5)–C(6)–C(7)	−3.3(3)
O(1)–C(6)–C(7)–Cl(1)	−120.30(15)	O(1)–C(6)–C(7)–Cl(2)	121.22(14)
O(1)–C(6)–C(7)–C(8)	0.5(2)	C(5)–C(6)–C(7)–Cl(1)	58.95(17)
C(5)–C(6)–C(7)–Cl(2)	−59.52(17)	C(5)–C(6)–C(7)–C(8)	179.77(14)
Cl(1)–C(7)–C(8)–C(9)	−61.68(17)	Cl(2)–C(7)–C(8)–C(9)	58.20(17)
C(6)–C(7)–C(8)–C(9)	178.20(14)	C(7)–C(8)–C(9)–C(10)	86.50(19)
C(7)–C(8)–C(9)–C(14)	−93.80(19)	C(8)–C(9)–C(10)–C(11)	−177.64(16)
C(14)–C(9)–C(10)–C(11)	2.7(3)	C(9)–C(10)–C(11)–C(12)	−2.0(3)
C(10)–C(11)–C(12)–N(2)	179.12(16)	C(10)–C(11)–C(12)–C(13)	0.0(3)
O(2)–N(2)–C(12)–C(11)	171.8(15)	O(2)–N(2)–C(12)–C(13)	−9.0(15)
O(3)–N(2)–C(12)–C(11)	0.3(19)	O(3)–N(2)–C(12)–C(13)	179.4(19)
O(2A)–N(2)–C(12)–C(11)	161.9(7)	O(2A)–N(2)–C(12)–C(13)	−18.9(7)
O(3A)–N(2)–C(12)–C(11)	−36(2)	O(3A)–N(2)–C(12)–C(13)	143(2)
N(2)–C(12)–C(13)–C(14)	−177.82(15)	C(11)–C(12)–C(13)–C(14)	1.3(3)
C(12)–C(13)–C(14)–C(9)	−0.6(3)	C(8)–C(9)–C(14)–C(13)	179.00(15)
C(10)–C(9)–C(14)–C(13)	−1.3(2)		

2,2-Dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(4-nitrophenyl)propane-1,3-dione (3h)

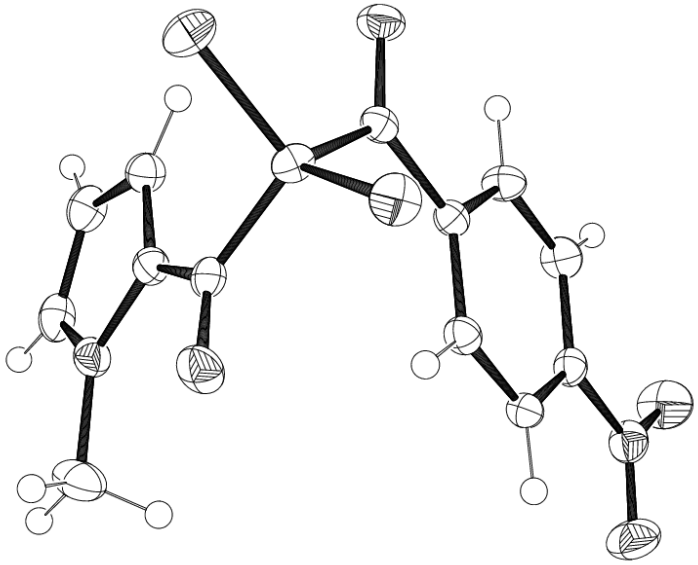


Table 1. Crystal data and structure refinement for mjh77.

Identification code	mjh77	
Chemical formula (moiety)	$C_{14}H_{10}Cl_2N_2O_4$	
Chemical formula (total)	$C_{14}H_{10}Cl_2N_2O_4$	
Formula weight	341.14	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	orthorhombic, Pbca	
Unit cell parameters	a = 12.4615(6) Å	α = 90°
	b = 13.4977(5) Å	β = 90°
	c = 17.2015(7) Å	γ = 90°
Cell volume	2893.3(2) $Å^3$	
Z	8	
Calculated density	1.566 g/cm^3	
Absorption coefficient μ	0.468 mm^{-1}	
F(000)	1392	
Crystal colour and size	colourless, 0.30 × 0.30 × 0.10 mm^3	
Reflections for cell refinement	5529 (θ range 3.0 to 28.5°)	
Data collection method	Xcalibur, Atlas, Gemini ultra	
	thick-slice ω scans	
θ range for data collection	3.0 to 28.6°	
Index ranges	h –13 to 16, k –17 to 17, l –22 to 22	
Completeness to θ = 25.0°	99.9 %	
Reflections collected	13352	
Independent reflections	3223 (R_{int} = 0.0326)	
Reflections with $F^2>2\sigma$	2709	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.8724 and 0.9547	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0258, 1.7441	
Data / restraints / parameters	3223 / 0 / 201	
Final R indices [$F^2>2\sigma$]	R1 = 0.0323, wR2 = 0.0693	
R indices (all data)	R1 = 0.0426, wR2 = 0.0753	
Goodness-of-fit on F^2	1.036	
Extinction coefficient	0.0011(2)	
Largest and mean shift/su	0.001 and 0.000	
Largest diff. peak and hole	0.34 and –0.27 e $Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for mjh77. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cl(1)	0.96530(3)	0.68376(3)	0.49929(2)	0.02529(12)
Cl(2)	0.86897(4)	0.77442(3)	0.63311(2)	0.02767(12)
N(1)	0.80306(11)	0.45779(9)	0.71317(8)	0.0220(3)
N(3)	0.63074(13)	0.32619(10)	0.35286(8)	0.0267(3)
O(1)	0.97291(9)	0.53449(9)	0.61518(7)	0.0267(3)
O(2)	0.69494(9)	0.73649(8)	0.53144(7)	0.0257(3)
O(3)	0.53965(11)	0.32316(10)	0.32733(9)	0.0416(4)
O(4)	0.69592(11)	0.25930(9)	0.34525(8)	0.0381(3)
C(1)	0.88406(16)	0.37973(12)	0.71018(11)	0.0331(4)
C(2)	0.71109(15)	0.45094(12)	0.75386(9)	0.0266(4)
C(3)	0.64886(15)	0.53307(12)	0.74071(10)	0.0267(4)
C(4)	0.70455(13)	0.59275(11)	0.68908(9)	0.0223(3)
C(5)	0.80106(13)	0.54619(11)	0.67161(9)	0.0198(3)
C(6)	0.88685(13)	0.57611(11)	0.62146(9)	0.0187(3)
C(7)	0.86411(13)	0.66990(10)	0.57049(9)	0.0189(3)
C(8)	0.75525(13)	0.66758(10)	0.52641(9)	0.0176(3)
C(9)	0.72851(12)	0.57725(10)	0.47950(9)	0.0174(3)
C(10)	0.62405(13)	0.57198(12)	0.45005(10)	0.0240(4)
C(11)	0.59111(14)	0.49003(12)	0.40858(10)	0.0247(4)
C(12)	0.66410(13)	0.41437(11)	0.39686(9)	0.0204(3)
C(13)	0.76770(13)	0.41807(11)	0.42406(9)	0.0205(3)
C(14)	0.79976(13)	0.50013(11)	0.46578(9)	0.0195(3)

Table 3. Bond lengths [Å] and angles [°] for mjh77.

Cl(1)–C(7)	1.7678(16)	Cl(2)–C(7)	1.7760(15)
N(1)–C(1)	1.460(2)	N(1)–C(2)	1.346(2)
N(1)–C(5)	1.3911(19)	N(3)–O(3)	1.218(2)
N(3)–O(4)	1.2214(19)	N(3)–C(12)	1.471(2)
O(1)–C(6)	1.2155(19)	O(2)–C(8)	1.1989(18)
C(1)–H(1A)	0.980	C(1)–H(1B)	0.980
C(1)–H(1C)	0.980	C(2)–H(2A)	0.950
C(2)–C(3)	1.372(2)	C(3)–H(3A)	0.950
C(3)–C(4)	1.385(2)	C(4)–H(4A)	0.950
C(4)–C(5)	1.390(2)	C(5)–C(6)	1.432(2)
C(6)–C(7)	1.566(2)	C(7)–C(8)	1.554(2)
C(8)–C(9)	1.500(2)	C(9)–C(10)	1.399(2)
C(9)–C(14)	1.388(2)	C(10)–H(10A)	0.950
C(10)–C(11)	1.379(2)	C(11)–H(11A)	0.950
C(11)–C(12)	1.382(2)	C(12)–C(13)	1.374(2)
C(13)–H(13A)	0.950	C(13)–C(14)	1.379(2)
C(14)–H(14A)	0.950		

C(1)–N(1)–C(2)	123.88(14)	C(1)–N(1)–C(5)	127.82(14)
C(2)–N(1)–C(5)	108.11(14)	O(3)–N(3)–O(4)	123.80(14)
O(3)–N(3)–C(12)	118.44(14)	O(4)–N(3)–C(12)	117.75(14)
N(1)–C(1)–H(1A)	109.5	N(1)–C(1)–H(1B)	109.5
N(1)–C(1)–H(1C)	109.5	H(1A)–C(1)–H(1B)	109.5
H(1A)–C(1)–H(1C)	109.5	H(1B)–C(1)–H(1C)	109.5
N(1)–C(2)–H(2A)	125.1	N(1)–C(2)–C(3)	109.88(14)
H(2A)–C(2)–C(3)	125.1	C(2)–C(3)–H(3A)	126.5
C(2)–C(3)–C(4)	107.00(15)	H(3A)–C(3)–C(4)	126.5
C(3)–C(4)–H(4A)	126.0	C(3)–C(4)–C(5)	108.01(14)
H(4A)–C(4)–C(5)	126.0	N(1)–C(5)–C(4)	106.99(14)
N(1)–C(5)–C(6)	122.56(14)	C(4)–C(5)–C(6)	130.45(14)
O(1)–C(6)–C(5)	125.59(14)	O(1)–C(6)–C(7)	118.92(14)
C(5)–C(6)–C(7)	115.49(13)	Cl(1)–C(7)–Cl(2)	108.17(8)
Cl(1)–C(7)–C(6)	110.15(11)	Cl(1)–C(7)–C(8)	106.66(10)
Cl(2)–C(7)–C(6)	107.24(10)	Cl(2)–C(7)–C(8)	109.98(10)
C(6)–C(7)–C(8)	114.51(12)	O(2)–C(8)–C(7)	119.75(13)
O(2)–C(8)–C(9)	122.03(14)	C(7)–C(8)–C(9)	118.22(12)
C(8)–C(9)–C(10)	116.30(13)	C(8)–C(9)–C(14)	123.99(14)
C(10)–C(9)–C(14)	119.70(14)	C(9)–C(10)–H(10A)	119.8
C(9)–C(10)–C(11)	120.35(15)	H(10A)–C(10)–C(11)	119.8
C(10)–C(11)–H(11A)	120.9	C(10)–C(11)–C(12)	118.18(15)
H(11A)–C(11)–C(12)	120.9	N(3)–C(12)–C(11)	119.15(15)
N(3)–C(12)–C(13)	118.05(14)	C(11)–C(12)–C(13)	122.80(14)
C(12)–C(13)–H(13A)	120.7	C(12)–C(13)–C(14)	118.59(15)
H(13A)–C(13)–C(14)	120.7	C(9)–C(14)–C(13)	120.36(15)
C(9)–C(14)–H(14A)	119.8	C(13)–C(14)–H(14A)	119.8

Table 4. Anisotropic displacement parameters ($Å^2$) for mjh77. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	0.0196(2)	0.0282(2)	0.0281(2)	0.00313(16)	0.00662(16)	–0.00370(16)
Cl(2)	0.0279(2)	0.02288(19)	0.0323(2)	–0.00833(16)	0.00047(18)	–0.00497(17)
N(1)	0.0265(8)	0.0190(6)	0.0205(7)	0.0010(5)	–0.0041(6)	–0.0020(6)
N(3)	0.0312(9)	0.0243(7)	0.0245(7)	–0.0012(6)	–0.0008(6)	–0.0050(6)
O(1)	0.0180(6)	0.0349(6)	0.0271(6)	0.0031(5)	–0.0017(5)	0.0062(5)
O(2)	0.0246(6)	0.0209(5)	0.0316(6)	–0.0008(5)	–0.0030(5)	0.0060(5)
O(3)	0.0357(8)	0.0373(7)	0.0517(9)	–0.0114(6)	–0.0154(7)	–0.0045(6)
O(4)	0.0436(8)	0.0263(6)	0.0445(8)	–0.0127(6)	–0.0032(7)	0.0041(6)
C(1)	0.0362(11)	0.0211(8)	0.0420(10)	0.0046(7)	–0.0064(9)	0.0033(8)
C(2)	0.0352(10)	0.0256(8)	0.0190(8)	0.0019(7)	0.0004(7)	–0.0109(8)
C(3)	0.0266(9)	0.0310(8)	0.0224(8)	–0.0017(7)	0.0054(7)	–0.0057(8)
C(4)	0.0220(9)	0.0231(7)	0.0218(8)	0.0003(6)	0.0021(7)	0.0000(7)
C(5)	0.0230(9)	0.0179(7)	0.0183(7)	–0.0004(6)	–0.0023(7)	–0.0016(7)
C(6)	0.0194(8)	0.0197(7)	0.0170(7)	–0.0036(6)	–0.0045(6)	–0.0014(7)
C(7)	0.0168(8)	0.0181(7)	0.0219(8)	–0.0017(6)	0.0034(6)	–0.0013(6)
C(8)	0.0169(8)	0.0173(7)	0.0185(7)	0.0029(6)	0.0017(6)	–0.0007(6)
C(9)	0.0164(8)	0.0179(7)	0.0180(7)	0.0020(6)	0.0002(6)	–0.0005(6)
C(10)	0.0205(8)	0.0217(7)	0.0297(9)	–0.0012(7)	–0.0009(7)	0.0037(7)
C(11)	0.0182(8)	0.0282(8)	0.0277(8)	–0.0011(7)	–0.0042(7)	–0.0018(7)
C(12)	0.0247(9)	0.0197(7)	0.0169(7)	0.0004(6)	0.0006(6)	–0.0033(7)
C(13)	0.0219(8)	0.0197(7)	0.0199(7)	0.0016(6)	0.0009(6)	0.0037(7)
C(14)	0.0170(8)	0.0222(7)	0.0195(7)	0.0018(6)	0.0000(6)	0.0017(7)

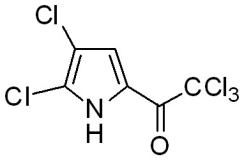
Table 5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for mjh77.

	x	y	z	U
H(1A)	0.8618	0.3245	0.7434	0.050
H(1B)	0.9529	0.4059	0.7286	0.050
H(1C)	0.8918	0.3564	0.6565	0.050
H(2A)	0.6921	0.3972	0.7868	0.032
H(3A)	0.5805	0.5465	0.7628	0.032
H(4A)	0.6809	0.6546	0.6691	0.027
H(10A)	0.5755	0.6251	0.4587	0.029
H(11A)	0.5202	0.4857	0.3886	0.030
H(13A)	0.8162	0.3652	0.4143	0.025
H(14A)	0.8710	0.5039	0.4852	0.023

Table 6. Torsion angles [°] for mjh77.

C(1)–N(1)–C(2)–C(3)	–175.86(15)	C(5)–N(1)–C(2)–C(3)	–0.54(18)
N(1)–C(2)–C(3)–C(4)	0.56(19)	C(2)–C(3)–C(4)–C(5)	–0.36(19)
C(3)–C(4)–C(5)–N(1)	0.04(18)	C(3)–C(4)–C(5)–C(6)	179.73(15)
C(1)–N(1)–C(5)–C(4)	175.39(15)	C(1)–N(1)–C(5)–C(6)	–4.3(2)
C(2)–N(1)–C(5)–C(4)	0.30(17)	C(2)–N(1)–C(5)–C(6)	–179.42(14)
N(1)–C(5)–C(6)–O(1)	–7.4(2)	N(1)–C(5)–C(6)–C(7)	171.70(13)
C(4)–C(5)–C(6)–O(1)	172.94(16)	C(4)–C(5)–C(6)–C(7)	–8.0(2)
O(1)–C(6)–C(7)–Cl(1)	10.26(17)	O(1)–C(6)–C(7)–Cl(2)	–107.23(14)
O(1)–C(6)–C(7)–C(8)	130.45(15)	C(5)–C(6)–C(7)–Cl(1)	–168.91(11)
C(5)–C(6)–C(7)–Cl(2)	73.60(14)	C(5)–C(6)–C(7)–C(8)	–48.72(17)
Cl(1)–C(7)–C(8)–O(2)	–109.14(14)	Cl(1)–C(7)–C(8)–C(9)	71.79(14)
Cl(2)–C(7)–C(8)–O(2)	7.92(18)	Cl(2)–C(7)–C(8)–C(9)	–171.14(11)
C(6)–C(7)–C(8)–O(2)	128.75(15)	C(6)–C(7)–C(8)–C(9)	–50.32(18)
O(2)–C(8)–C(9)–C(10)	–7.9(2)	O(2)–C(8)–C(9)–C(14)	173.43(15)
C(7)–C(8)–C(9)–C(10)	171.11(13)	C(7)–C(8)–C(9)–C(14)	–7.5(2)
C(8)–C(9)–C(10)–C(11)	–177.70(15)	C(14)–C(9)–C(10)–C(11)	1.0(2)
C(9)–C(10)–C(11)–C(12)	–0.3(2)	C(10)–C(11)–C(12)–N(3)	179.94(14)
C(10)–C(11)–C(12)–C(13)	–0.7(2)	O(3)–N(3)–C(12)–C(11)	0.8(2)
O(3)–N(3)–C(12)–C(13)	–178.67(15)	O(4)–N(3)–C(12)–C(11)	–178.00(15)
O(4)–N(3)–C(12)–C(13)	2.6(2)	N(3)–C(12)–C(13)–C(14)	–179.64(13)
C(11)–C(12)–C(13)–C(14)	0.9(2)	C(12)–C(13)–C(14)–C(9)	–0.2(2)
C(8)–C(9)–C(14)–C(13)	177.89(14)	C(10)–C(9)–C(14)–C(13)	–0.7(2)

2,2,2-Trichloro-1-(4,5-dichloro-1*H*-pyrrol-2-yl)ethanone (1c)



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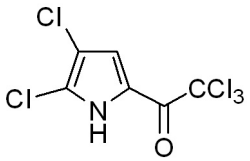

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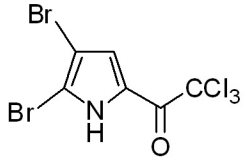

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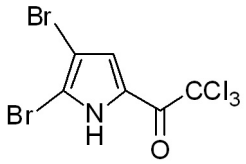
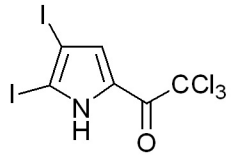
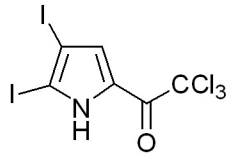


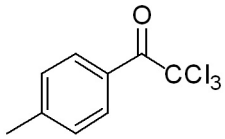
2,2,2-Trichloro-1-(4,5-diiodo-1*H*-pyrrol-2-yl)ethanone (1e)

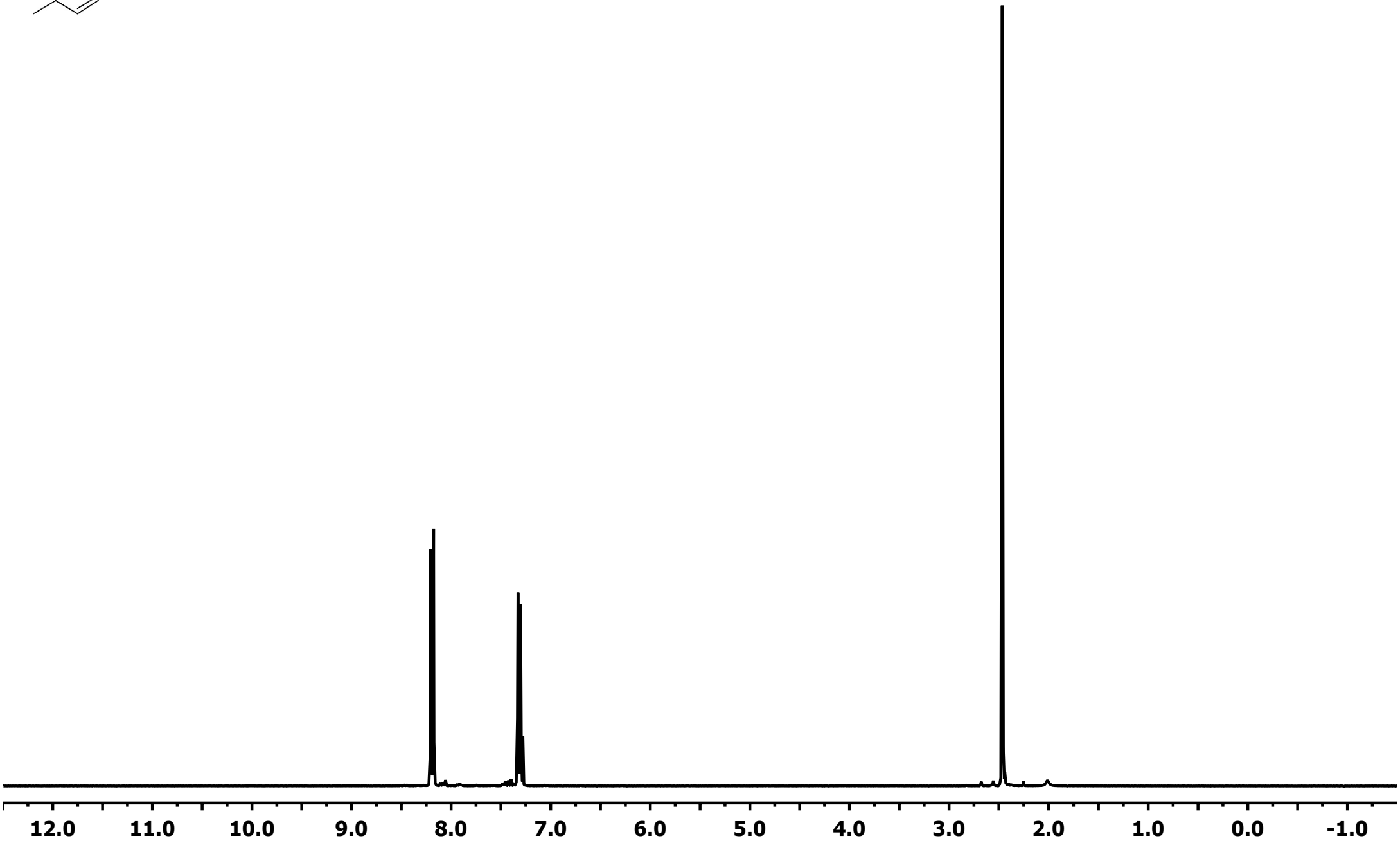


2,2,2-Trichloro-1-(4,5-diiodo-1*H*-pyrrol-2-yl)ethanone (1e)



2,2,2-Trichloro-1-(*p*-tolyl)ethanone (1f)





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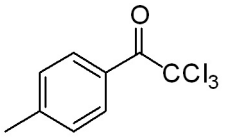
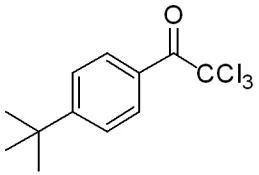
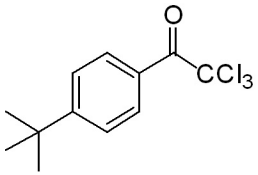


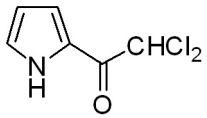
1-(4-(*tert*-Butyl)phenyl)-2,2,2-trichloroethanone (1g)



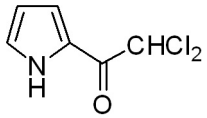
1-(4-(*tert*-Butyl)phenyl)-2,2,2-trichloroethanone (1g)



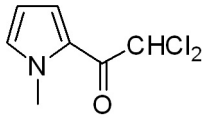
2,2-Dichloro-1-(1*H*-pyrrol-2-yl)ethanone (2a)



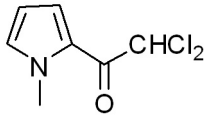
2,2-Dichloro-1-(1*H*-pyrrol-2-yl)ethanone (2a)



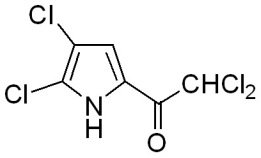
2,2-Dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)ethanone (2b)



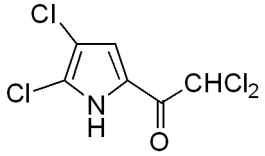
2,2-Dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)ethanone (2b)



2,2-Dichloro-1-(4,5-dichloro-1*H*-pyrrol-2-yl)ethanone (2c)



2,2-Dichloro-1-(4,5-dichloro-1*H*-pyrrol-2-yl)ethanone (2c)



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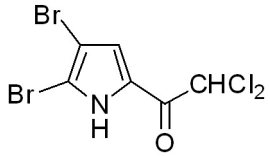

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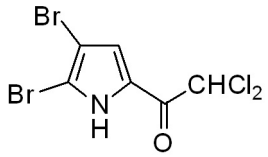
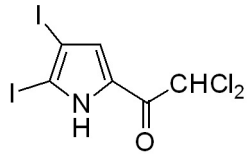
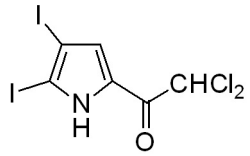


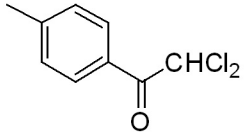
2,2-Dichloro-1-(4,5-diiodo-1*H*-pyrrol-2-yl)ethanone (2e)



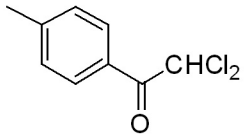
2,2-Dichloro-1-(4,5-diiodo-1*H*-pyrrol-2-yl)ethanone (2e)



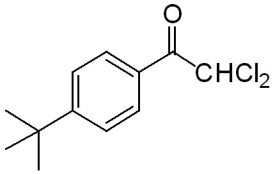
2,2-Dichloro-1-(*p*-tolyl)ethanone (2f)



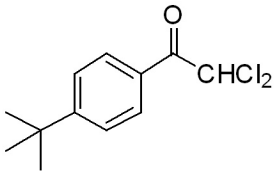
2,2-Dichloro-1-(*p*-tolyl)ethanone (2f)



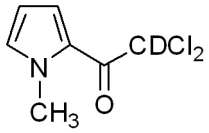
1-(4(*t*-Butyl)phenyl)-2,2-dichloroethanone (2g)



1-(4(*t*-Butyl)phenyl)-2,2-dichloroethanone (2g)



2,2-Dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)ethanone ((2-*d*)-2b)



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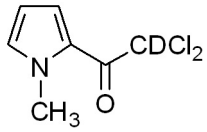
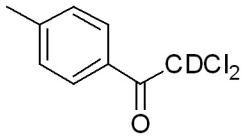


2-Deutero-2,2-dichloro-1-(*p*-tolyl)ethanone ((2-*d*)-2f)



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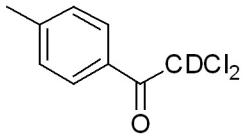
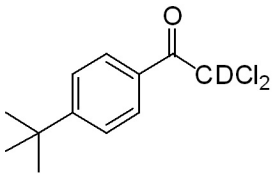
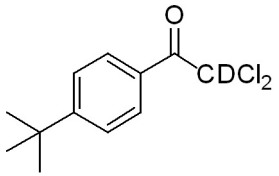


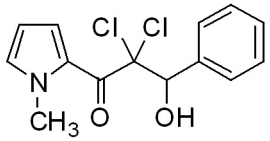
1-(4-(*tert*-Butyl)phenyl)-2-deutero-2,2-dichloroethanone ((2-*d*)-2g)



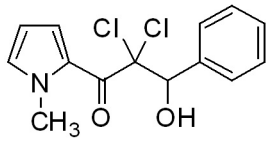
1-(4-(*tert*-Butyl)phenyl)-2-deutero-2,2-dichloroethanone ((2-*d*)-2g)



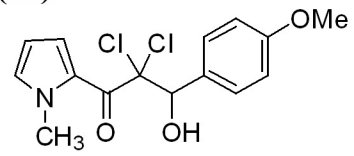
2,2-Dichloro-3-hydroxy-1-(1-methyl-1*H*-pyrrol-2-yl)-3-phenylpropan-1-one (3a)



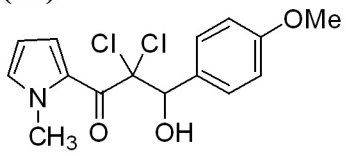
2,2-Dichloro-3-hydroxy-1-(1-methyl-1*H*-pyrrol-2-yl)-3-phenylpropan-1-one (3a)



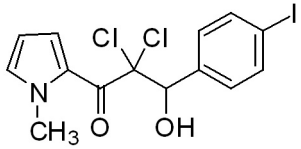
2,2-Dichloro-3-hydroxy-3-(4-methoxyphenyl)-1-(1-methyl-1*H*-pyrrol-2-yl)propan-1-one (3b)



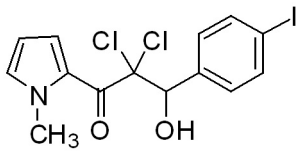
2,2-Dichloro-3-hydroxy-3-(4-methoxyphenyl)-1-(1-methyl-1*H*-pyrrol-2-yl)propan-1-one (3b)

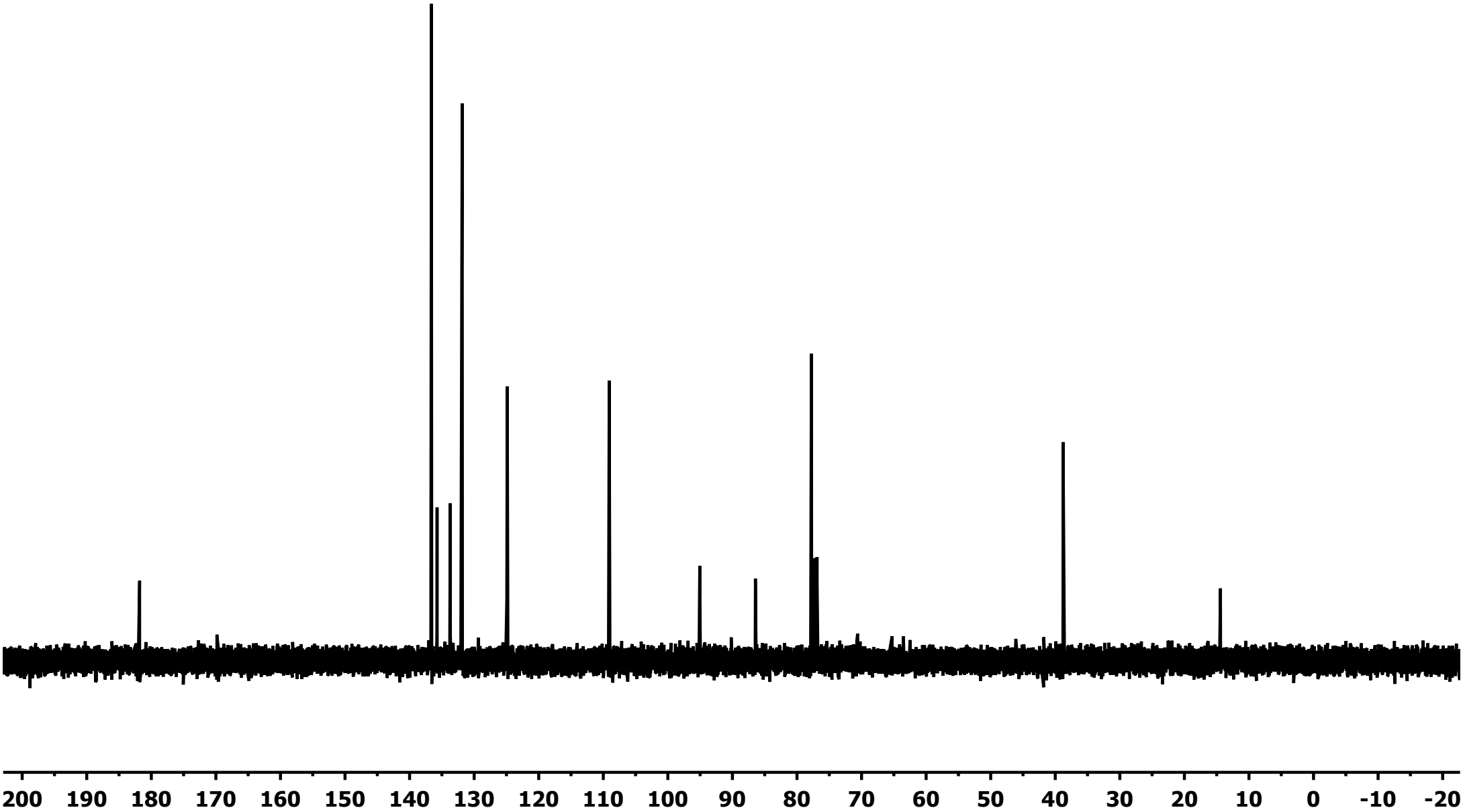


2,2-Dichloro-3-hydroxy-3-(4-iodophenyl)-1-(1-methyl-1*H*-pyrrol-2-yl)propan-1-one (3c)

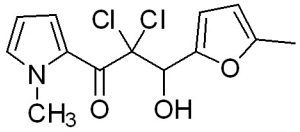


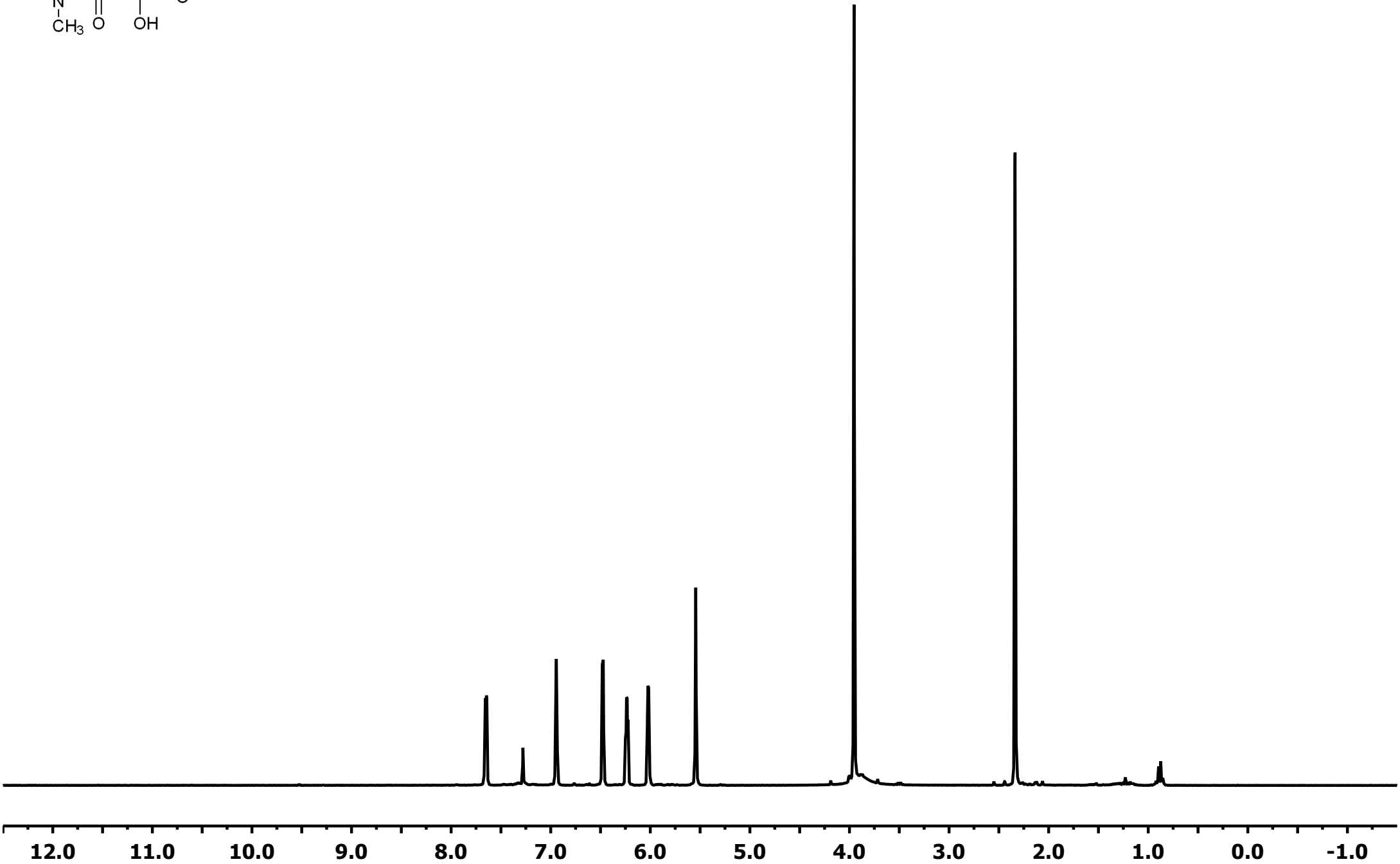
2,2-Dichloro-3-hydroxy-3-(4-iodophenyl)-1-(1-methyl-1*H*-pyrrol-2-yl)propan-1-one (3c)



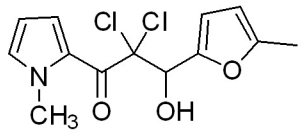


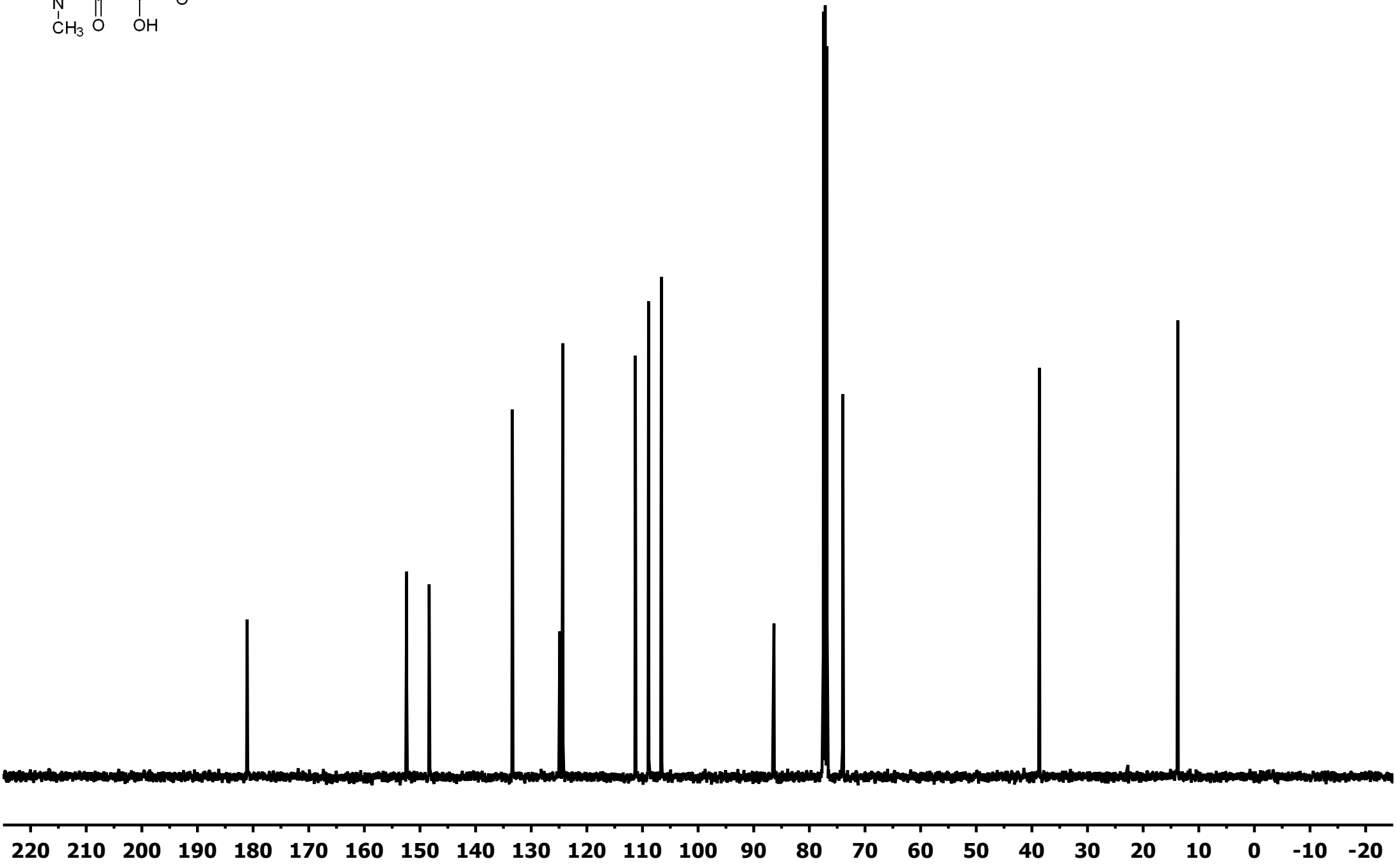
2,2-Dichloro-3-hydroxy-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(5-methylfuran-2-yl)propan-1-one (3d)



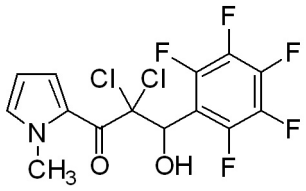


2,2-Dichloro-3-hydroxy-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(5-methylfuran-2-yl)propan-1-one (3d)

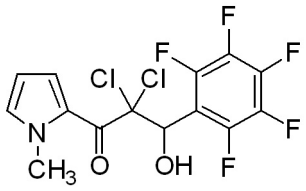




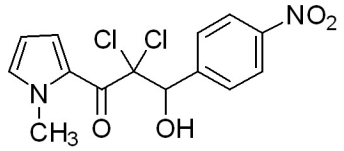
2,2-Dichloro-3-hydroxy-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(perfluorophenyl)propan-1-one (3e)



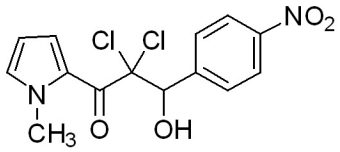
2,2-Dichloro-3-hydroxy-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(perfluorophenyl)propan-1-one (3e)



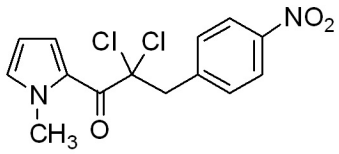
2,2-Dichloro-3-hydroxy-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(4-nitrophenyl)propan-1-one (3f)



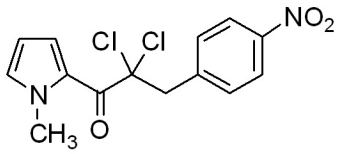
2,2-Dichloro-3-hydroxy-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(4-nitrophenyl)propan-1-one (3f)



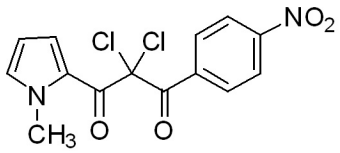
2,2-Dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(4-nitrophenyl)propan-1-one (3g)



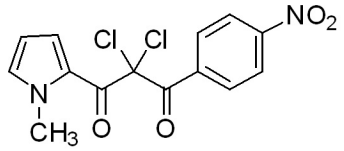
2,2-Dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(4-nitrophenyl)propan-1-one (3g)



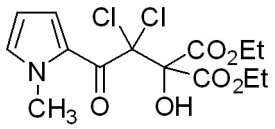
2,2-Dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(4-nitrophenyl)propane-1,3-dione (3h)



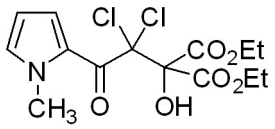
2,2-Dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)-3-(4-nitrophenyl)propane-1,3-dione (3h)



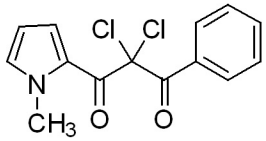
Diethyl 2-(1,1-dichloro-2-(1-methyl-1*H*-pyrrol-2-yl)-2-oxoethyl)-2-hydroxymalonate (3i)



Diethyl 2-(1,1-dichloro-2-(1-methyl-1*H*-pyrrol-2-yl)-2-oxoethyl)-2-hydroxymalonate (3i)



2,2-Dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)-3-phenylpropane-1,3-dione (3j)



2,2-Dichloro-1-(1-methyl-1*H*-pyrrol-2-yl)-3-phenylpropane-1,3-dione (3j)