Supporting information

Synthesis of cyclic carbonates from epoxides and carbon dioxide catalysed by an easy-to-handle ionic iron(III) complex.

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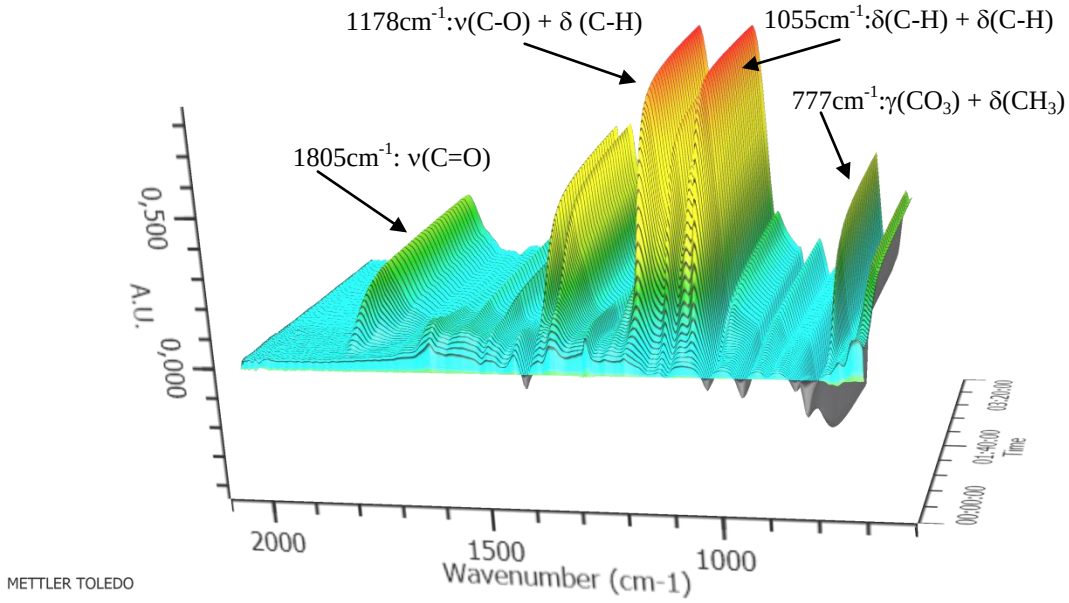
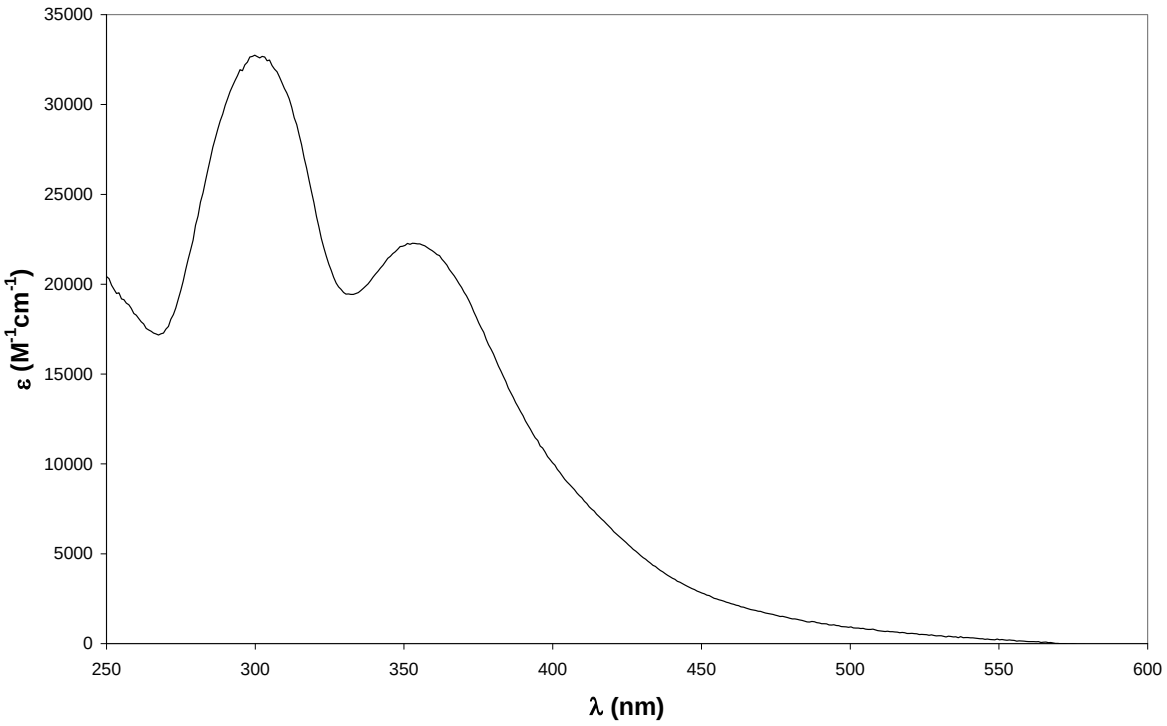
References:

D. D. Elleman, S. L. Manatt, C. D. Pearce, *The Journal of Chemical Physics*, 1965, **42**, 650.
C. Qi, H. Jiang, Z. Wang, B. Zou, S. Yang, *Synlett*, 2007, **2**, 255.

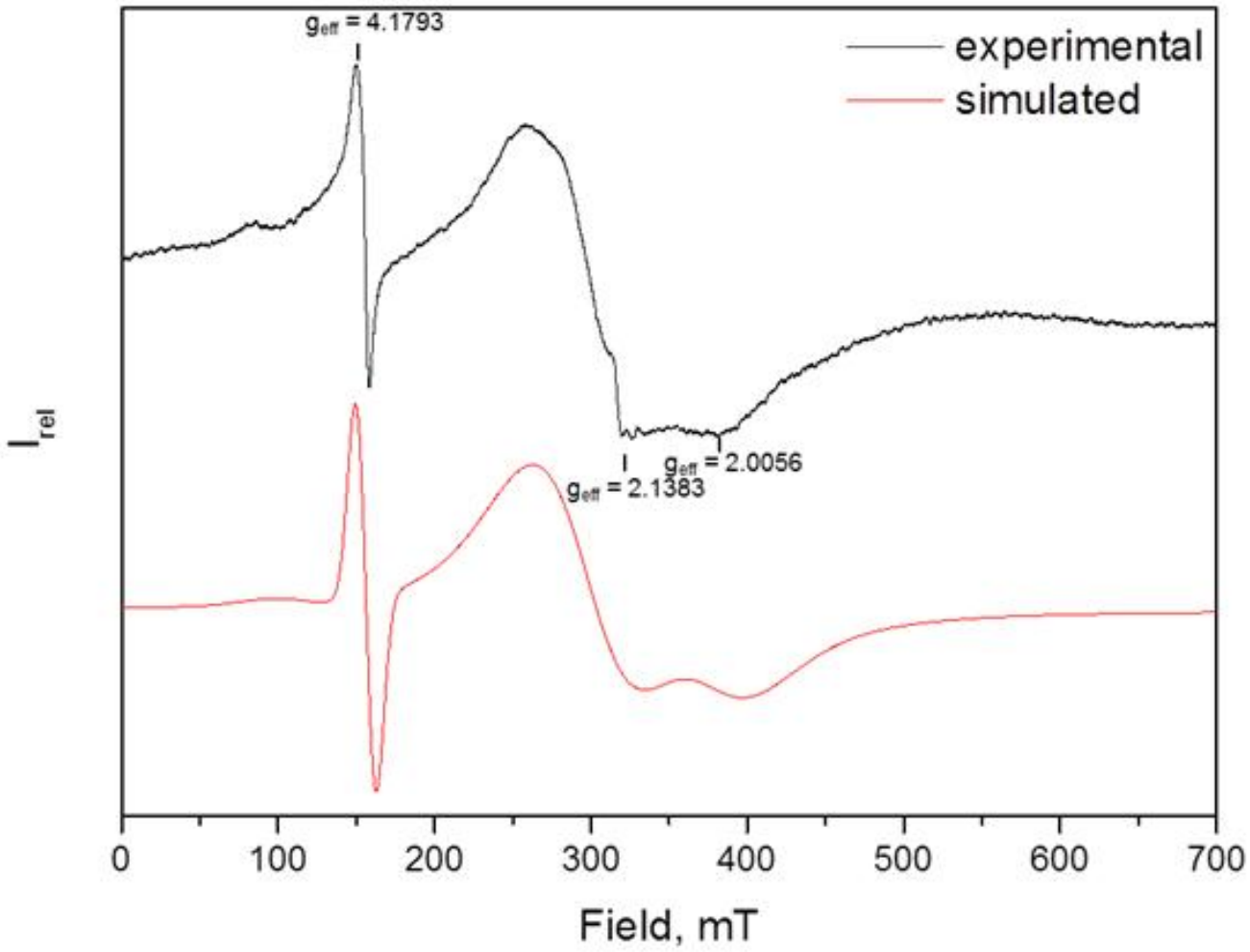
Time-resolved FT-IR/ATR spectrum for the formation of propylene carbonate from propylene oxide and CO_2 (80°C, 30bar CO_2, 0.2 mol% cat.(**3**), CH_2Cl_2 as solvent).



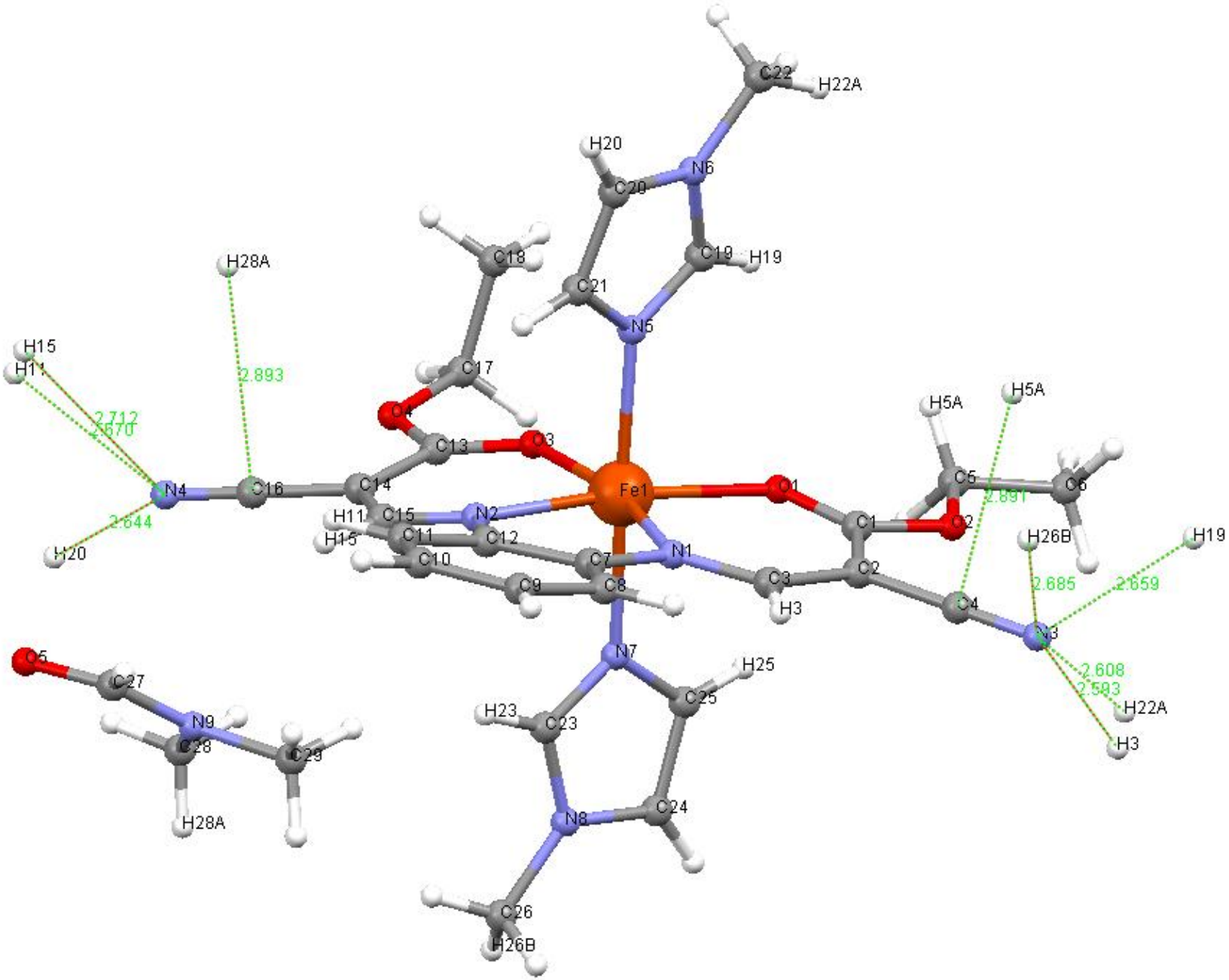
UV/VIS-Spectrum of Fe(III)complex **3** in acetonitrile.



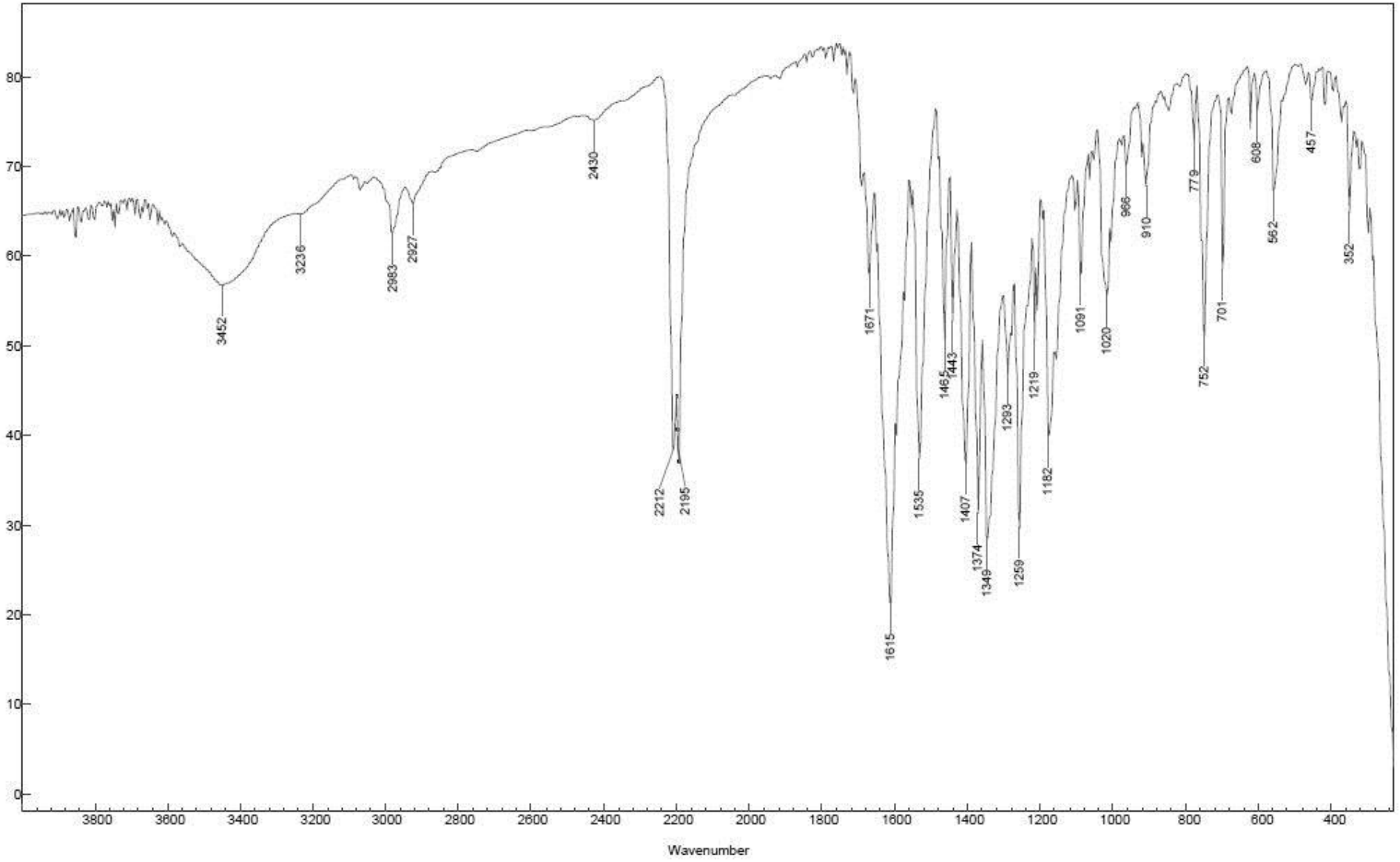
The ESR measurements of complex **3** (performed in quartz tubes at 123 K (9.45 GHz, 1mW microwave power)). The analysis and simulation of the ESR data was done with the Jes-Fa Series software package (Version 2.2.0).



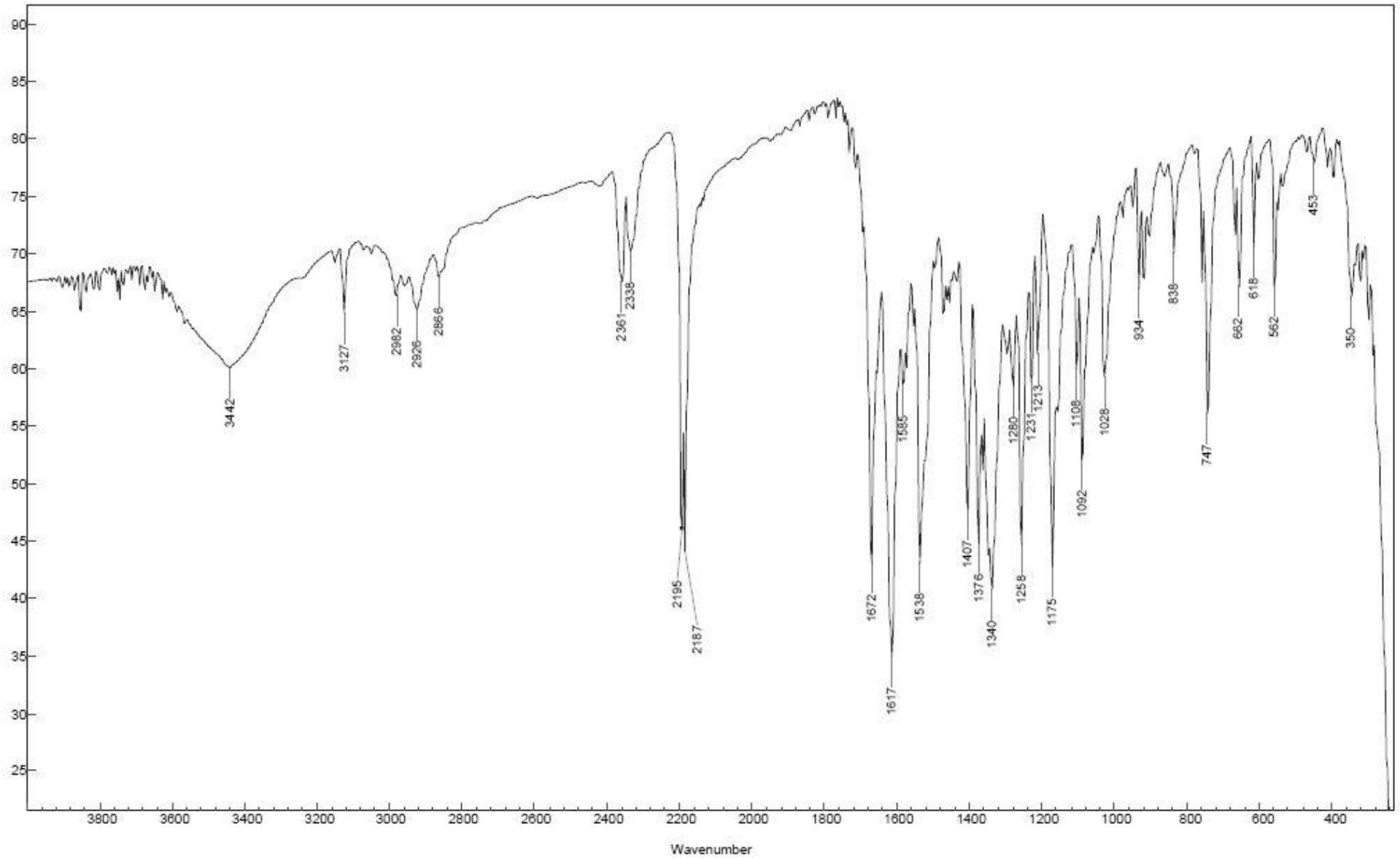
Mercury 3.0 drawing of **4** showing intermolecular interactions shorter than 3 Å involving the nitrile groups of the ligand.



FT-IR spectrum of complex **3** in KBr.



FT- IR spectrum of complex **4** in KBr.



Estimation of the cyclic carbonate yields in the reaction mixture via ^{1}H-NMR spectroscopy with an internal standard:

$$n_{cc} = \frac{I_{cc}}{I_{st}} \times \frac{N_{st}}{N_{cc}} \times \frac{m_{st}}{M_{st}} \times \frac{m_{ges\,\mathrm{Probe}}}{m_{\mathrm{Probe}}}$$

CC: Cyclic carbonate St: Standard (*1,1,2,2*-tetrachloroethane, chloroform)

n_{cc} : amount for cyclic carbonate in mole

I_{cc} : ^{1}H integration of cyclic carbonates

I_{st} : ^{1}H integration of standard

N_{st} : number of NMR active nuclei for the signal of integration I_{st}

N_{cc} : number of NMR active nuclei for the signal of integration I_{cc}

m_{st} : mass of standard in probe (20-30 mg)

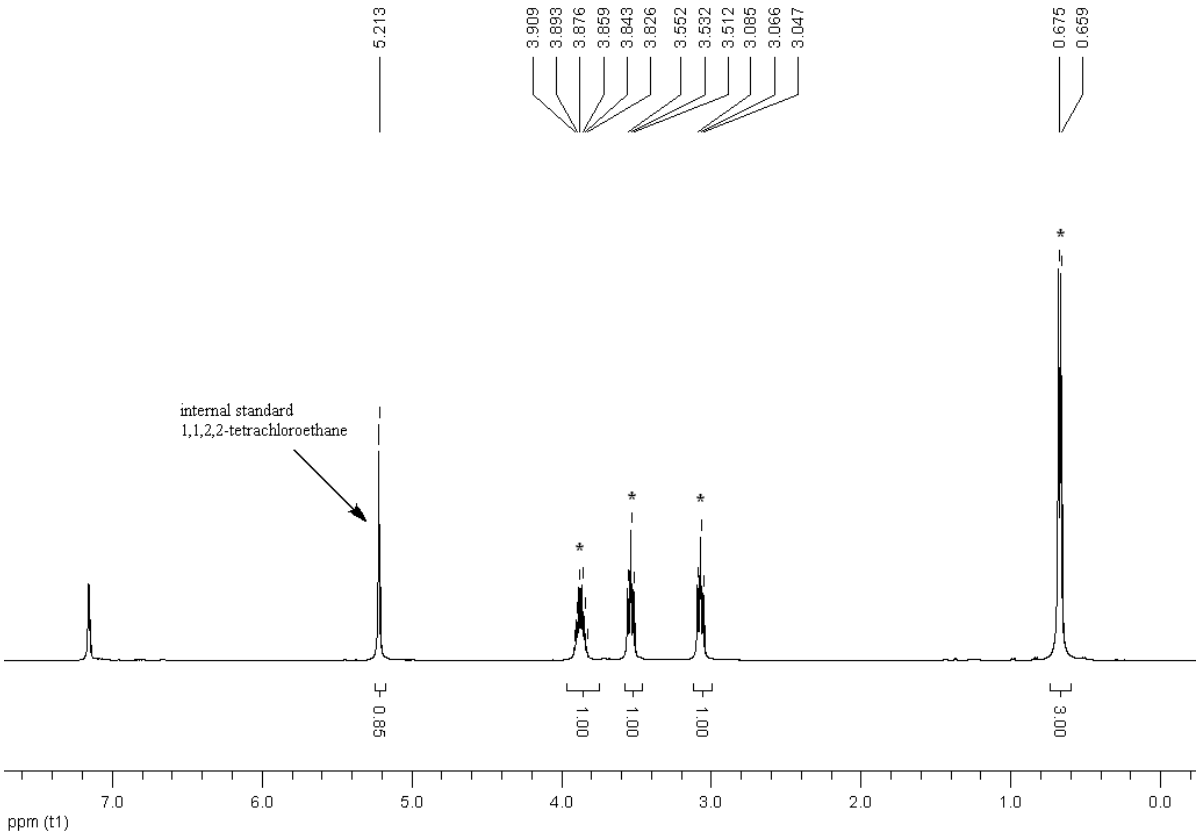
M_{st} : molar mass of standard

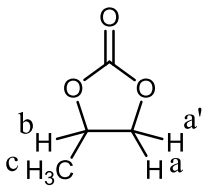
m_{total_probe} : total mass of product mixture

m_{probe} : mass of product mixture in probe (20-30 mg)

Estimation of **4-methyl-1,3-dioxolan-2-one** (PC):

^{1}H NMR spectrum (400MHz, benzene-d_6): *=cyclic carbonate

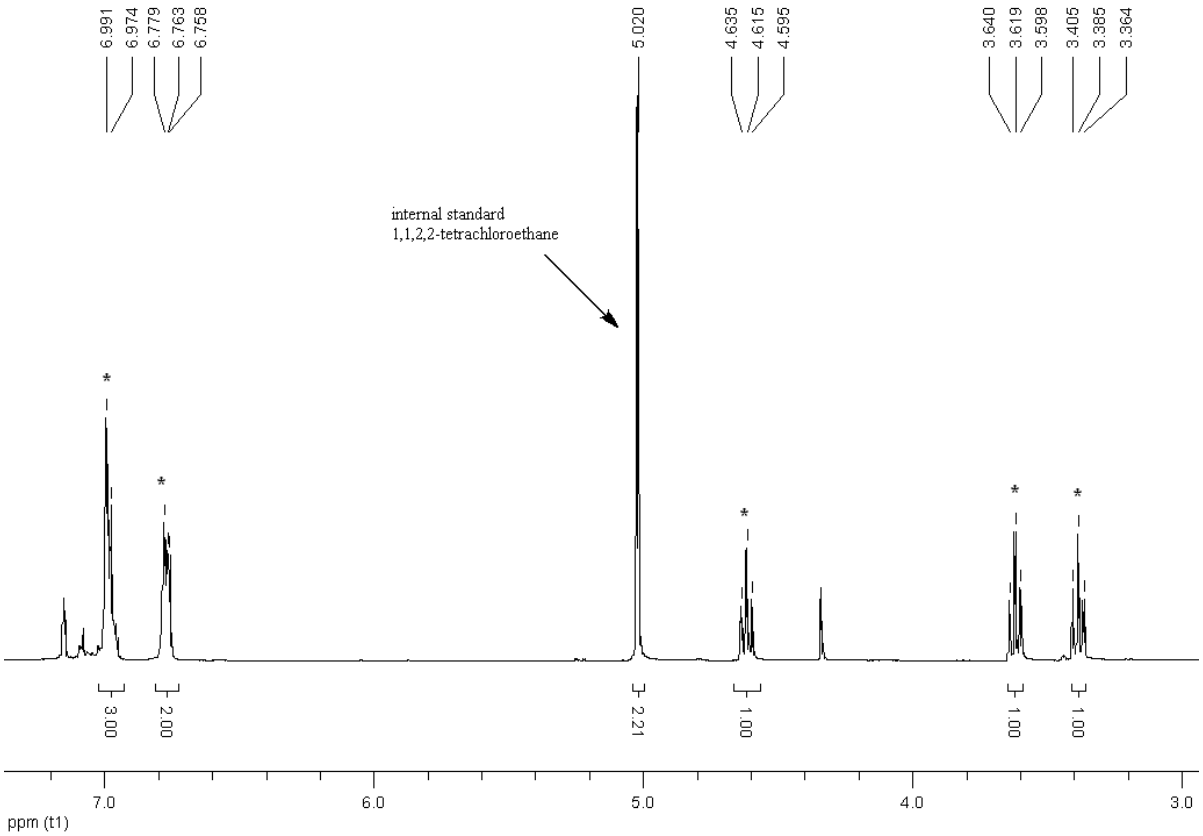


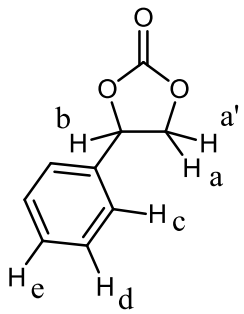


4-methyl-1,3-dioxolan-2-one (propylene carbonate, PC)
^{1}H NMR (400 MHz, benzene-d_6): δ ppm 0.67 (d, *J*=6.20 Hz, **Hc**, 3H), 3.07 (t, *J*=7.7 Hz, **Ha**, 1H), 3.53 (t, *J*=8.0 Hz, **Ha'**, 1H), 3.87 (m, **Hb**, 1H).

Estimation of **4-phenyl-1,3-dioxolan-2-one** (SC):

^{1}H NMR spectrum (400MHz, benzene-d_6): *=cyclic carbonate

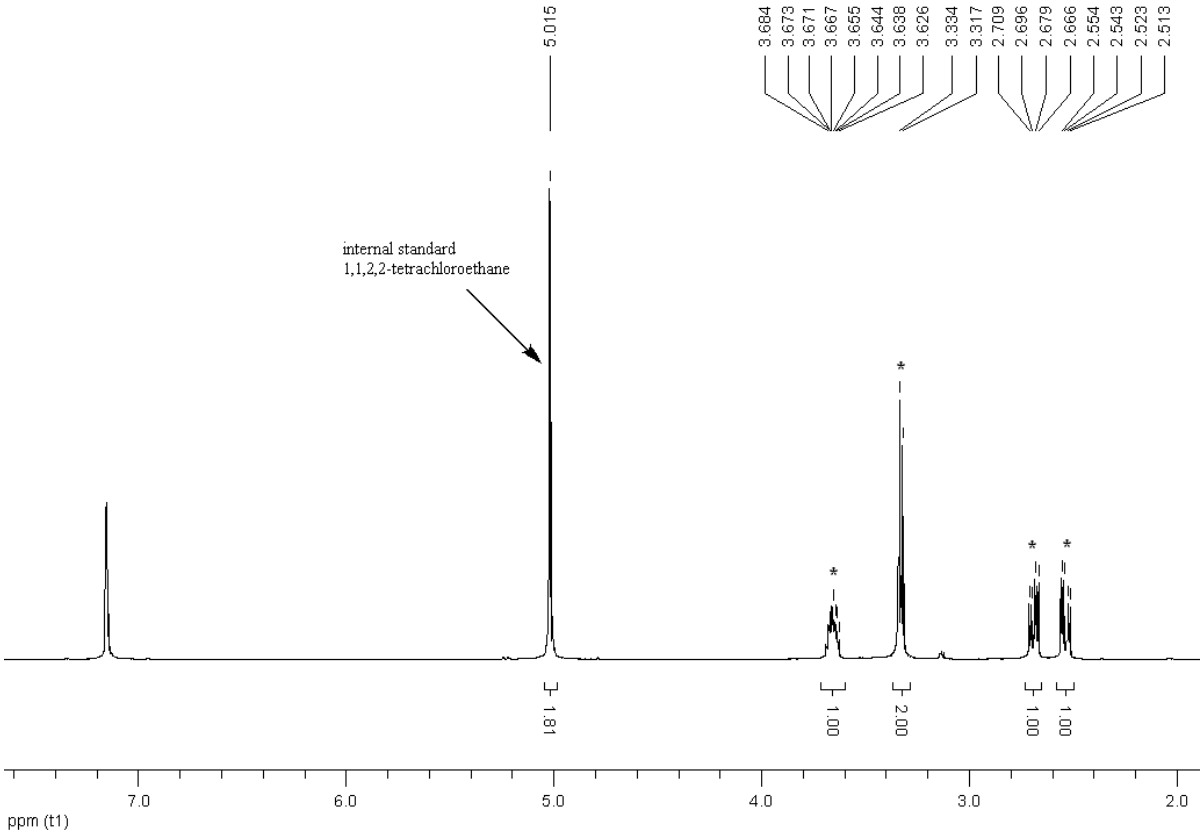


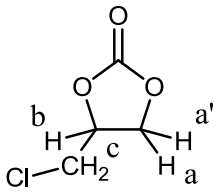


4-phenyl-1,3-dioxolan-2-one (styrene carbonate, SC)
^{1}H NMR (400 MHz, benzene-d_6): δ ppm 3.38 (t, *J*=8.2 Hz, **Ha**, 1H), 3.62 (t, *J*=8.3 Hz, **Ha'**, 1H), 4.61 (m, **Hb**, 1H), 6.77 (d, *J*=6.3 Hz, **Hc**, 2H), 6.97 - 7.00 (m, **Hd**, **He**, 3H).

Estimation of **4-chloromethyl-1,3-dioxolan-2-one**:

^{1}H NMR spectrum (400MHz, benzene-d_6): *=cyclic carbonate



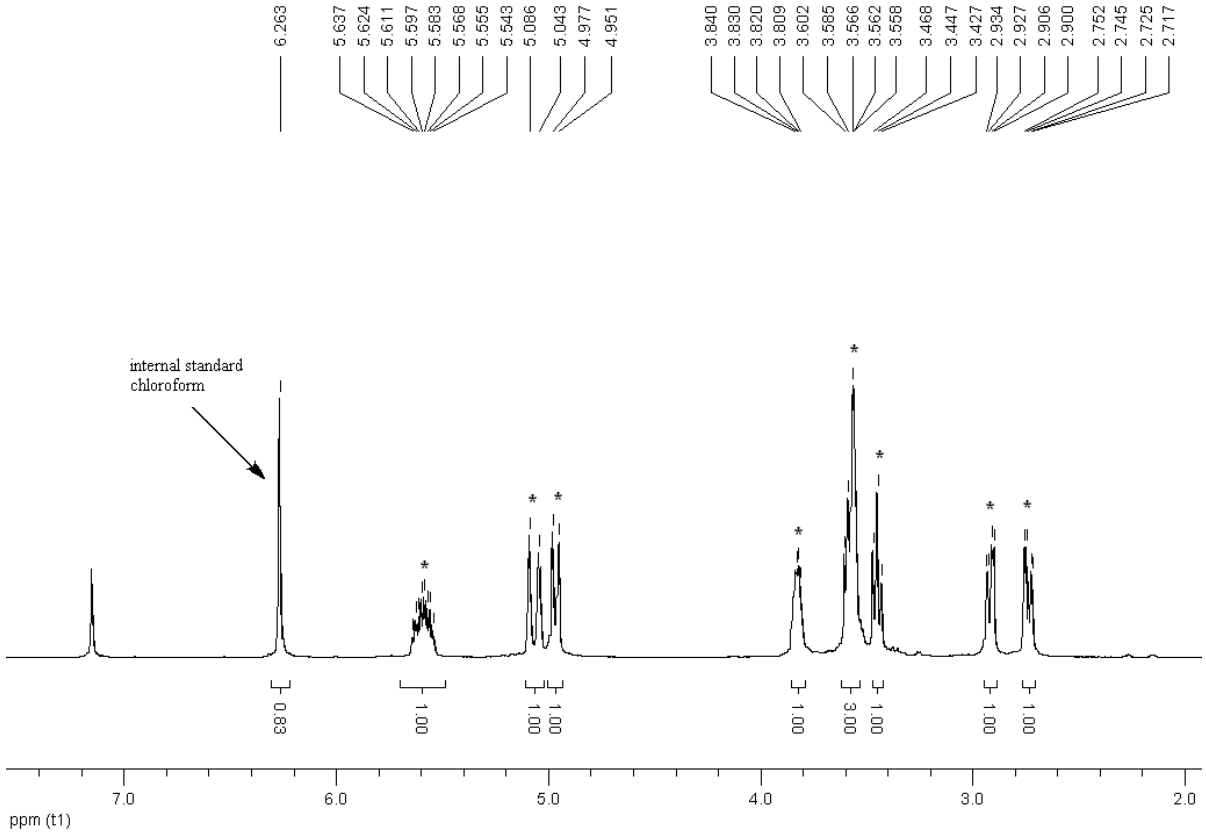


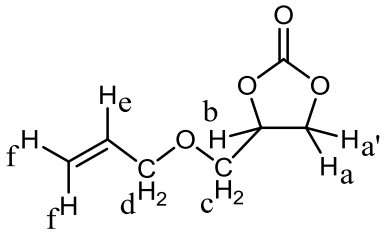
4-chloromethyl-1,3-dioxolan-2-one

^{1}H NMR (400 MHz, benzene-d_6) δ ppm 2.53 (dd, J=4.1 Hz, 12.1 Hz, **Ha**, 1H), 2.69 (dd, J=5.1 Hz, 12.1 Hz, **Ha'**, 1H), 3.33 (m, **Hc**, 2H), 3.65 (m, **Hb**, 1H).

Estimation of **4-Allyloxymethyl-1,3-dioxolan-2-one**:

^{1}H NMR spectrum (400MHz, benzene-d_6): *=cyclic carbonate

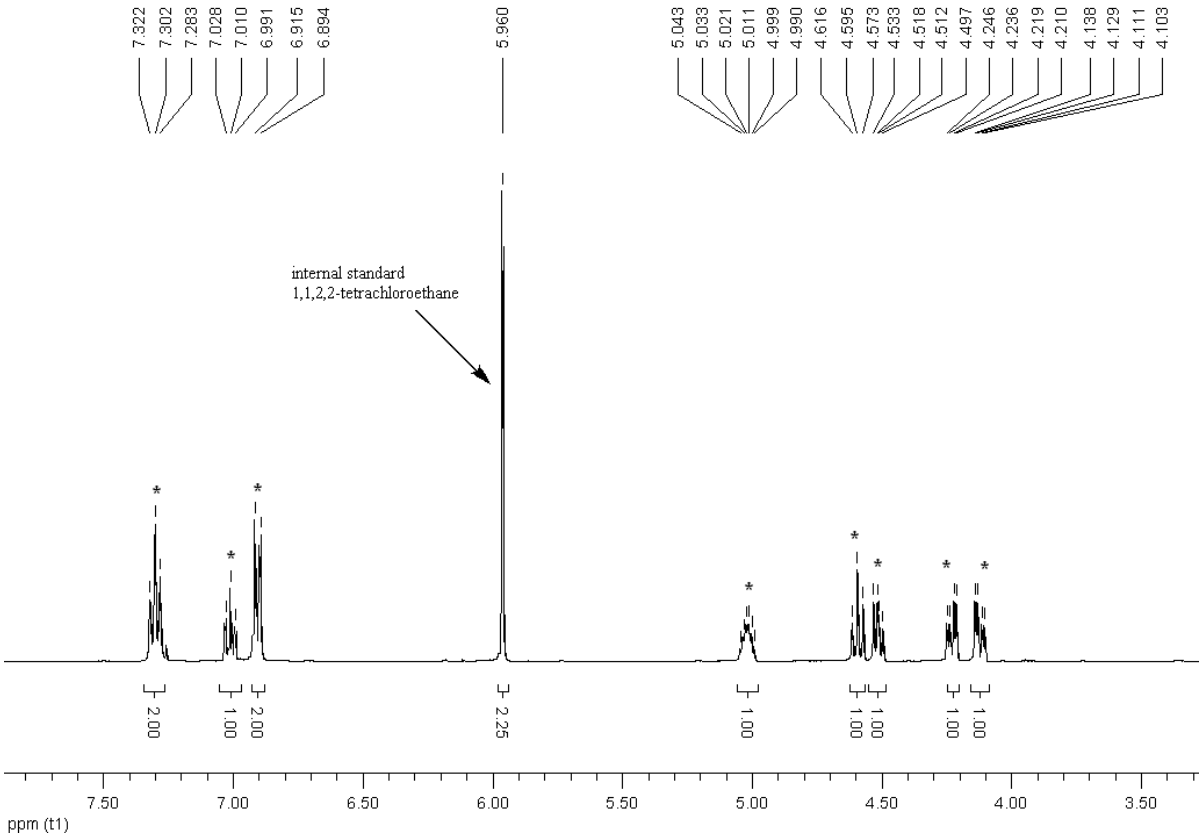


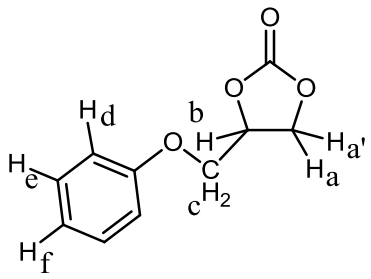


4-Allyloxymethyl-1,3-dioxolan-2-one:
^{1}H-NMR (400 MHz, benzene-d_6) δ ppm 2.73 (dd, J=3.1 Hz, 10.9 Hz, **Ha**, 1H,), 2.92 (dd, J=2.7 Hz, 10.9 Hz, **Ha'**, 1H), 3.45 (t, J=8.3Hz, **Hc**, 1H), 3.57 (m, **Hc**, **Hd**, 3H), 3.83 (m, **Hb**, 1H), 4.96 (d, J=10.4 Hz, **Hf**, 1H), 5.06 (d, J=17.3 Hz, **Hf**, 1H), 5.60 (dq, 1H, J=5.2 Hz, 10.4 Hz, **He**, 1H).

Estimation of **4-phenyloxymethyl-1,3-dioxolan-2-one**:

^{1}H NMR spectrum (400MHz, benzene-d_6): *=cyclic carbonate

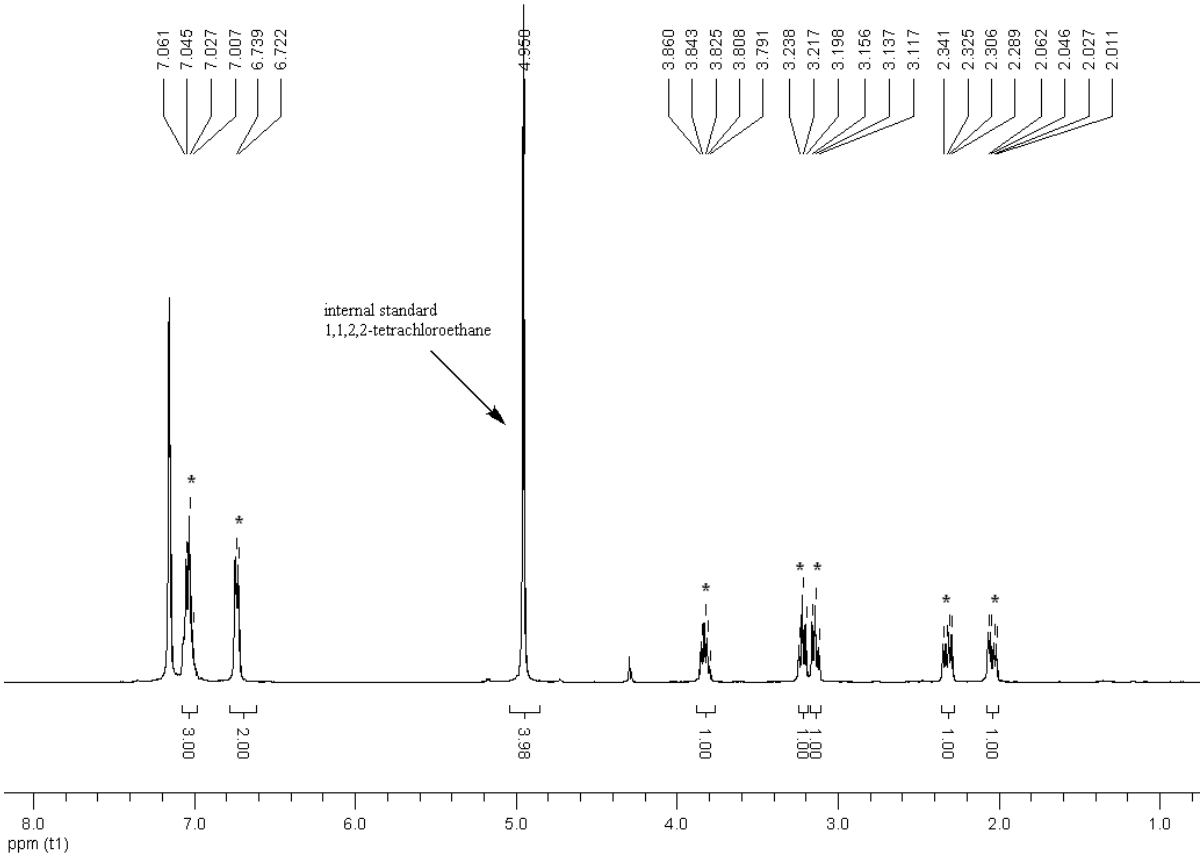


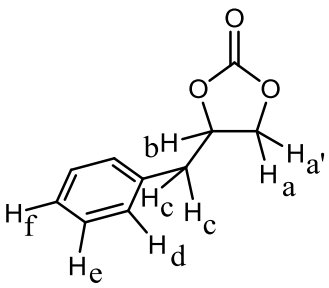


4-phenyloxymethyl-1,3-dioxolan-2-one:
^{1}H-NMR (400 MHz, $CDCl_3$) δ ppm 4.12 (dd, J=3.5 Hz, 10.7 Hz, **Ha**, 1H), 4.23 (dd, J=3.9 Hz, 10.7 Hz, **Ha'**, 1H), 4.51 (dd, J=6.0 Hz, 8.4 Hz, **Hc**, 1H), 4.59 (t, J=8.5 Hz, **Hc**, 1H), 5.02 (m, **Hb**, 1H), 6.90 (d, J=8.3 Hz, **Hd**, 1H), 7.01 (t, J=7.4 Hz, **Hf**, 1H), 7.30 (t, J=7.6 Hz, **He**, 2H).

Estimation of **4-benzyl-dioxolan-2-one**:

^{1}H NMR spectrum (400MHz, benzene-d_6): *=cyclic carbonate



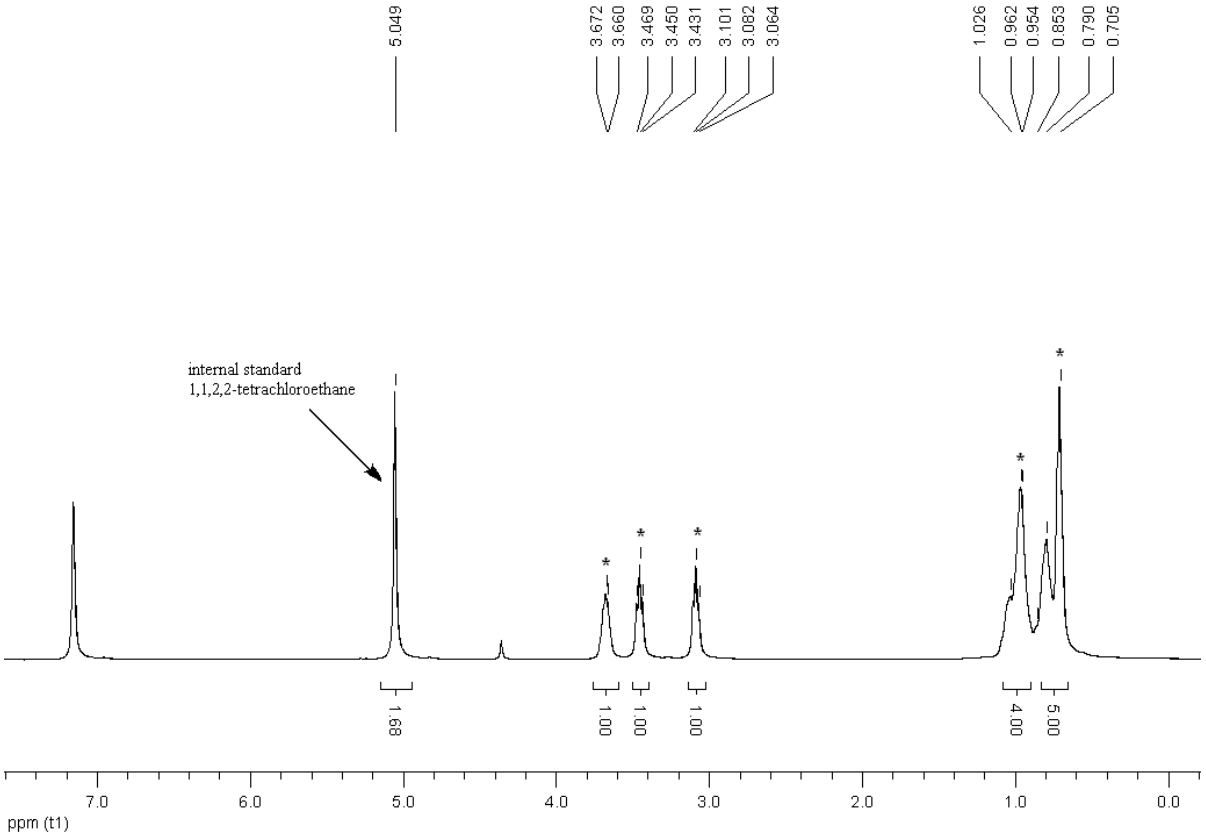


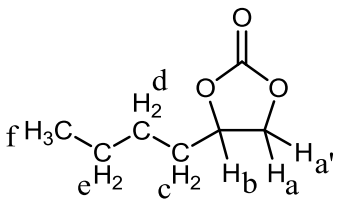
4-benzyl-1,3-dioxolan-2-one

^{1}H NMR (400 MHz, benzene-d_6) δ ppm 2.04 (dd, J=6.3 Hz, 14.1 Hz, **Ha**, 1H), 2.32 (dd, J=6.7 Hz, 14.1 Hz, **Ha'**, 1H), 3.14 (t, J=7.7 Hz, **Hc**, 1H), 3.22 (t, J=8.1 Hz, **Hc**, 1H), 3.83 (p, J=6.8 Hz, **Hb**, 1H), 6.73 (d, J=6.8 Hz, **Hd**, 3H), 7.04 (m, **He**, **Hf**, 3H).

Estimation of **4-butyl-dioxolan-2-one**:

^{1}H NMR spectrum (400MHz, benzene-d_6): *=cyclic carbonate





4-butyl-1,3-dioxolan-2-one:
^{1}H NMR (400 MHz, benzene-d_6) δ ppm 0.69-1.03 (m, **Hc**, **Hd**, **He**, Hf, 9H), 3.09 (t, J=7.5 Hz, **Ha**, 1H), 3.46 (t, J=7.8 Hz, **Ha'**, 1H), 3.68 (m, **Hb**, 1H).