Electronic Supplementary Material (ESI) for Polymer Chemistry.

Metallocene catalysts for the ring-opening co-polymerisation of epoxides and cyclic anhydrides

Matthew S. Shaw,[a] Morgan R. Bates,[a] Matthew D. Jones,[b] Benjamin D. Ward.[a]

[a] School of Chemistry, Cardiff University, Main Building, Park Place, Cardiff CF10 3AT, UK.

[b] Department of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, UK.

Email: WardBD@Cardiff.ac.uk

Contents

Experimental

Cp_2TiCl_2, Cp_2ZrCl_2 and Cp_2HfCl_2 were purchased and used without further purification. Anhydrous toluene and dichloromethane were collected from an MBraun SPS800 solvent purification system fitted with an alumina column, before degassing and re-saturation with argon. Anhydrous THF was distilled over molten potassium in an argon atmosphere. Anhydrides were extracted into hot chloroform, concentrated, dried, and then sublimed under vacuum. Epoxides and $CDCl_3$ were dried over CaH_2, degassed *via* freeze-pump-thaw, and distilled. DMAP was sublimed under vacuum and used to prepare stock solutions (78 mg mL^{-1} in dry THF) which were remade regularly. All reactants used in small scale polymerisations, alkoxide syntheses and stoichiometric reactions were stored in a nitrogen dry box.

NMR experiments were performed on Bruker Fourier 300, Avance III HD 400 or 500 spectrometers, with the chemical shifts (δ) referenced to residual solvent resonances (δ^H, δ^C = 0 for $Si(CH_3)_4$). Electrospray ionisation mass spectrometry analyses were performed by analytical services, Cardiff University School of Chemistry. Polymers were characterised using an Agilent 1260 Infinity II Multi Detector GPC/SEC fitted with a 5 µm Mixed-D PLgel column and calibrated by polystyrene standards. Analysis was performed using THF as an eluent (1 mL min^{-1} flow rate), with samples made up to 3 mg mL^{-1} before auto injection. MALDI-ToF experiments were performed in positive mode on a Bruker AutoFlex speed MALDI-ToF mass spectrometer, with samples prepared by vortex mixing DCTB (50 µL of 20 mg mL^{-1} in THF), polymer sample (10 µL of 10 mg mL^{-1} in THF) and NaOAc (5 µL of 50 mg mL^{-1} in THF).

For each small scale polymerisation run, in a nitrogen-filled glove box, an oven dried 7 mL screw-cap vial was charged with a metallocene (1 eq., 3.2 or 6.4 µmol), anhydride (400 eq.) and a magnetic stirrer bar. Anhydrous toluene (1 mL), epoxide (400 eq.) and stock DMAP solution (1 or 2 eq.) were then added by autopipette, before the vial was sealed and placed in a 20-well aluminium heating block. The temperature was controlled by a thermocouple placed in another 7 mL vial containing paraffin oil (2 mL) as a reference. After continuous stirring for a given time, the reaction mixtures were removed from the heat and aliquots taken for ^1H NMR analysis. Polymeric material was then isolated by adding dichloromethane (0.5 mL) before precipitating in isopropanol. The resulting solid was then filtered, washed with isopropanol and dried *in vacuo*.

For large scale polymerisation, phthalic anhydride was used as received, toluene and limonene oxide (*(+)-Limonene 1,2-epoxide,* mixture of *cis*/*trans* isomers) were dried over molecular sieves, and DMAP was sublimed under vacuum. Phthalic anhydride (190 g, 1280 mmol, 400 eq.), limonene oxide (195 g, 210 mL, 1280 mmol, 400 eq.), zirconocene dichloride (935 mg, 3.2 mmol, 1 eq.), DMAP (782 mg, 6.4 mmol, 2 eq.) and toluene (500 mL) were charged into an argon-purged 2 L reactor. The reactor was fitted with an oil bubbler and heated to 100 °C with mechanical stirring. During this time, aliquots were taken *via* syringe against a flow of argon to monitor conversion, and extra toluene was added as the solvent level reduced. After 3 days, the reaction mixture was poured onto isopropanol, where after settling the supernatant was decanted. The polymer was then washed with isopropanol, before filtering and drying *in vacuo*.

Syntheses of alkoxide complexes in the absence of cocatalyst were performed in Schlenk flasks and employed 20 equivalents of epoxide with each addition alongside dichloromethane (10 mL). To follow

the progress of the reaction, the mixtures were concentrated *in vacuo* and dried, before restarting with fresh solvent and epoxide. Stoichiometric reactions in the presence of DMAP were carried out in $CDCl_3$ in an NMR tube sealed with a J. Young tap. Reactions were set up in a nitrogen-filled glove box, with any subsequent addition of reagents (epoxide or anhydride) also done in a glove box. Heating of samples was done where detailed by placing the NMR tube in an oil bath heated to 60 °C.

For the attempted synthesis of poly(CHO) using [Cp_2ZrCl_2], identical reaction conditions described previously for small scale reactions were employed, but with the omission of the anhydride. After 24 hours, no polymeric material precipitated out of hexane, and the dry residue contained no polymers or oligomers of CHO, as determined by MALDI-ToF and Electrospray Ionisation Mass Spectrometry respectively.

Conversion *vs.* time graph for neat CHO-PA [Cp_2TiCl_2] polymerisations

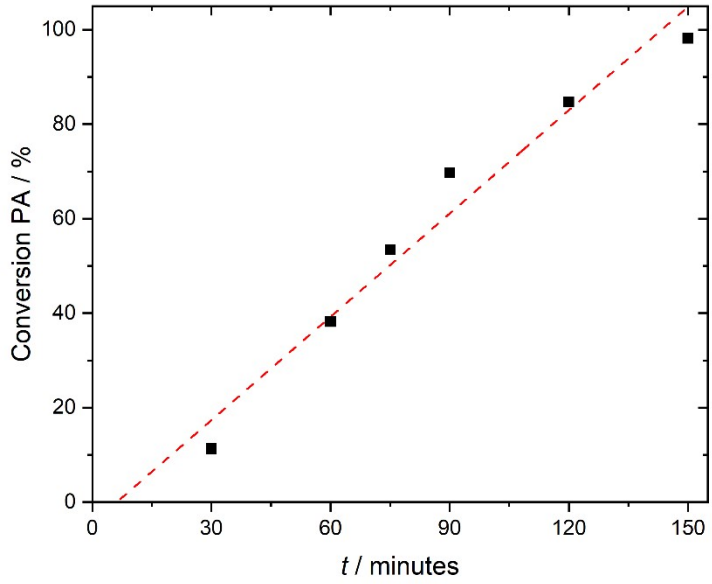


Figure S1: *Conversion PA versus time (as measured by ^{1}H NMR spectroscopy of reaction aliquots) of CHO-PA copolymerisations conduced with neat CHO as the solvent. The data show the expected linear pseudo zero-order dependency of conversion upon time. Conditions; 6.4 µmol [Cp_2TiCl_2], 1:2:2000:400 [Cp_2TiCl_2]:[DMAP]:[CHO]:[PA], 80 °C.*

NMR and Mass Spectra from Stoichiometric Experiments

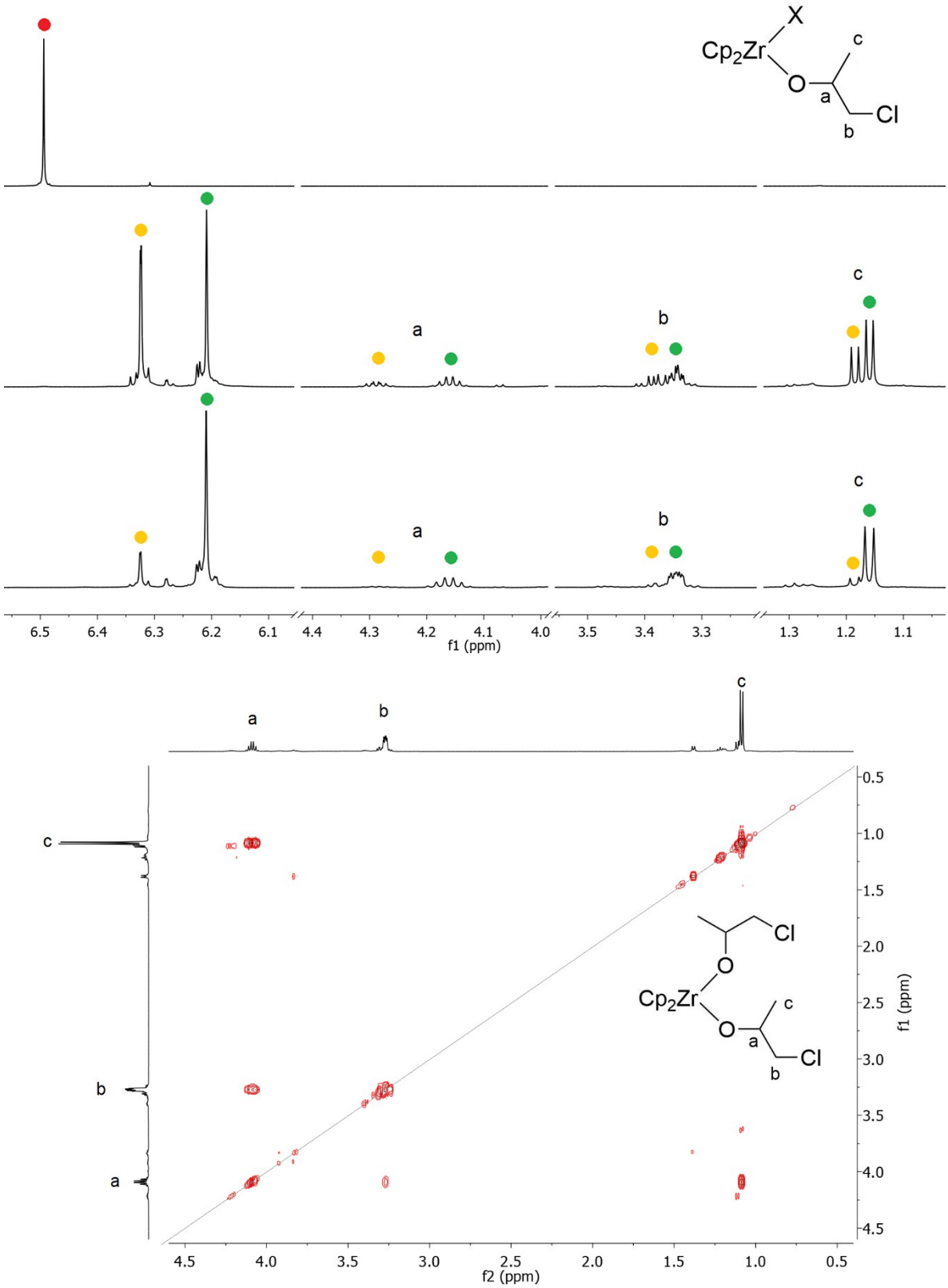


Figure S2: *Stacked ^{1}H NMR spectra ($CDCl_3$, 500 MHz) of top: Cp_2ZrCl_2 (red), middle: after reaction with propylene oxide and bottom: after addition of more propylene oxide (^{1}H-^{1}H COSY NMR below this) Yellow resonances represent the mono(alkoxide) product (X = Cl) and green the bis(alkoxide) (X = $OCH(Me)CH_2Cl$). The COSY spectrum highlights the coupling of a-b and a-c (but not b-c).*

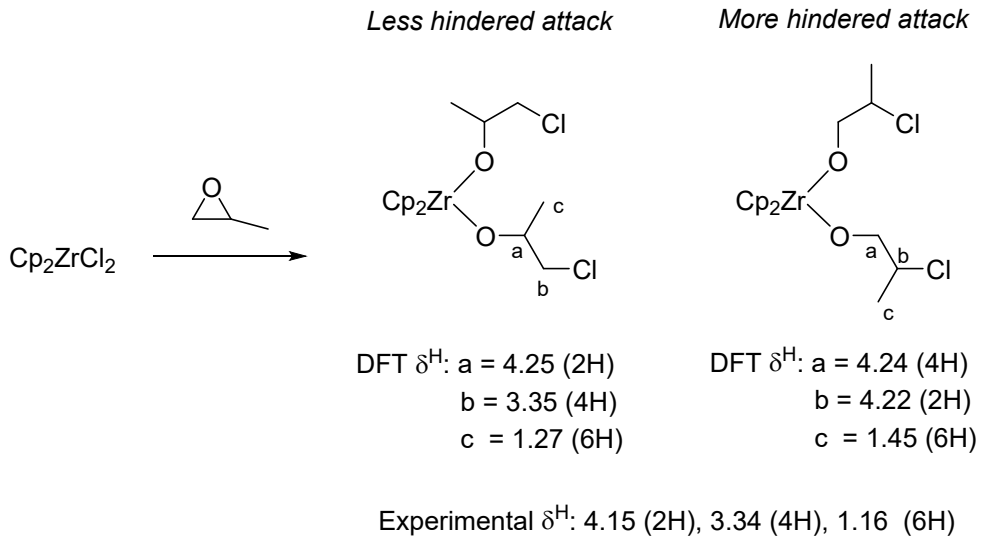


Figure S3: *DFT predicted ^{1}H NMR chemical shifts (Gaussian 09, in $CDCl_3$, ethanol used to convert calculated shielding tensors to chemical shifts) for both isomers of the bis(alkoxide) complex resulting from the reaction of zirconocene dichloride with excess propylene oxide. Note the far closer agreement with the experimental chemical shifts for the isomer resulting from chloride attack at the least hindered position of propylene oxide.*

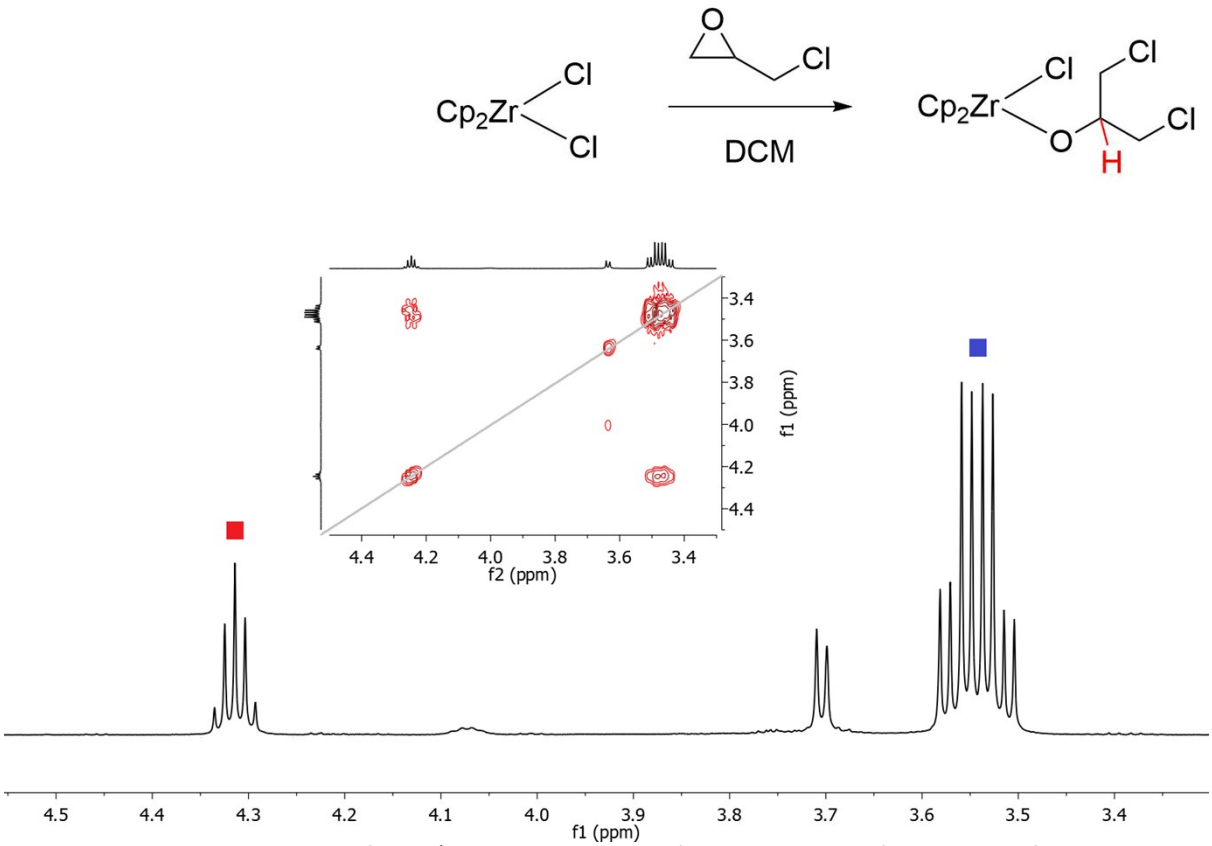


Figure S4: *Alkoxide region of the ^{1}H NMR spectrum ($CDCl_3$, 500 MHz) reaction of Cp_2ZrCl_2 with epichlorohydrin, with ^{1}H-^{1}H COSY insert. Red = 1:4:6:4:1 (J = 5.3 Hz) quintet resulting from coupling only to four chemically equivalent protons (blue), indicating reaction at the least hindered position.*

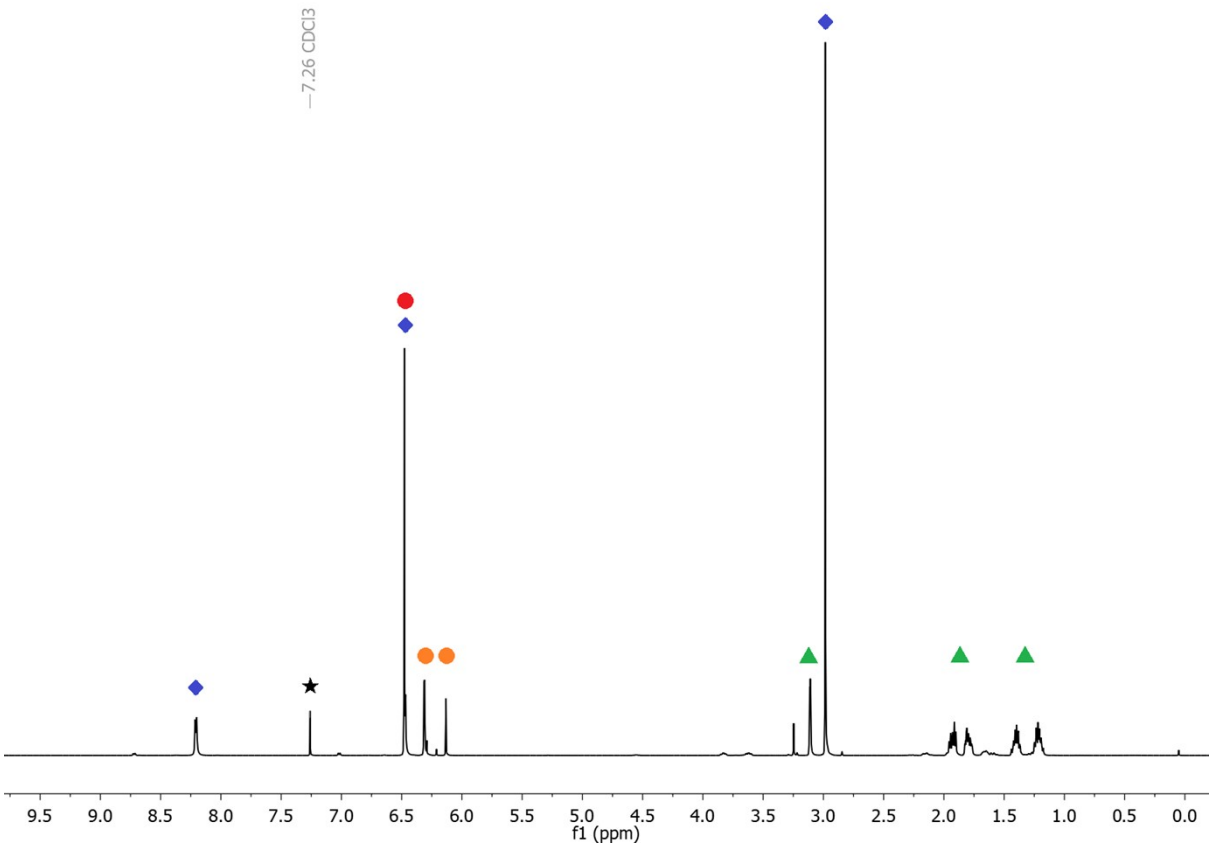


***Figure S5**: [1]H NMR spectrum ($CDCl_3$, 500 MHz) of a 1:2:2 mixture of Cp_2ZrCl_2: DMAP: CHO. Black star = $CDCl_3$, blue diamonds = DMAP, red circle = Cp_2ZrCl_2, green triangles = CHO, orange circles = new metallocene resonances.*

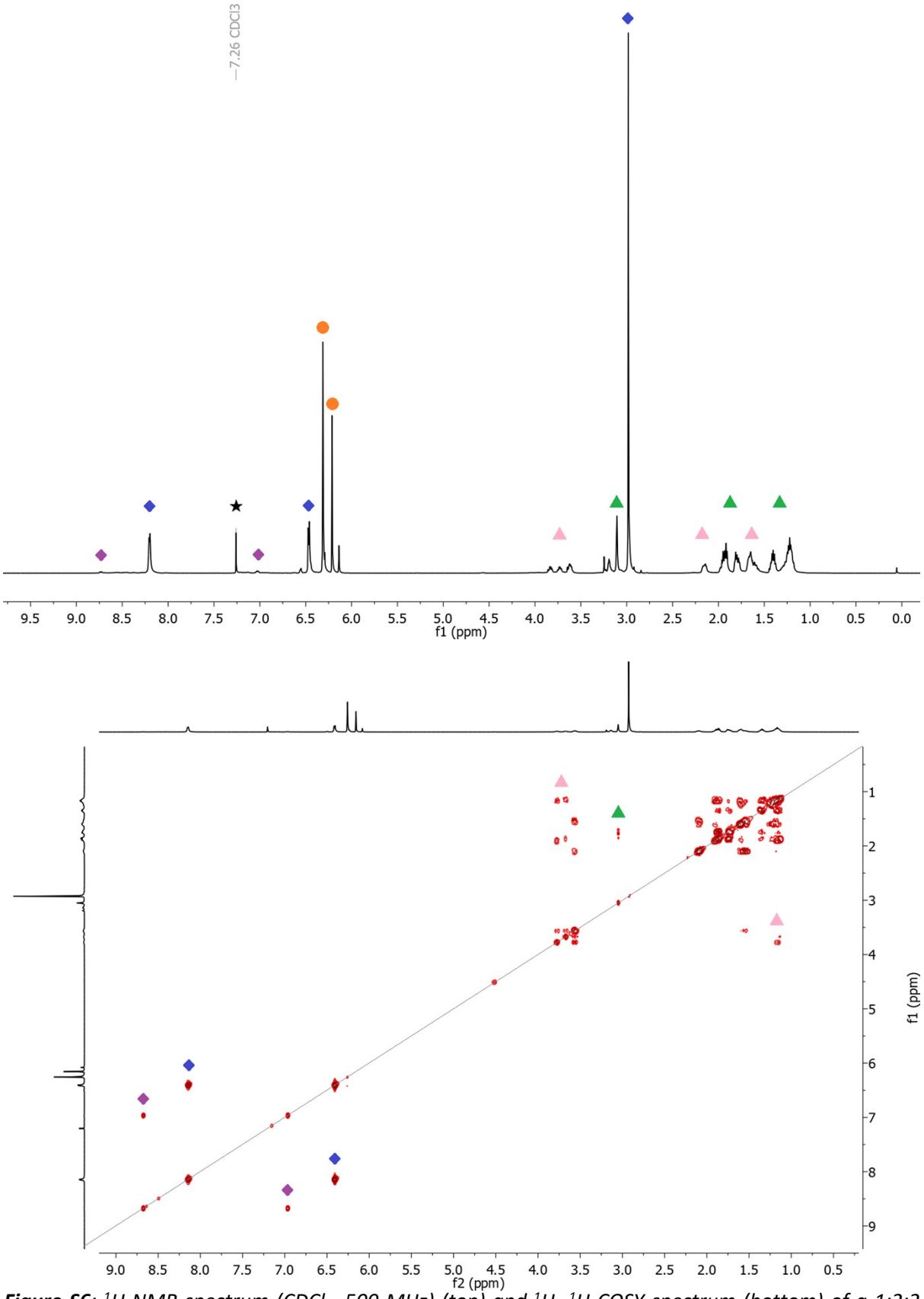


***Figure S6**: ^{1}H NMR spectrum ($CDCl_3$, 500 MHz) (top) and ^{1}H ^{1}H COSY spectrum (bottom) of a 1:2:2 mixture of Cp_2ZrCl_2: DMAP: CHO after being heated to 60 °C. Black star = $CDCl_3$, blue diamonds = DMAP, red circle = Cp_2ZrCl_2, green triangles = CHO, orange circles = new metallocene resonances, purple diamonds = reacted DMAP, pink triangles = ring-opened CHO.*

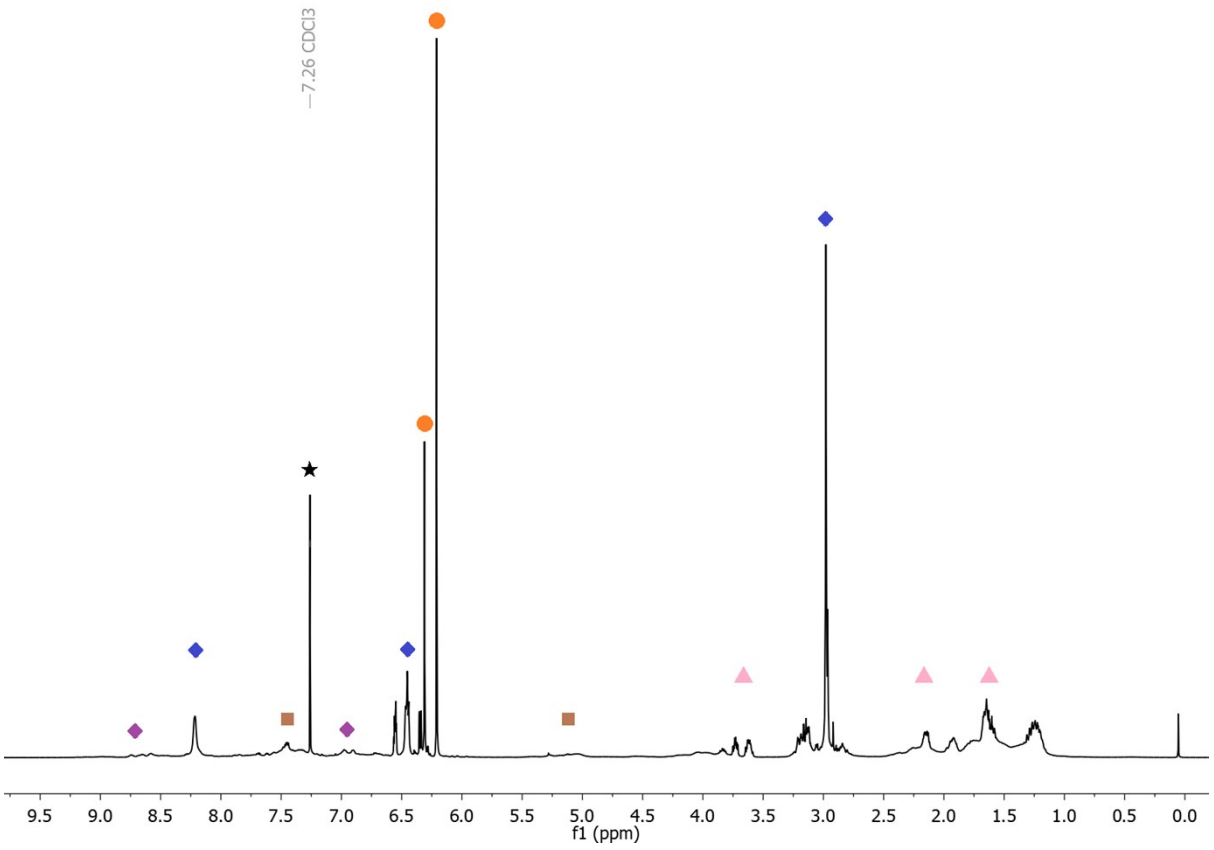


***Figure S7**: [1]H NMR spectrum ($CDCl_3$, 500 MHz) of a 1:2:2:2 mixture of Cp_2ZrCl_2: DMAP: CHO: PA. Black star = $CDCl_3$, blue diamonds = DMAP, red circle = Cp_2ZrCl_2, green triangles = CHO, orange circles = new metallocene resonances, purple diamonds = reacted DMAP, pink triangles = ring-opened CHO. Brown squares = resonances associated with ring-opened PA.*

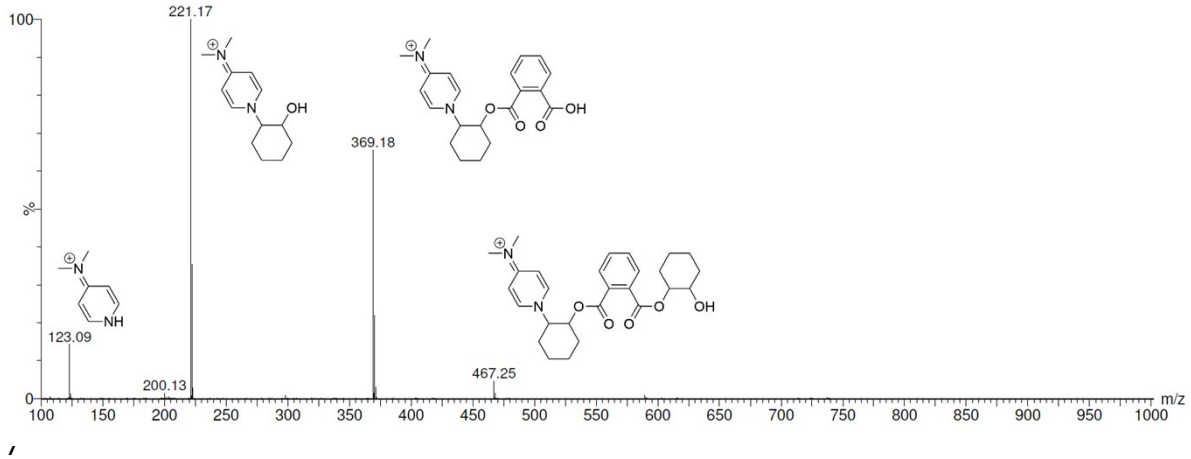


Figure S8: *Positive mode electrospray ionisation mass spectrum of the products of a 1:2:4:2 reaction of Cp_2ZrCl_2: DMAP: CHO: PA conducted in $CDCl_3$, with structures of characterisable ions indicated.*

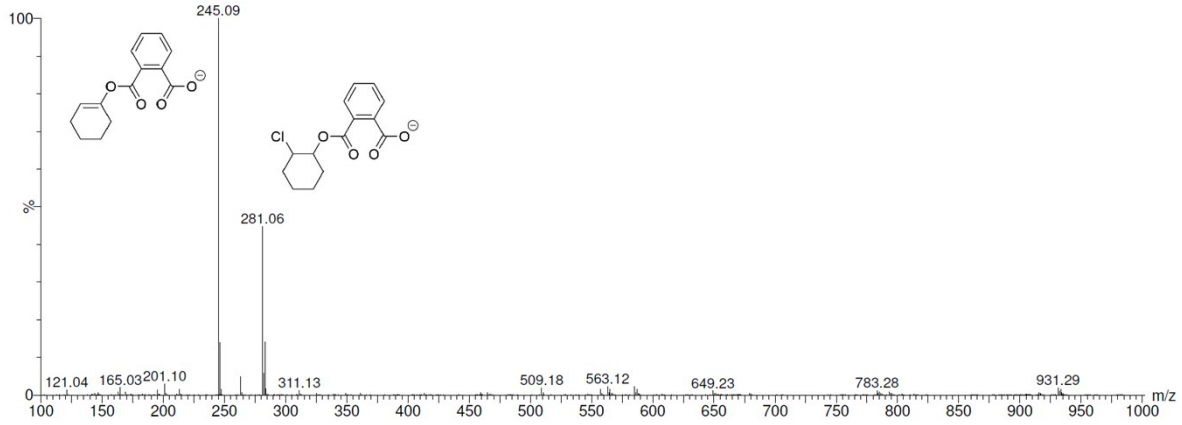


Figure S9: *Negative mode electrospray ionisation mass spectrum of the products of a 1:2:4:2 reaction of Cp_2ZrCl_2: DMAP: CHO: PA conducted in $CDCl_3$, with structures of characterisable ions indicated.*

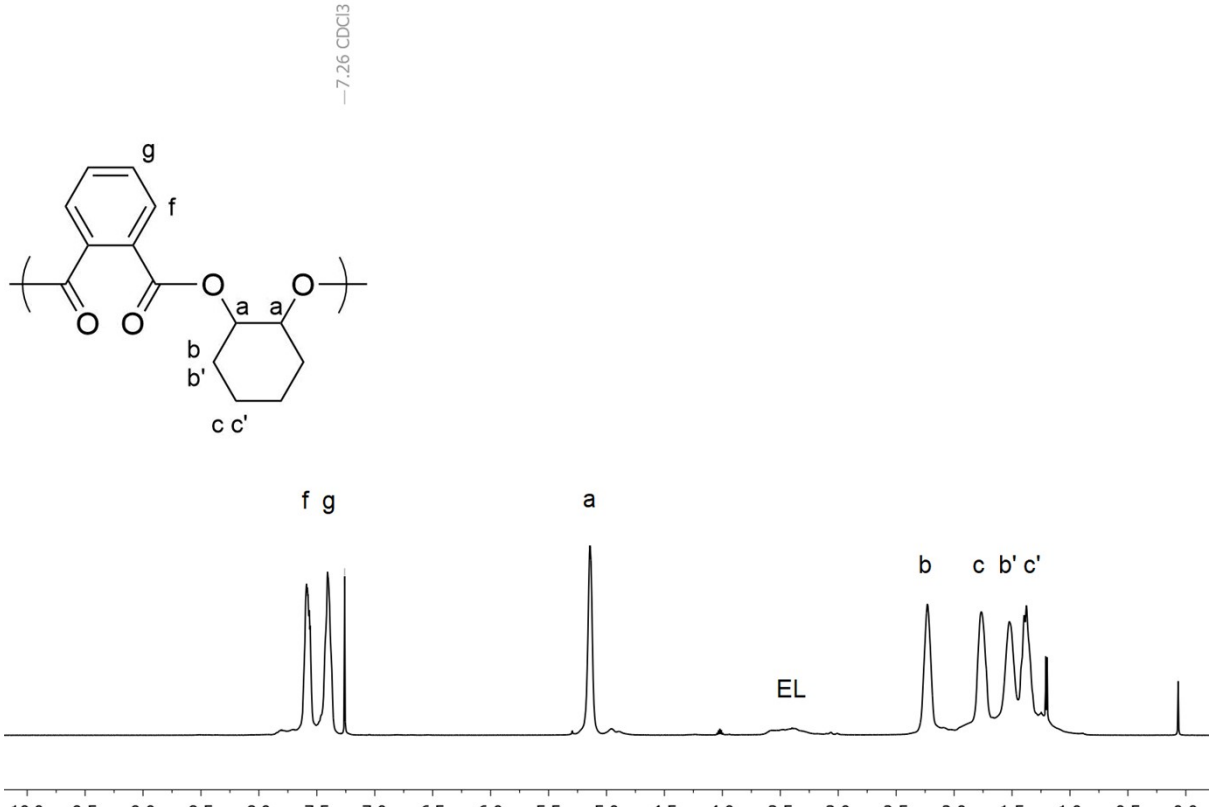


Figure S10: *Representative ^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of the CHO-PA copolymer. EL = ether linkages.*

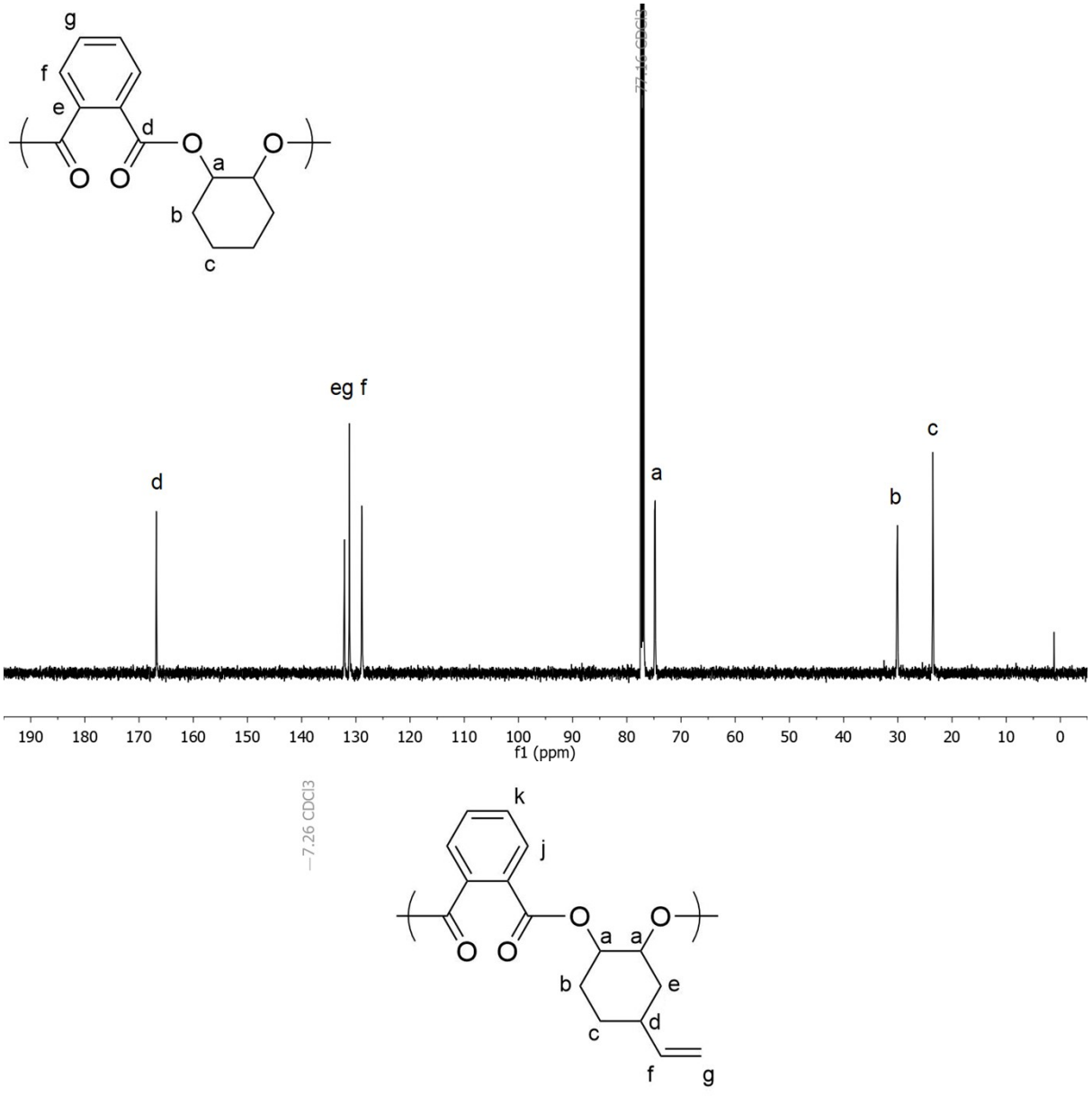
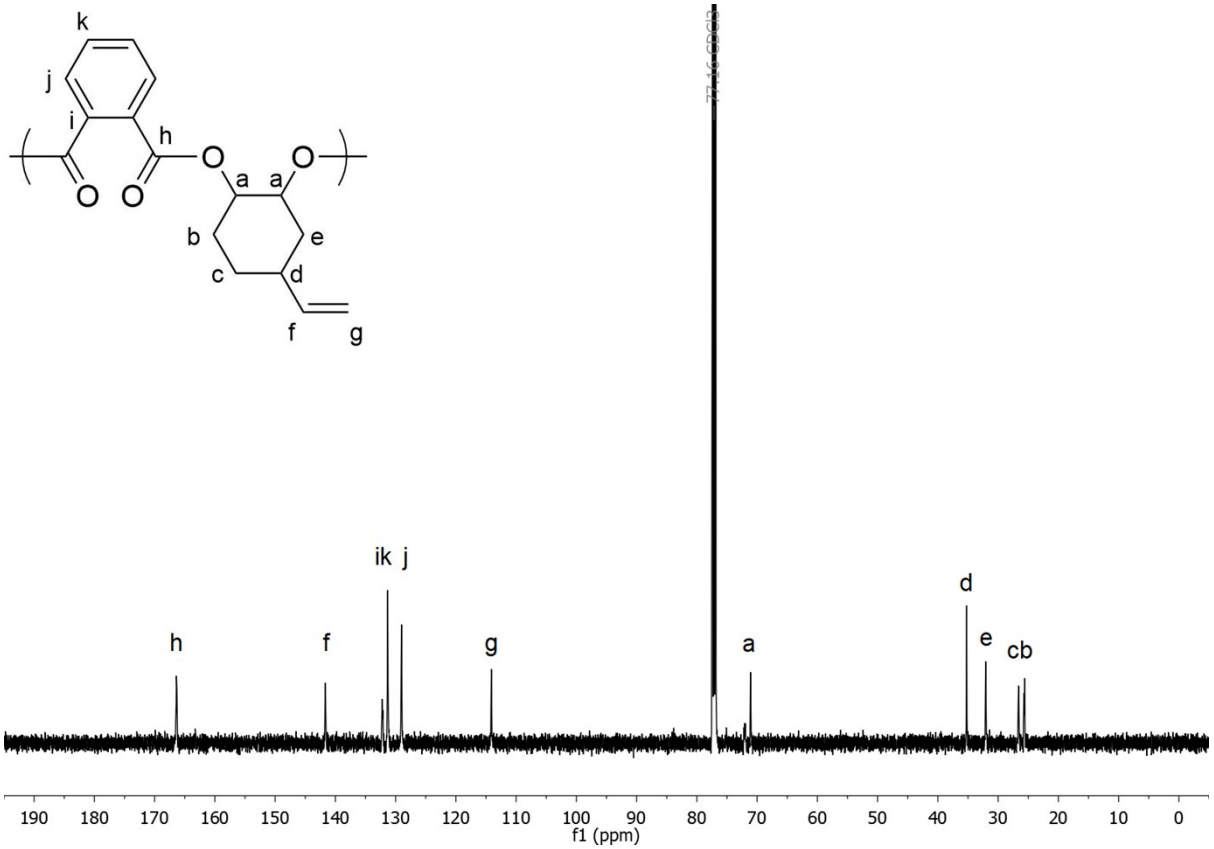


Figure S12: *Representative ^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of the VCHO-PA copolymer.*



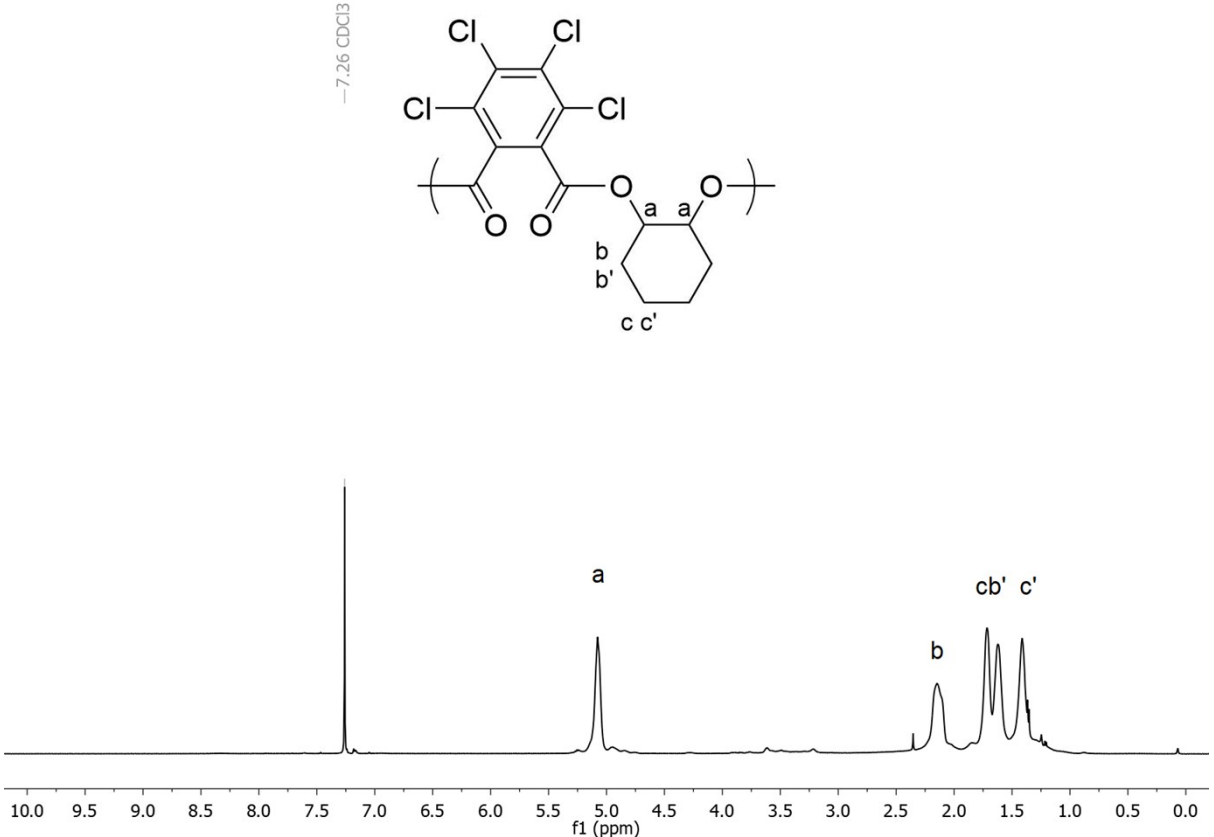
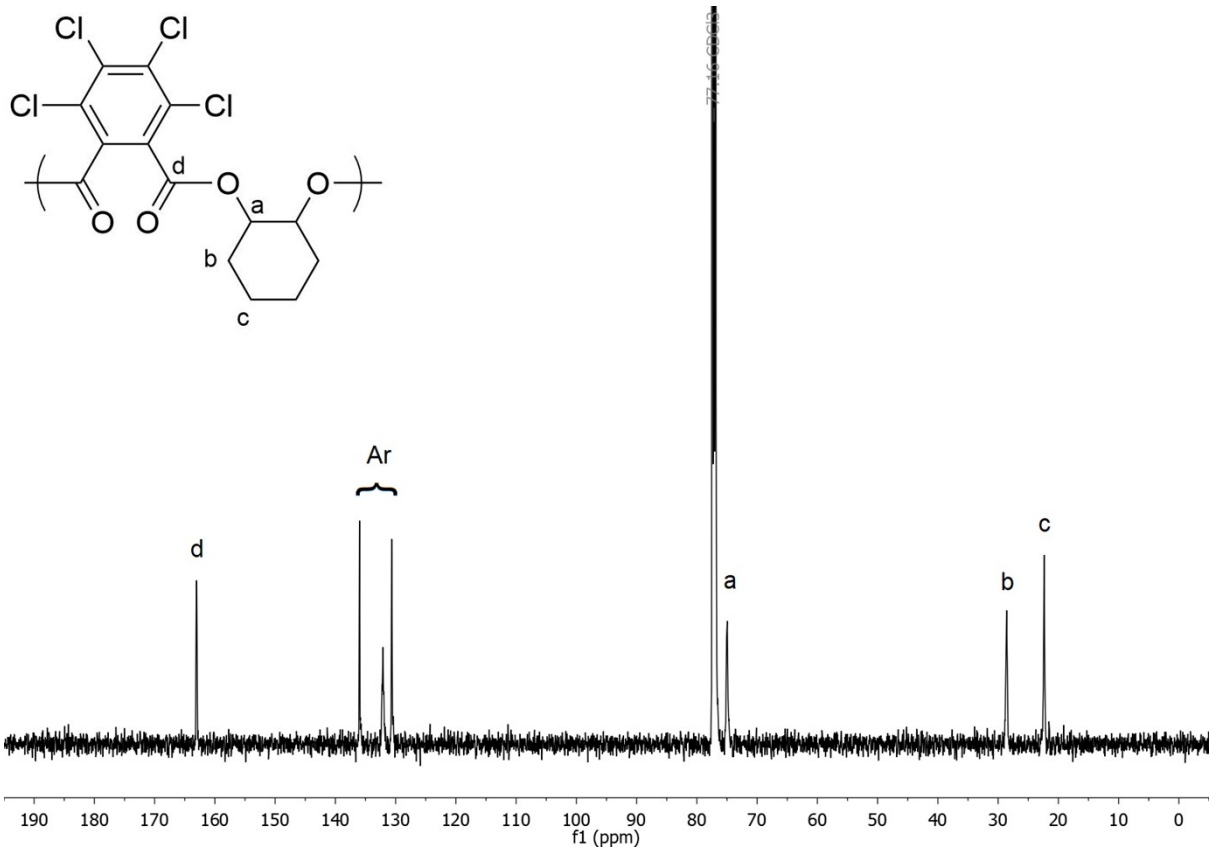


Figure S14: *Representative ^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of the CHO-TCPA copolymer.*



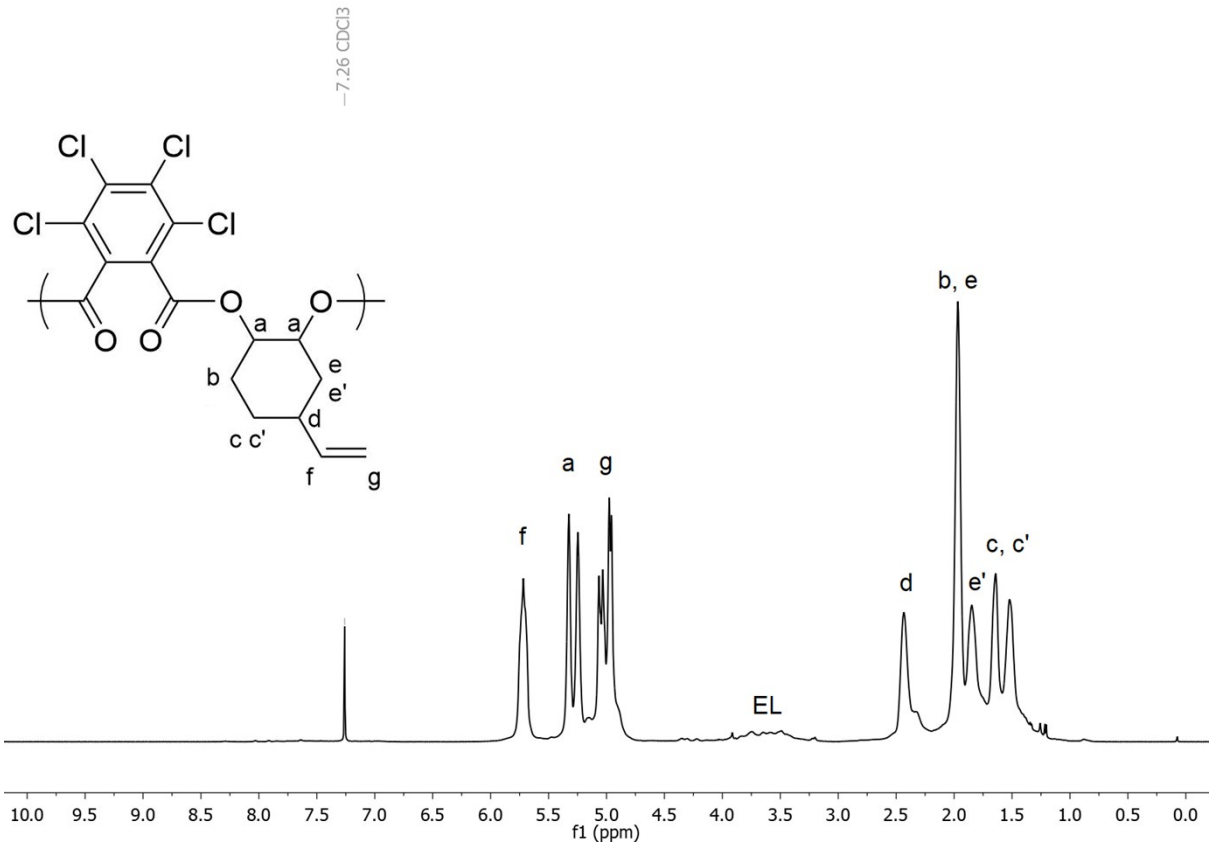
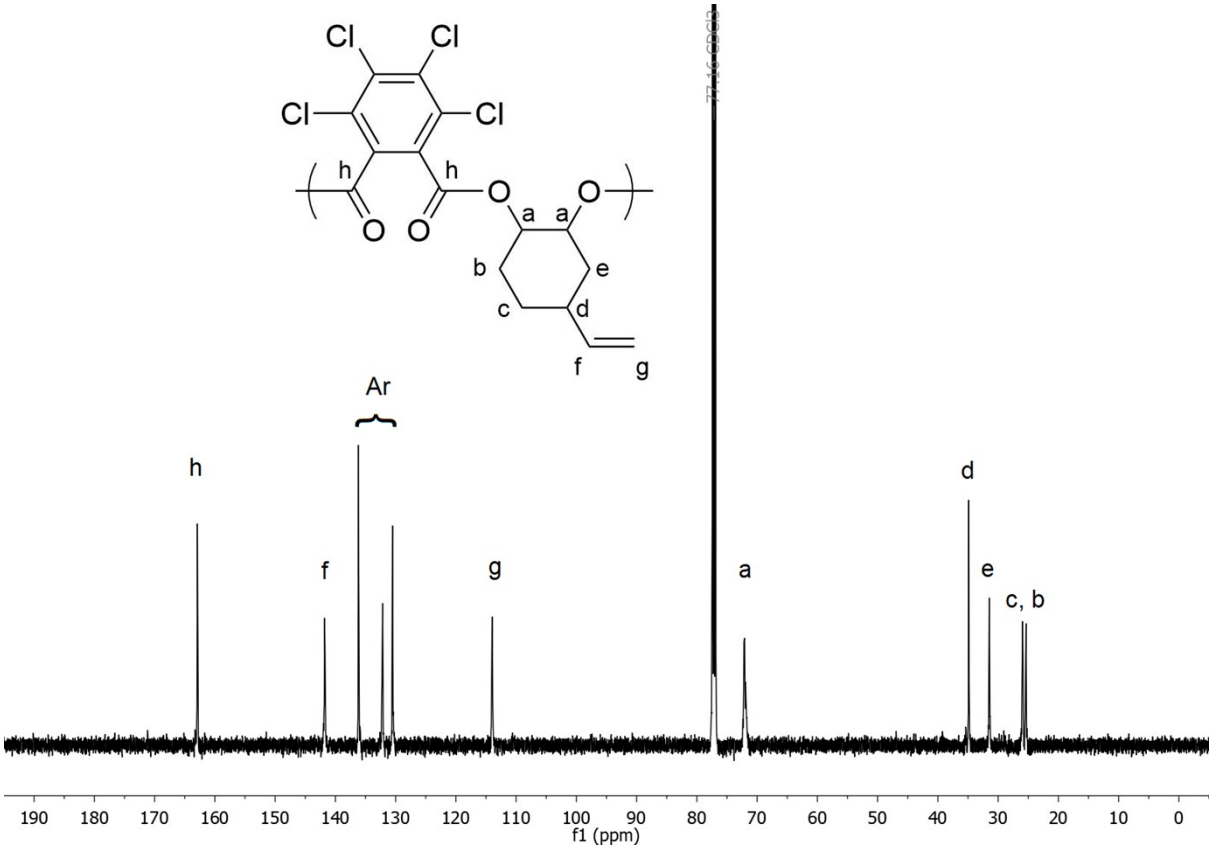


Figure S16: *Representative ^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of the VCHO-TCPA copolymer. EL = ether linkages.*



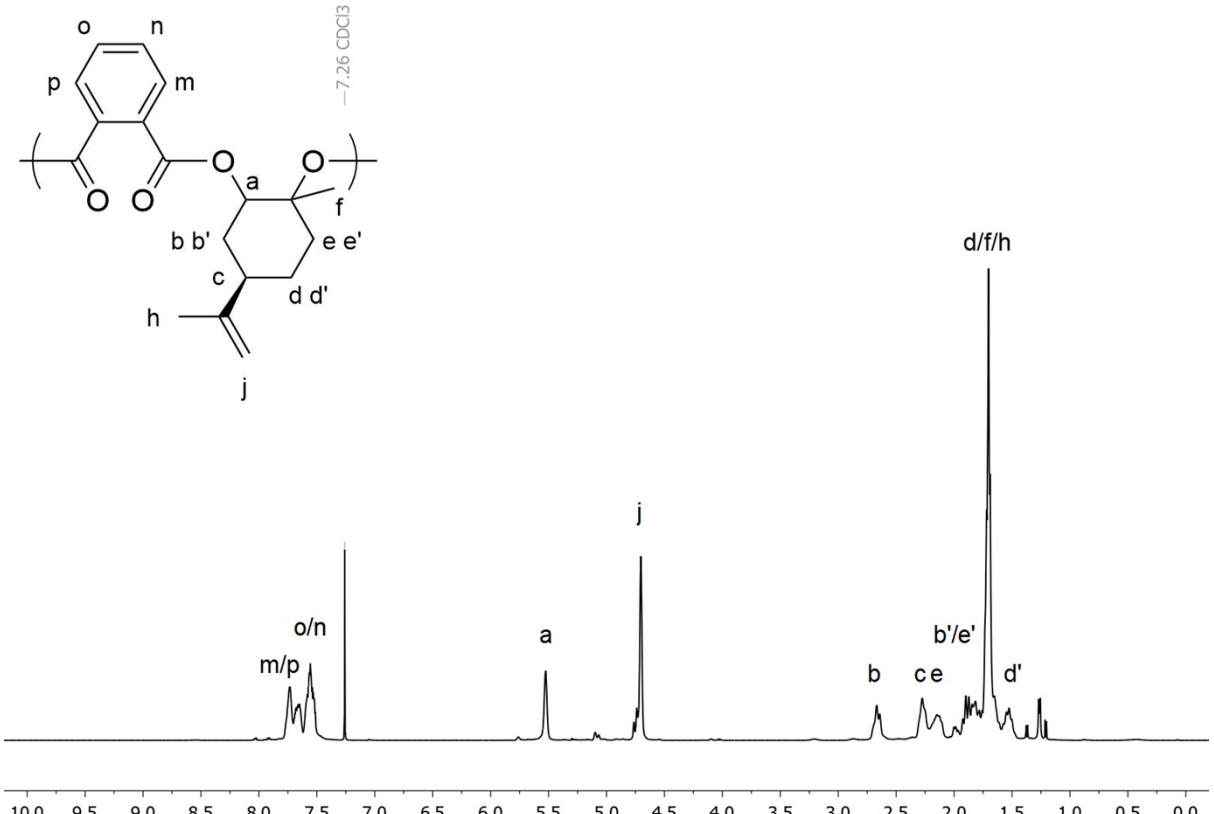


Figure S18: *Representative ^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of the LO-PA copolymer.*

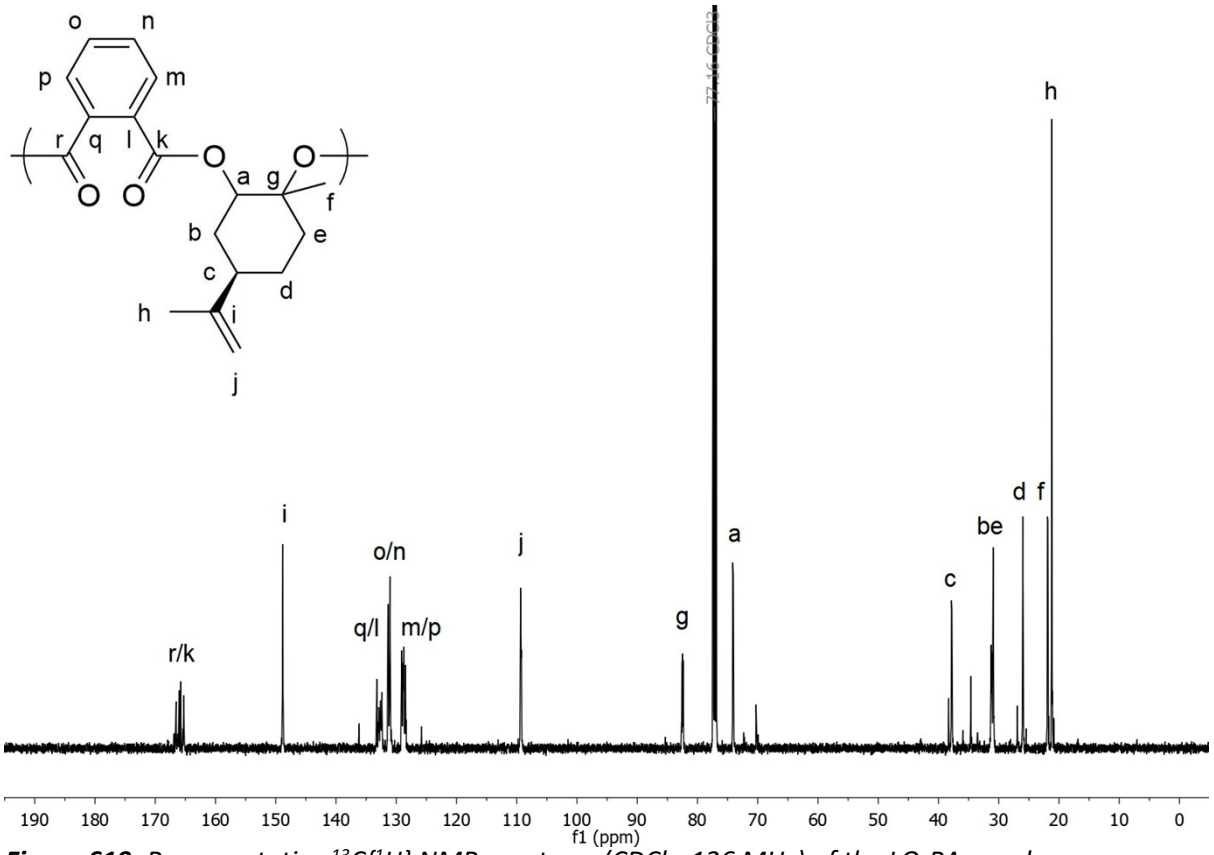


Figure S19: *Representative $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 126 MHz) of the LO-PA copolymer.*

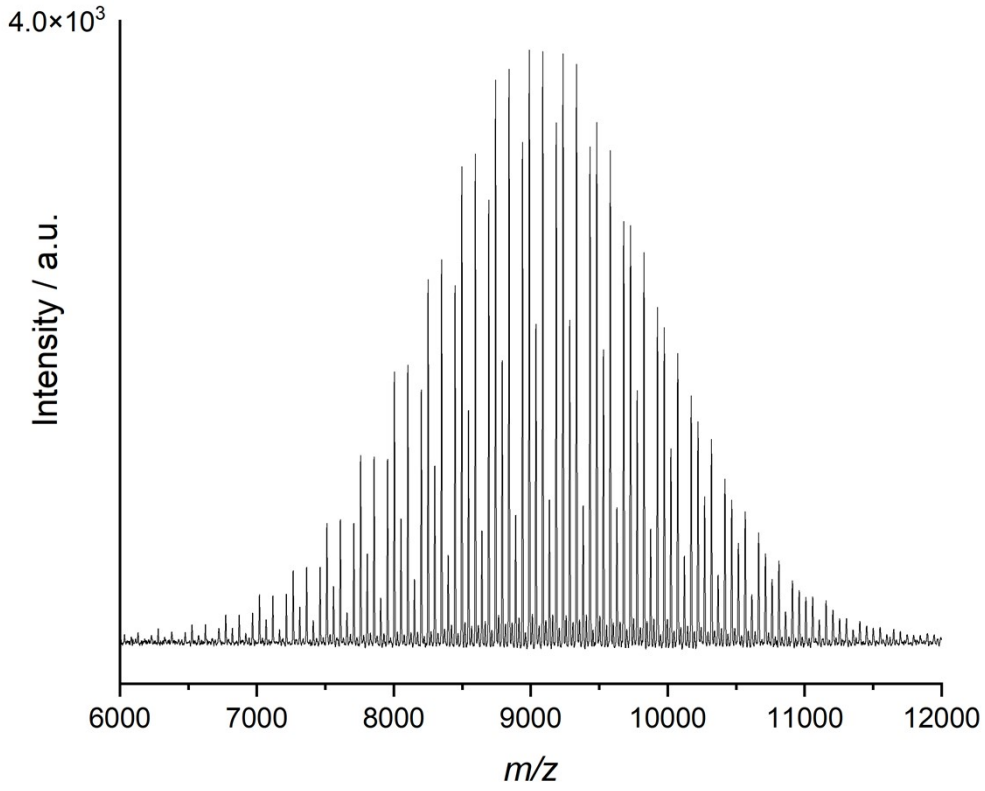


Figure S20: *MALDI-ToF spectrum of the CHO-PA copolymer ([Cp_2TiCl_2], entry 1, table 1).*

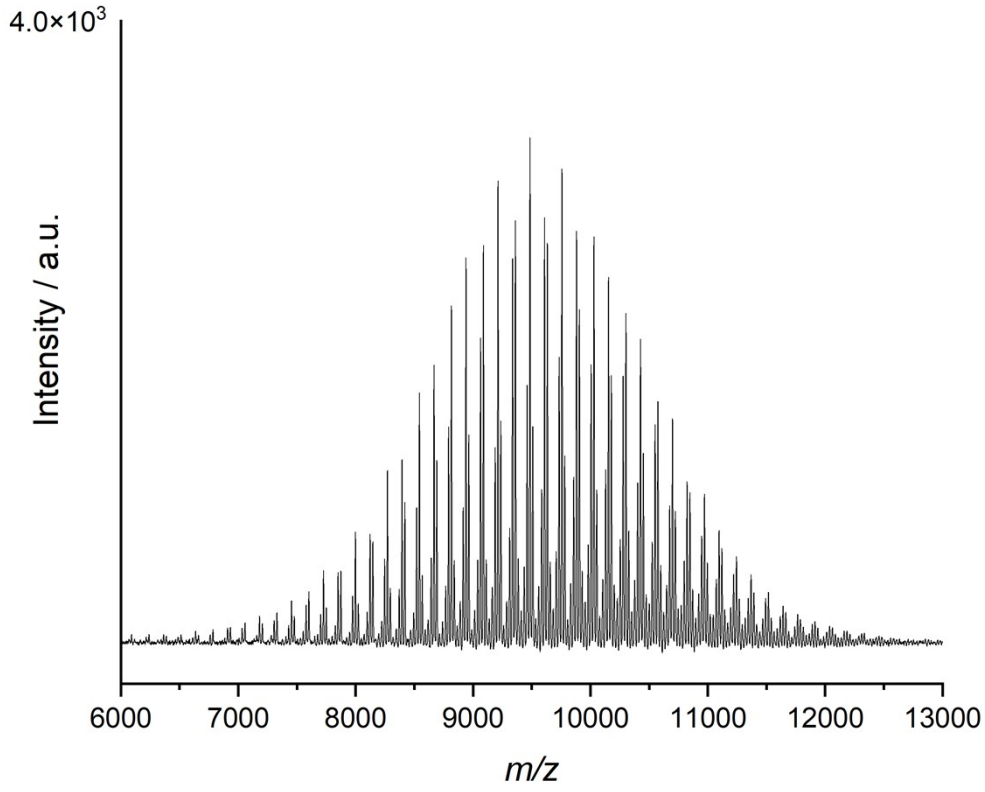


Figure S21: *MALDI-ToF spectrum of the VCHO-PA copolymer ([Cp_2ZrCl_2], entry 6, table 1).*

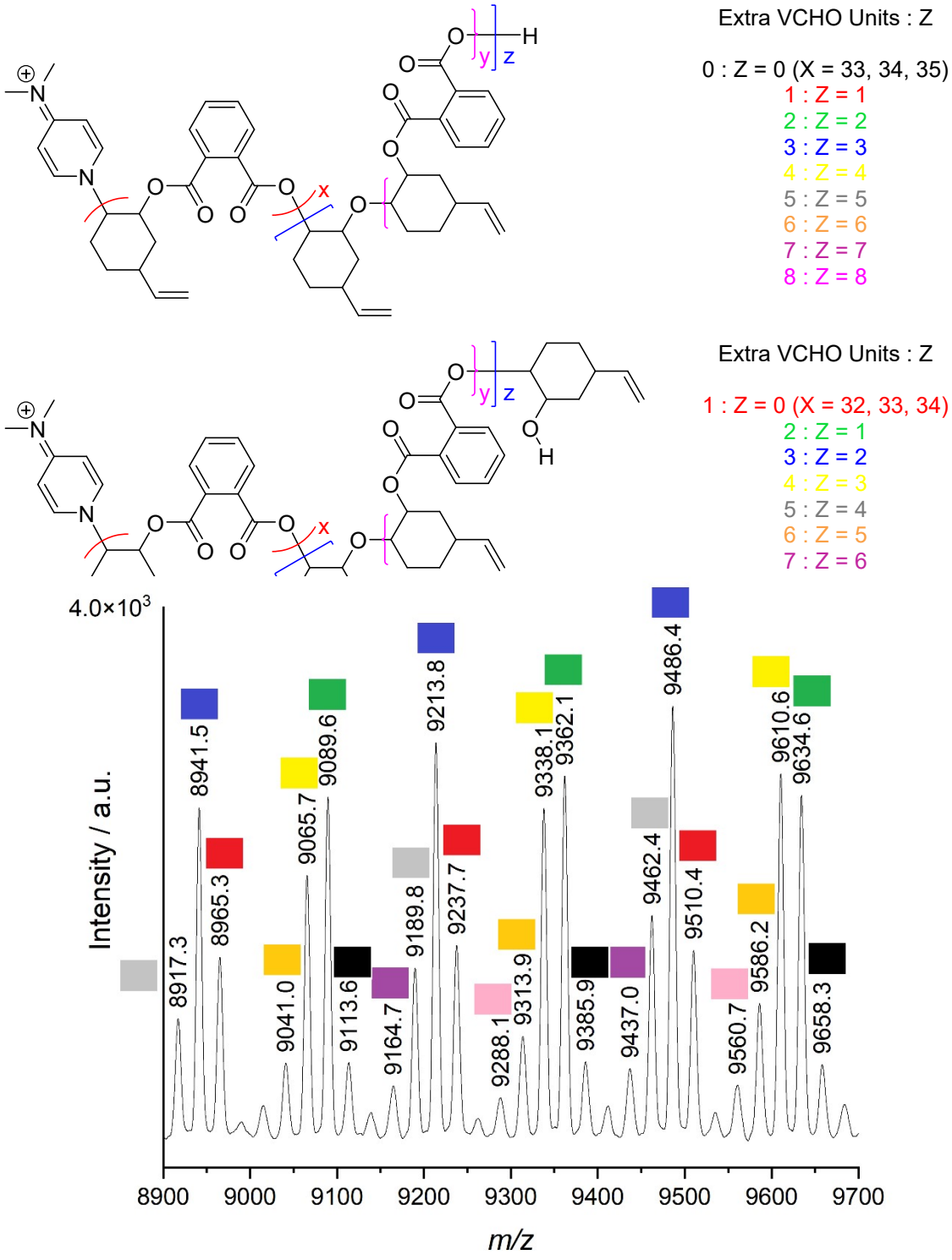


Figure S22: *Portion of the MALDI-ToF spectrum of the VCHO-PA copolymer ([Cp_2ZrCl_2], entry 6, table 1). Each labelled series represents a different number of additional epoxide units either terminating the polymer chain, within the polyester chain, or both, given these possibilities are indistinguishable by MALDI-ToF. This sample has a relatively low (80 %) ester selectivity, and so the appearance of series related to up to 8 additional VCHO units is to be expected.*

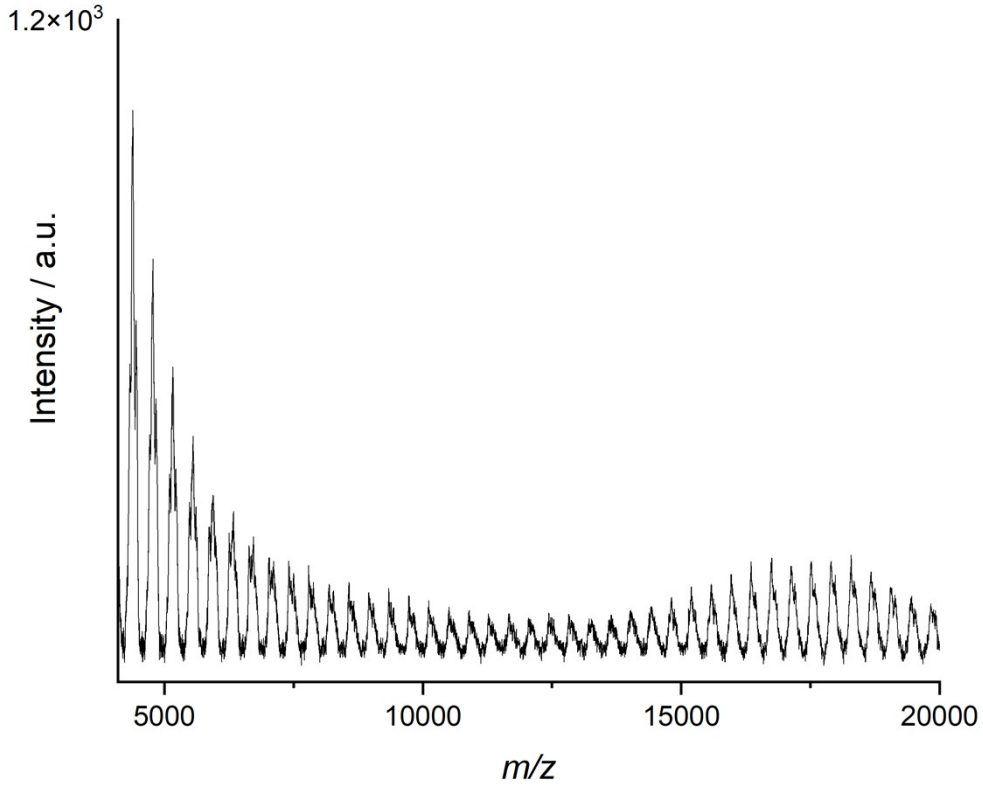


Figure S23: *MALDI-ToF spectrum of the CHO-TCPA copolymer (entry 4, table 2).*

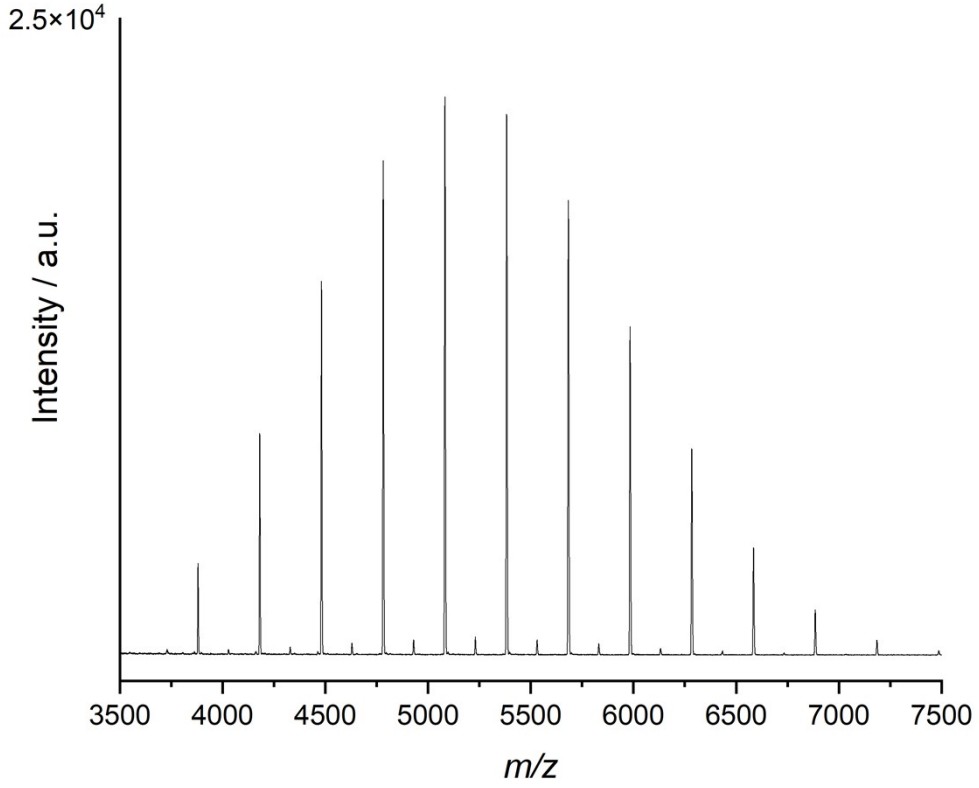


Figure S24: *MALDI-ToF spectrum of the LO-PA copolymer ([Cp_2ZrCl_2], entry 2, table 3).*

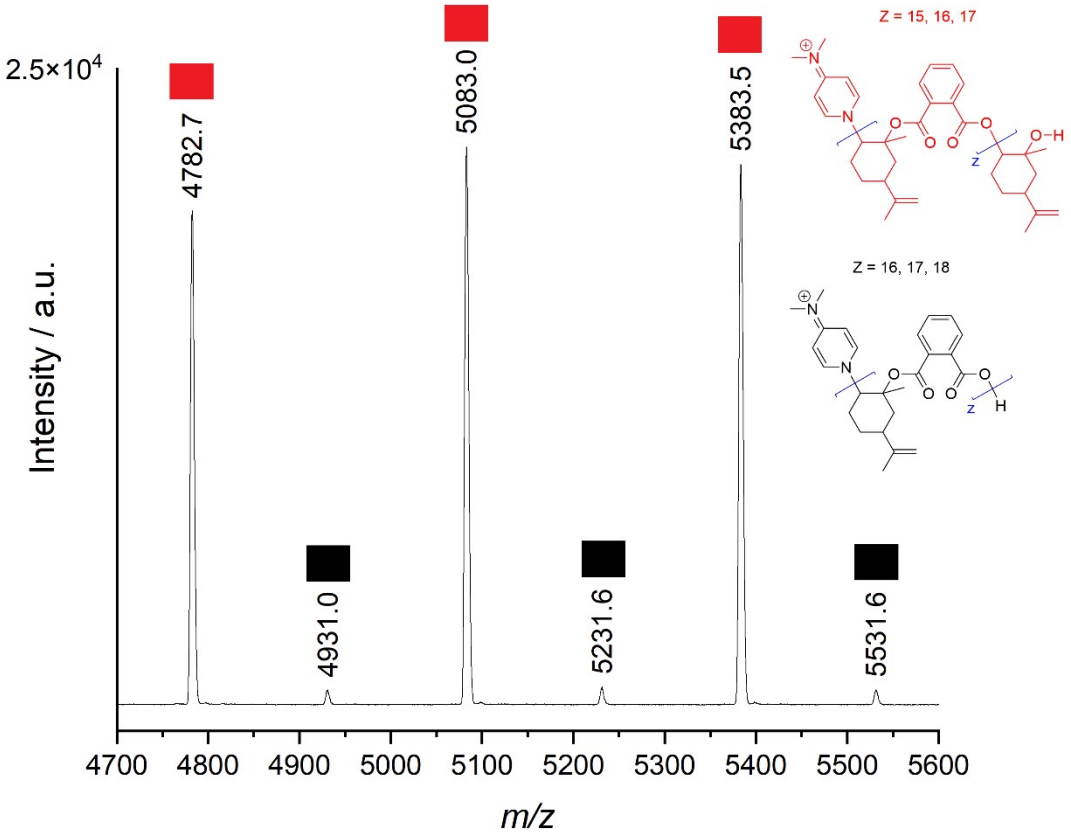


Figure S25: *Portion of the MALDI-ToF spectrum of the LO-PA copolymer ([Cp_2ZrCl_2], entry 2, table 3), with labelled series. Given the lack of polyether resonances observed in the ^{1}H NMR spectrum, the position of the "extra" LO unit in the red series is assigned as an end group.*

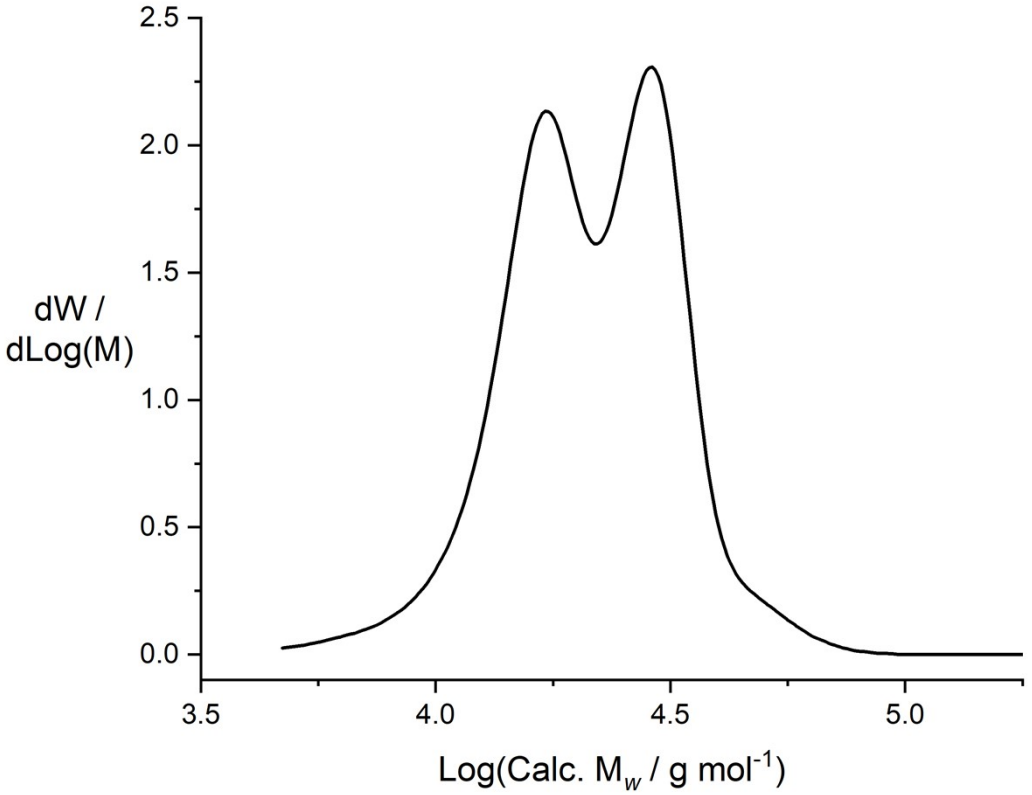


Figure S26: *Representative fitted GPC curve (viscometry detection) of the CHO-PA copolymer ([Cp_2TiCl_2], entry 1, table 1).*

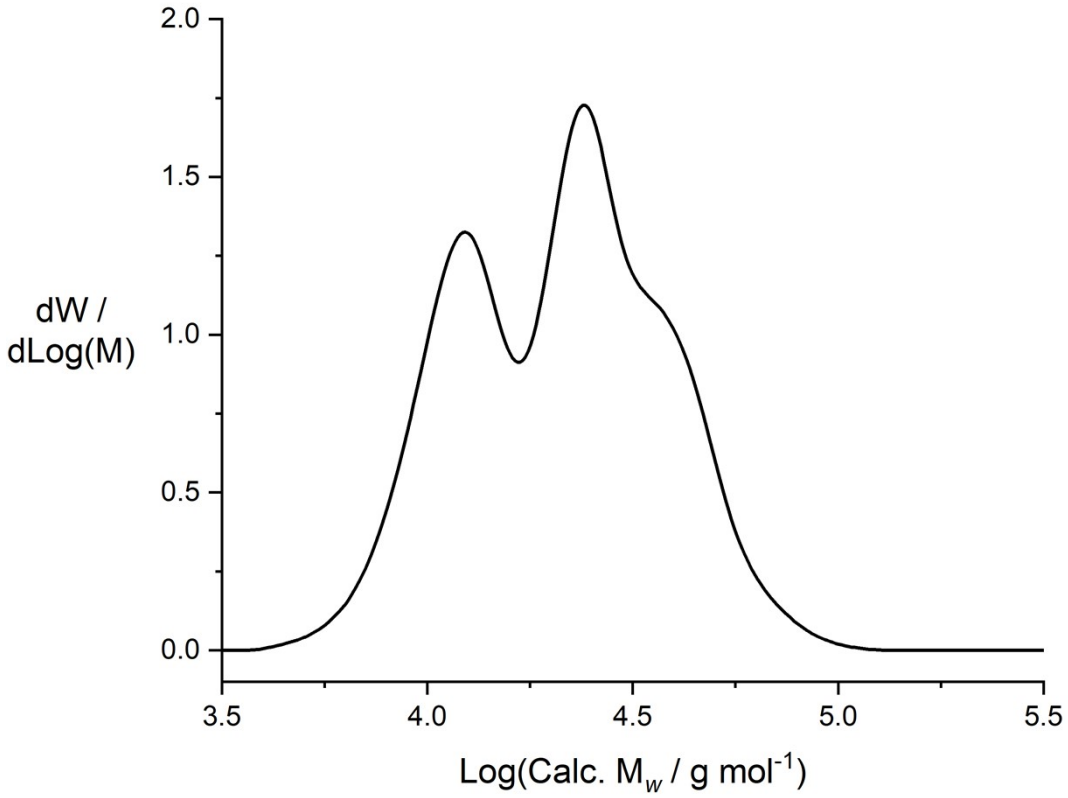


Figure S27: *Representative fitted GPC curve (viscometry detection) of the VCHO-PA copolymer ([Cp_2HfCl_2], entry 7, table 1).*

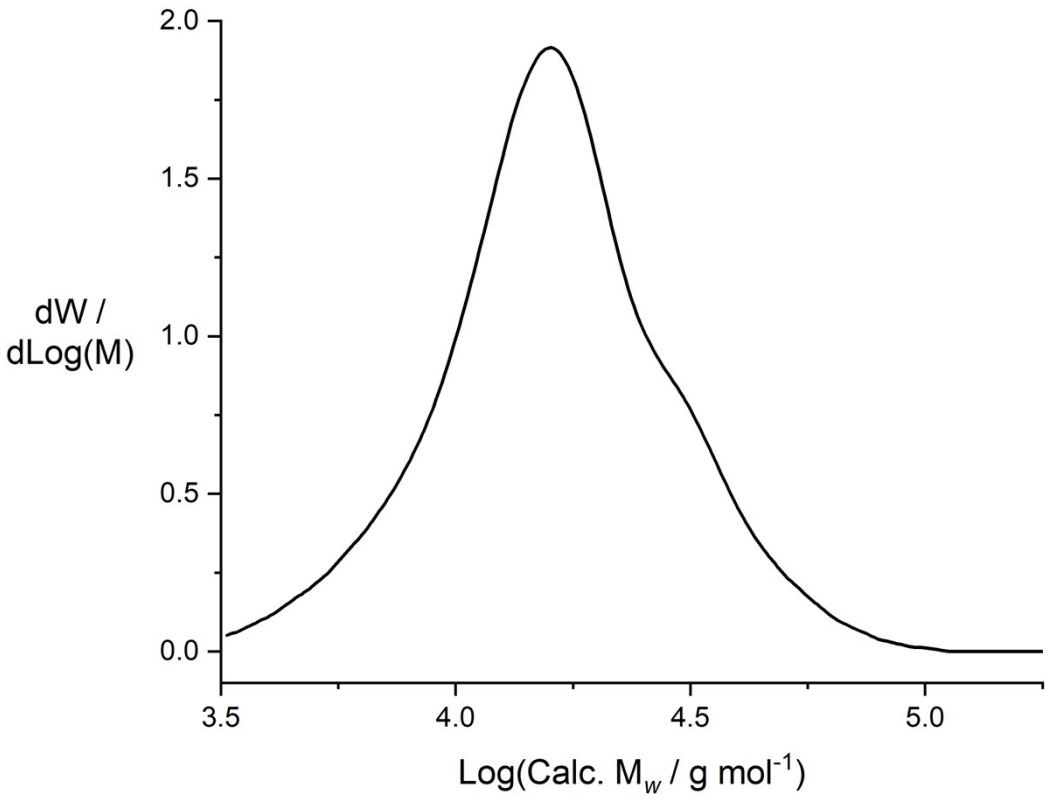


Figure S28: *Representative fitted GPC curve (viscometry detection) of the CHO-TCPA copolymer ([Cp_2TiCl_2], entry 1, table 2.*

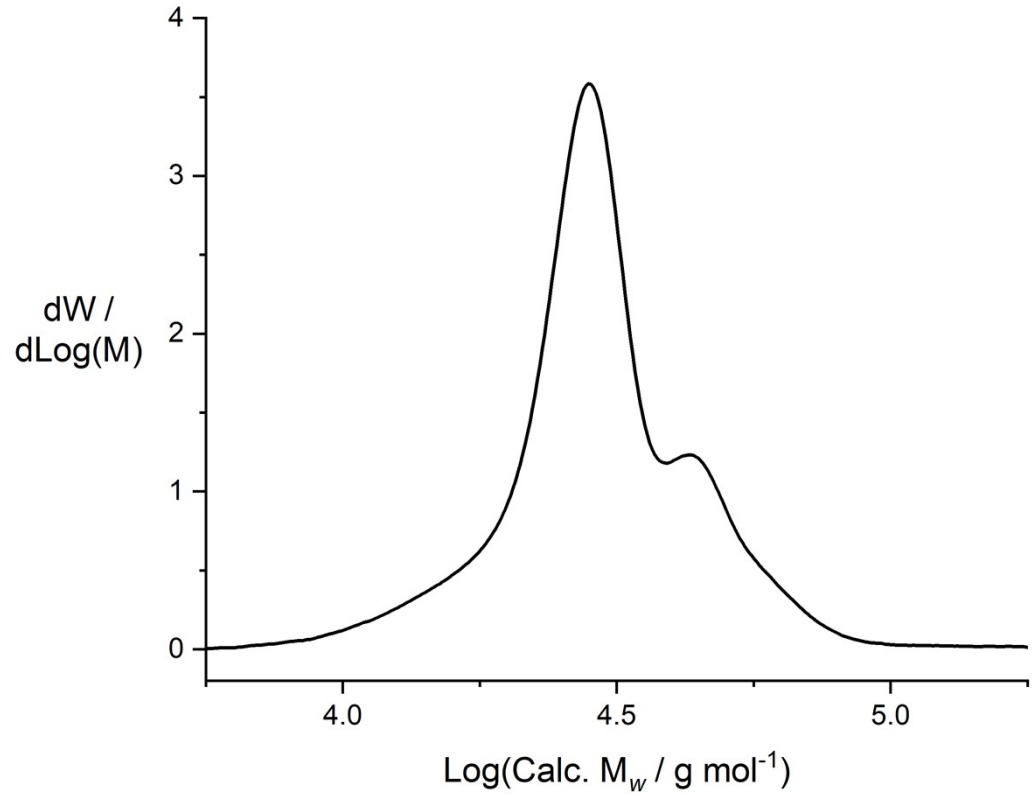


Figure S29: *Representative fitted GPC curve (viscometry detection) of the VCHO-TCPA copolymer ([Cp_2ZrCl_2], entry 6, table 2).*

Figure S30: *Representative fitted GPC curve (viscometry detection) of the LO-PA copolymer ([Cp_2ZrCl_2], entry 2, table 3).*

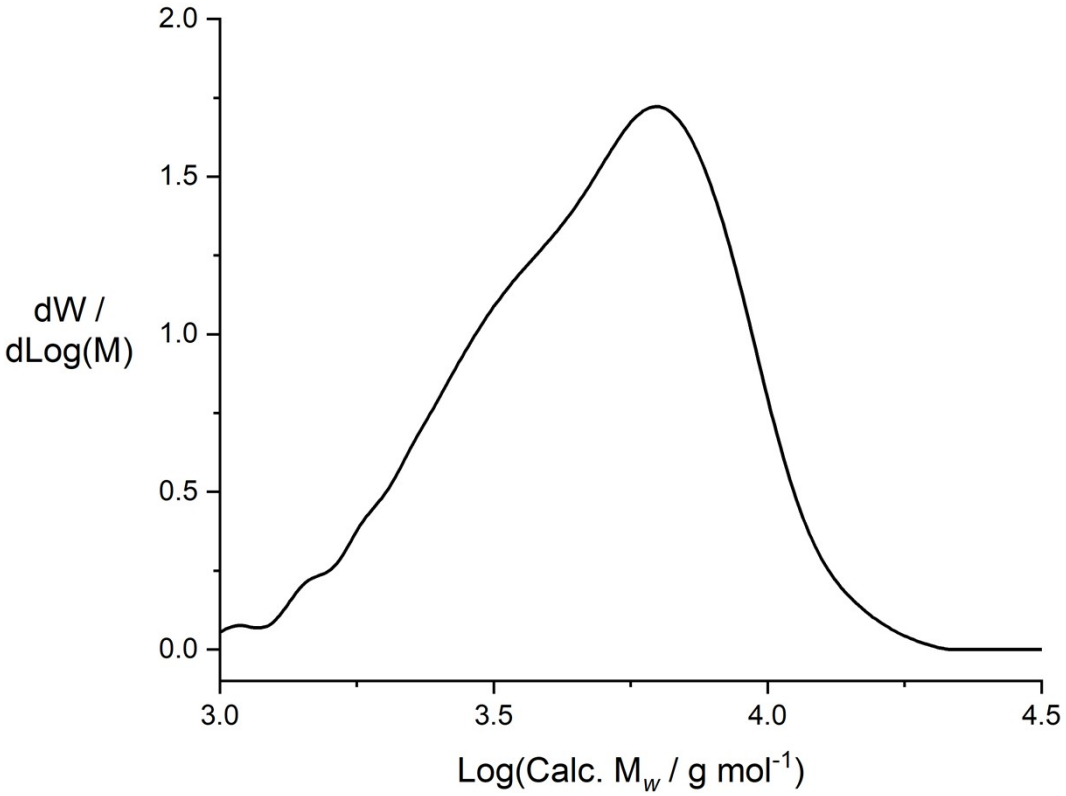


Figure S31: *Representative fitted GPC curve (viscometry detection) of the LO-PA copolymer made on the large scale.*

Density Functional Theory: Computational Details

Density Functional Theory calculations were performed in Gaussian 09 (revision D.01) using the M06 functional alongside the def2tzvp basis set.[1–4] Input geometries were optimised without symmetry constraints, and the resulting structures were confirmed as either minima or saddle points by performing frequency calculations. Solvent effects were incorporated into the calculations using the polarisable continuum model for toluene.[5] Natural Bond Order analyses were called using the Gaussian 09 interface and performed using NBO version 6.0.[6] Relative energies are quoted in kcal mol^{-1} and are temperature (70 °C) and concentration (Monomers: All Ti-containing species: DMAP = 400:1:2) corrected through use of the GoodVibes Program.[7] Prediction of NMR chemical shifts was done for $[Cp_2Zr(OCH(Me)CH_2Cl)_2]$ and $[Cp_2Zr(OCH_2CHMeCl)_2]$ using ethanol (δ^H = 1.25, 3.72 in $CDCl_3$) as a reference to convert the shielding tensors produced by Gaussian into comparable chemical shifts.[8]

1 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. J. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, *Gaussian 09, Revision D.01*, Gaussian Inc., Wallingford, CT, 2016.

2 Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215–241.

3 F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297–3305.

4 F. Weigend, *Phys. Chem. Chem. Phys.*, 2006, **8**, 1057–1065.

5 J. Tomasi, B. Mennucci and R. Cammi, *Chem. Rev.*, 2005, **105**, 2999–3094.

6 E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. E. Bohmann, C. M. Morales, C. R. Landis and F. Weinhold, *NBO 6.0*, Theoretical Chemistry Institute, University of Wisconsin, Madison, 2013.

7 G. Luchini, J. Alegre-Requena, J. Rodriguez-Guerra, J. Chen and R. Paton, *GoodVibes*, bobbypaton/GoodVibes: GoodVibes v3.0.0. Zenodo. https://doi.org/10.5281/zenodo.3346166, 2019.

8 G. R. Fulmer, A. J. M. Miller, N. H. Sherden, H. E. Gottlieb, A. Nudelman, B. M. Stoltz, J. E. Bercaw and K. I. Goldberg, *Organometallics*, 2010, **29**, 2176–2179.

Density Functional Theory: Tabulated Energies

Table S1: *DFT computed energies (m06/def2tzvp) of structures from both frequency calculations in Gaussian 09 and from the GoodVibes program after concentration (monomers: Ti-containing species: DMAP = 400:1:2) and temperature (70 °C) correction. Chemical structures corresponding to each entry can be seen in Scheme 4 of the main manuscript.*

	Gaussian 09 Output		GoodVibes (70 °C, 400:1:2) Output	
Structure	**H / Hartree**	**G / Hartree**	**H / Hartree**	**G(T) / Hartree**
Ethylene Oxide	-153.696725	-153.724852	-153.696877	-153.720063
Succinic Anhydride	-380.394255	-380.429249	-380.394021	-380.425938
Acetate	-228.523993	-228.556372	-228.523703	-228.561707
DMAP	-381.940350	-381.983732	-381.940514	-381.989102
S / $[Cp_2Ti(OAc)_2]$	-1693.105642	-1693.175486	-1693.104467	-1693.187085
Int1a	-1693.059268	-1693.131380	-1693.058162	-1693.147911
Int1b	-1846.763255	-1846.842767	-1846.762070	-1846.861663
Int1c	-1846.812433	-1846.893588	-1846.811221	-1846.912740
Int1-DMAP	-2075.027698	-2075.122340	-2075.026510	-2075.145636
TS1	-1846.757832	-1846.837518	-1846.756651	-1846.849363
Int2	-1846.833097	-1846.914622	-1846.831980	-1846.925839
Int3	-2227.237107	-2227.332174	-2227.235441	-2227.355187
TS2	-2227.181070	-2227.273785	-2227.179493	-2227.288052
Int4	-2227.225563	-2227.320206	-2227.224042	-2227.333242
TS3	-2227.200983	-2227.293280	-2227.199521	-2227.315864
Int5	-2227.250483	-2227.348298	-2227.248873	-2227.371741

Density Functional Theory: QTAIM

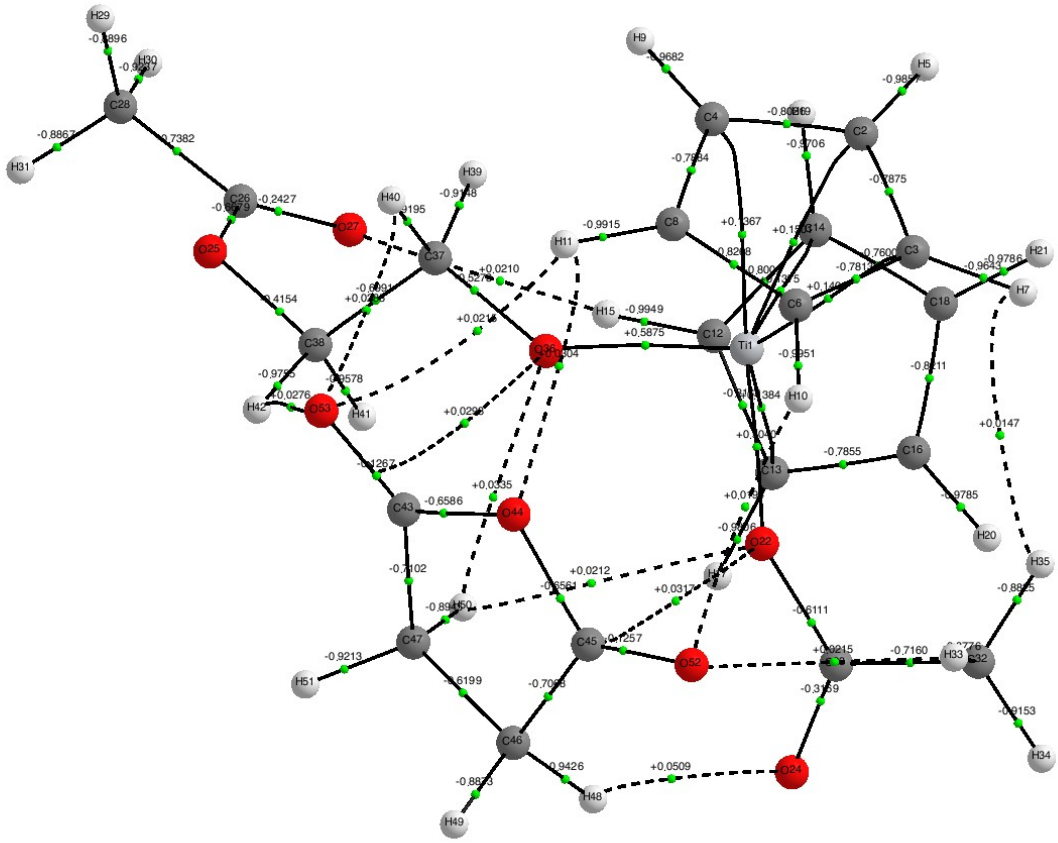


Figure S32: *Visualised output from QTAIM analysis of Int3, detailing bond critical points (green markers) between the C^{43}=O^{53} bond of succinic anhydride and O^{36} of the inserting alkoxide, and between succinic anhydride protons (H^{48}, H^{50}) and acetate oxygens (O^{24}, O^{22}). The magnitude of the number is the Hessian of the electron density at that point, rho. As calculated using Gaussian 09.*

Density Functional Theory: XYZ Coordinates of Structures

Ethylene Oxide:

C	-0.65268	-0.48434	0.00000
C	0.00000	0.81274	0.00000
O	0.75332	-0.37903	0.00000
H	-1.09491	-0.86202	0.91858
H	-1.09491	-0.86202	-0.91858
H	0.03965	1.39293	0.91859
H	0.03965	1.39293	-0.91859

Succinic Anhydride:

O	-0.00001	0.98398	0.00000
C	-0.75694	-1.23985	-0.00001
C	0.75694	-1.23985	-0.00001
H	-1.19995	-1.71452	0.87589
H	-1.19995	-1.71455	-0.87588
H	1.19995	-1.71454	0.87588
H	1.19996	-1.71455	-0.87588
C	1.13850	0.21069	-0.00001
C	-1.13848	0.21071	-0.00004
O	2.21440	0.70852	0.00002
O	-2.21441	0.70850	0.00003

Acetate:

C	-1.33661	-0.05021	-0.00238
H	-1.73920	0.62120	-0.76395
H	-1.72000	-1.05814	-0.16668
H	-1.70417	0.30918	0.96252
C	0.19455	0.00000	-0.00573
O	0.69854	1.14421	0.00101
O	0.80342	-1.09058	0.00108

DMAP:

C	-1.94211	-1.12455	-0.00003
N	-2.65240	-0.00001	-0.00001
C	-0.56550	-1.18962	-0.00004
H	-2.50959	-2.05314	-0.00009
C	0.18041	0.00005	-0.00008
C	-0.56544	1.18968	0.00004
C	-1.94210	1.12455	0.00006
H	-0.08294	2.15768	-0.00003
H	-2.50954	2.05317	0.00021
H	-0.08293	-2.15756	0.00006
N	1.54131	-0.00003	-0.00012
C	2.26352	-1.24820	0.00011
H	2.03555	-1.85212	0.88533
H	3.33187	-1.04483	0.00084
H	2.03671	-1.85171	-0.88568
C	2.26359	1.24818	0.00001
H	2.03648	1.85168	0.88569
H	2.03594	1.85200	-0.88536
H	3.33192	1.04468	-0.00055

S / $Cp_2Ti(OAc)_2$:

Ti	0.64173	-0.00021	-0.00109	C	-2.67102	1.39073	-2.25662
C	2.13470	-1.81824	-0.12894	H	-2.96819	0.36962	-2.50715
C	2.50017	-0.91695	-1.15578	H	-3.55986	1.99891	-2.10392
C	0.86674	-2.34043	-0.45118	H	-2.08837	1.77427	-3.09492
H	2.72784	-2.07280	0.73684				
C	1.44290	-0.85670	-2.07438				
H	3.42283	-0.36016	-1.21185				
C	0.43239	-1.73840	-1.63780				
H	0.29427	-3.03096	0.14747				
H	1.38569	-0.20676	-2.93469				
H	-0.54436	-1.86119	-2.07700				
C	0.44427	1.74259	1.62915				
C	0.88349	2.33835	0.44091				
C	1.44919	0.85645	2.06975				
H	-0.53200	1.87376	2.06686				
C	2.14776	1.80650	0.12108				
H	0.31519	3.03012	-0.16020				
C	2.50679	0.90590	1.15128				
H	1.38702	0.20961	2.93200				
H	2.74315	2.05434	-0.74510				
H	3.42537	0.34254	1.20921				
O	-0.68732	0.73980	-1.20455				
C	-1.83584	1.34361	-1.00886				
O	-2.21321	1.79343	0.04980				
O	-0.68017	-0.74047	1.21412				
C	-1.83426	-1.33187	1.01605				
O	-2.23230	-1.73822	-0.05273				
C	-2.64859	-1.42601	2.27524				
H	-2.94192	-0.41627	2.57207				
H	-3.54030	-2.02767	2.11365				
H	-2.05253	-1.84223	3.08815				

Int1a:

Ti	0.85166	0.01218	0.00105
C	-0.68825	1.52939	0.83902
C	-0.92791	1.41400	-0.55281
C	0.58631	2.10041	1.01882
H	-1.40627	1.22349	1.58759
C	0.21385	1.88765	-1.22170
H	-1.83415	0.97325	-0.96974
C	1.15088	2.31263	-0.25263
H	1.08044	2.27995	1.96262
H	0.37444	1.88463	-2.29086
H	2.14110	2.69387	-0.45256
C	1.19450	-2.28344	0.25375
C	0.62009	-2.08206	-1.01519
C	0.25463	-1.87497	1.22740
H	2.19231	-2.64784	0.44904
C	-0.66366	-1.53415	-0.82921
H	1.11272	-2.25330	-1.96132
C	-0.89870	-1.42278	0.56363
H	0.42047	-1.86877	2.29575
H	-1.39175	-1.24139	-1.57336
H	-1.81165	-0.99926	0.98377
O	-3.45905	-0.20879	-1.09455
C	-4.02877	-0.03084	0.00802
O	-3.46846	0.14215	1.11488
O	2.64059	0.04488	1.07830
C	3.29306	0.01776	-0.00627
O	2.63427	0.00782	-1.08729
C	4.77364	-0.03899	-0.00929
H	5.07754	-1.08876	0.00860
H	5.17267	0.41187	-0.91575
H	5.17721	0.44385	0.87848
C	-5.55133	-0.00015	-0.01976
H	-5.93577	-0.80141	-0.65289
H	-5.97813	-0.07656	0.98026
H	-5.87658	0.94306	-0.46594

Int1b:

Ti	1.11213	-0.13206	-0.09428
C	1.04017	-1.61855	-1.91135
C	2.16875	-0.80556	-2.08089
C	-0.11543	-0.80247	-1.99178
H	1.05202	-2.68020	-1.70863
C	1.71893	0.52765	-2.25074
H	3.19794	-1.12906	-2.06823
C	0.31339	0.51030	-2.23344
H	-1.14964	-1.08867	-1.81654
H	2.33710	1.40035	-2.39737
H	-0.32371	1.37775	-2.31114
C	1.86156	0.51672	2.07438
C	2.39015	1.42824	1.13453
C	2.42667	-0.74204	1.82347
H	1.11166	0.74038	2.81858
C	3.26329	0.72145	0.29361
H	2.11241	2.46645	1.02915
C	3.27146	-0.63334	0.70639
H	2.20264	-1.65551	2.35287
H	3.83409	1.13657	-0.52233
H	3.84898	-1.43239	0.26774
O	-0.24922	1.10123	0.33015
C	-0.64504	2.34505	0.19252
O	0.07638	3.20945	-0.25658
O	-3.02511	-1.02727	-0.95582
C	-3.57187	-0.44355	0.01369
O	-3.17013	-0.42636	1.19432
C	-4.87484	0.28655	-0.29157
H	-5.69601	-0.43405	-0.25723
H	-5.07893	1.06305	0.44675
H	-4.86032	0.71424	-1.29535
C	-2.06638	2.57637	0.59076
H	-2.41293	1.83716	1.31167
H	-2.19269	3.59711	0.94746
H	-2.68051	2.45305	-0.30657
O	0.18202	-1.79198	0.73586
C	-0.95247	-2.67350	0.60657
C	-0.68714	-1.99088	1.86441
H	-0.64878	-3.70887	0.48750
H	-1.76010	-2.27195	-0.01542
H	-0.20669	-2.51481	2.68513
H	-1.33456	-1.14080	2.07417

Int1c:

Ti	-0.39218	-0.30912	0.02302
C	0.63863	-1.25707	1.90895
C	-0.76153	-1.27923	2.13191
C	1.04876	0.08096	1.85925
H	1.28335	-2.11303	1.78202
C	-1.19688	0.04886	2.25214
H	-1.39083	-2.15279	2.20803
C	-0.09196	0.89083	2.05587
H	2.04382	0.42856	1.62717
H	-2.22118	0.35489	2.39290
H	-0.11273	1.97083	2.03181
C	0.45163	-1.19363	-2.04569
C	-0.94280	-1.14270	-2.14972
C	0.78497	-2.07497	-1.00071
H	1.14891	-0.58684	-2.60141
C	-1.48752	-2.02999	-1.19257
H	-1.50665	-0.49198	-2.80054
C	-0.42176	-2.61839	-0.49999
H	1.78305	-2.29798	-0.65278
H	-2.53656	-2.17930	-0.98501
H	-0.50597	-3.34520	0.29277
O	-2.10976	0.59119	-0.25452
C	-3.37614	0.37608	-0.06557
O	-3.83424	-0.61183	0.47556
O	0.60081	1.14348	-0.73755
C	1.14631	2.29274	-0.42894
O	2.23522	2.40416	0.08739
C	0.28920	3.46693	-0.80680
H	-0.70466	3.34851	-0.36837
H	0.74203	4.39967	-0.47791
H	0.15447	3.48621	-1.88966
C	-4.24485	1.48703	-0.59124
H	-5.28956	1.30489	-0.34936
H	-3.92608	2.44282	-0.17229
H	-4.12864	1.55936	-1.67429
C	3.89173	-0.33577	-0.95700
C	4.61358	0.02865	0.24816
O	3.64632	-1.00140	0.26557
H	3.08814	0.31534	-1.29433
H	4.38251	-0.93457	-1.72080
H	4.32792	0.94261	0.76331
H	5.64154	-0.29820	0.38250

Int1-DMAP:

Ti	1.80711	-0.48953	0.15078
C	3.64188	-1.99789	0.23494
C	3.93232	-1.00476	-0.72266
C	2.52344	-2.71584	-0.20810
H	4.16692	-2.16054	1.16281
C	3.03557	-1.16984	-1.79838
H	4.69871	-0.24669	-0.64820
C	2.15580	-2.20642	-1.47973
H	2.05626	-3.53445	0.31952
H	2.98139	-0.53798	-2.67058
H	1.32527	-2.54015	-2.08213
C	0.89504	1.02892	1.75491
C	2.28600	1.24659	1.69588
C	0.68975	-0.27454	2.24510
H	0.12236	1.71795	1.41737
C	2.93547	0.07642	2.11750
H	2.77284	2.13300	1.31648
C	1.94180	-0.87913	2.45085
H	-0.27176	-0.74568	2.38930
H	4.00366	-0.06126	2.18425
H	2.11712	-1.88175	2.81263
O	1.64943	0.98511	-0.99178
C	2.01730	2.20013	-1.34757
O	3.12099	2.63191	-1.10844
N	-0.22176	-1.15598	-0.23997
C	-1.11343	-0.17214	-0.48863
C	-2.46571	-0.35185	-0.50259
C	0.93514	2.95437	-2.04543
H	0.11538	3.12035	-1.33400
H	1.31387	3.90233	-2.42057
H	0.52720	2.35904	-2.86405
C	-3.00747	-1.62374	-0.24896
H	-0.03227	-3.17232	0.20641
C	-2.07389	-2.65547	-0.00837
C	-0.73520	-2.37535	-0.00762
H	-3.06120	0.54793	-0.65316
H	-0.74114	0.83613	-0.63488
H	-2.38749	-3.67097	0.18922
N	-4.33677	-1.83212	-0.22683
C	-5.24222	-0.72477	-0.47490
H	-5.05834	0.10475	0.21169
H	-6.26507	-1.06742	-0.34089
H	-5.13516	-0.33835	-1.49279
C	-4.86702	-3.15205	0.02473
H	-4.56363	-3.52919	1.00663
H	-5.95287	-3.11125	0.00287
H	-4.54094	-3.87190	-0.73301
O	-1.31652	2.75325	0.28798
C	-2.52383	3.10966	0.29251
O	-3.47195	2.53608	-0.27664
C	-2.83212	4.37400	1.08801
H	-3.87796	4.66786	1.00009
H	-2.19300	5.19082	0.74621
H	-2.59420	4.20752	2.14135

TS1:

Ti	-1.28873	-0.25350	0.00221
C	-1.89227	-0.21271	2.31757
C	-2.96324	-0.75298	1.57443
C	-1.70962	1.11523	1.91793
H	-1.28981	-0.75144	3.03297
C	-3.46699	0.27025	0.74606
H	-3.34244	-1.76143	1.64698
C	-2.67255	1.41512	0.92854
H	-0.92908	1.78046	2.25767
H	-4.30582	0.18101	0.07408
H	-2.74982	2.34702	0.38771
C	-0.44057	-1.16075	-2.02817
C	-1.25211	-0.06802	-2.37270
C	-1.25946	-2.14390	-1.43377
H	0.63006	-1.21216	-2.16037
C	-2.56399	-0.35317	-1.96228
H	-0.91396	0.86330	-2.80078
C	-2.57062	-1.65070	-1.38813
H	-0.92113	-3.08527	-1.02719
H	-3.41633	0.29649	-2.08713
H	-3.43084	-2.16222	-0.98365
O	-0.00615	1.09901	-0.24235
C	0.25926	2.37662	-0.41433
O	-0.55398	3.15295	-0.85876
O	3.52172	0.18475	-0.93062
C	4.25188	-0.38887	-0.09712
O	3.89353	-1.27974	0.71869
C	5.70836	0.04079	-0.03279
H	6.32920	-0.71313	0.45044
H	6.08699	0.25850	-1.03180
H	5.77485	0.96337	0.54940
C	1.64543	2.73694	0.01304
H	2.36741	2.01536	-0.38358
H	1.88806	3.75189	-0.29373
H	1.69868	2.67241	1.10435
O	0.07243	-1.47355	0.88531
C	1.13929	-1.03778	1.73154
C	1.66337	-1.56349	0.50117
H	1.22507	-1.61641	2.64841
H	1.19884	0.04023	1.87740
H	1.90094	-2.61227	0.41963
H	1.87389	-0.88165	-0.31346

Int2:

Ti	1.09469	-0.42014	0.02446
C	0.88412	-2.60489	-0.89983
C	2.16255	-2.54717	-0.29402
C	0.90222	-1.74761	-2.01574
H	0.05583	-3.22280	-0.58376
C	2.92565	-1.60217	-0.98410
H	2.48091	-3.11484	0.56609
C	2.14034	-1.10447	-2.05240
H	0.06477	-1.54314	-2.66527
H	3.92307	-1.27738	-0.72844
H	2.42996	-0.32027	-2.73400
C	0.21388	0.61204	2.01214
C	1.58506	0.41024	2.23002
C	-0.39658	-0.65017	1.88372
H	-0.25526	1.57334	1.87497
C	1.83696	-0.97111	2.21596
H	2.32498	1.18853	2.33144
C	0.60114	-1.62897	2.00935
H	-1.44290	-0.83480	1.68025
H	2.79933	-1.44339	2.34312
H	0.44909	-2.69644	1.95987
O	2.30376	1.08850	-0.37593
C	2.18421	2.37862	-0.21756
O	1.24146	2.94292	0.29598
O	-3.94813	0.99438	-0.68431
C	-4.65971	0.10333	0.02036
O	-4.20188	-0.57433	0.90005
C	-6.08147	0.08574	-0.43464
H	-6.12967	-0.11986	-1.50449
H	-6.63837	-0.66812	0.11535
H	-6.53115	1.06675	-0.27510
C	3.37086	3.13435	-0.75792
H	3.48356	2.92931	-1.82390
H	3.24887	4.20397	-0.60177
H	4.28399	2.79091	-0.26881
O	-0.40939	0.25729	-0.76575
C	-1.73625	0.10054	-1.08302
C	-2.56901	1.12973	-0.34662
H	-2.09339	-0.90874	-0.82068
H	-1.89637	0.21878	-2.16689
H	-2.43804	1.02638	0.73241
H	-2.27288	2.13665	-0.64307

Int3:

Ti	-0.45171	-1.16794	0.27358
C	-0.68258	-2.40586	2.30472
C	-1.95933	-1.94248	1.93273
C	0.11868	-1.28935	2.59281
H	-0.36619	-3.43644	2.34257
C	-1.95850	-0.53449	2.05966
H	-2.79506	-2.55645	1.62914
C	-0.68415	-0.13433	2.46351
H	1.16312	-1.31244	2.86947
H	-2.77618	0.12612	1.81134
H	-0.34894	0.88634	2.57532
C	1.23333	-2.15541	-1.14838
C	0.11972	-1.89940	-1.95659
C	0.85398	-3.08203	-0.16176
H	2.19591	-1.66794	-1.21732
C	-0.94124	-2.72019	-1.50911
H	0.05658	-1.16582	-2.74709
C	-0.49267	-3.45539	-0.41010
H	1.49001	-3.47038	0.62041
H	-1.93326	-2.75763	-1.93476
H	-1.07280	-4.16962	0.15356
O	-1.82350	-0.16986	-0.66271
C	-2.75296	-0.25686	-1.57773
O	-2.62317	0.19897	-2.69293
O	4.23459	1.35799	-0.07545
C	5.00880	0.35027	-0.49985
O	4.59609	-0.60218	-1.10539
C	6.43450	0.58543	-0.12540
H	6.51931	0.72901	0.95227
H	7.04518	-0.25699	-0.43886
H	6.79405	1.49927	-0.60041
C	-4.02713	-0.90243	-1.11113
H	-4.50589	-0.22671	-0.39755
H	-4.70280	-1.07839	-1.94537
H	-3.82389	-1.83706	-0.58509
O	0.83799	0.16897	0.18181
C	2.11678	0.41349	0.63523
C	2.84450	1.27101	-0.38075
H	2.68430	-0.52160	0.77009
H	2.10473	0.92592	1.61079
H	2.70233	0.85051	-1.38015
H	2.46652	2.29406	-0.35956
C	-0.39408	2.90999	0.54144
O	-1.62627	2.61175	1.08135
C	-2.59995	2.56298	0.10524
C	-2.00471	2.99668	-1.19963
C	-0.51308	2.93712	-0.95103
H	-2.35677	2.35197	-2.00369
H	-2.35849	4.01180	-1.39891
H	-0.08946	1.99126	-1.30838
H	0.07303	3.75480	-1.36699
O	-3.71208	2.24584	0.37162
O	0.54794	3.09335	1.24012

TS2

Ti	-1.25830	0.74079	-0.13227
C	-1.49690	2.76284	-1.44304
C	-2.65543	1.99457	-1.61824
C	-0.41411	2.04491	-1.97277
H	-1.43785	3.72724	-0.96367
C	-2.29518	0.81727	-2.31286
H	-3.64156	2.23665	-1.25528
C	-0.91971	0.85199	-2.53455
H	0.61653	2.36287	-1.96677
H	-2.95670	-0.00424	-2.53905
H	-0.32912	0.07073	-2.98816
C	0.23843	1.15717	1.73445
C	-0.87758	0.45677	2.22461
C	-0.20135	2.37565	1.20680
H	1.25286	0.79550	1.71461
C	-2.00091	1.29358	2.09089
H	-0.89029	-0.54570	2.62189
C	-1.60338	2.46161	1.43436
H	0.42057	3.12916	0.74614
H	-3.00232	1.03388	2.38658
H	-2.24506	3.29127	1.18135
O	-3.16918	0.04051	0.07529
C	-3.73584	-0.89159	0.77746
O	-3.36808	-1.31530	1.85538
O	4.31517	0.25853	-0.40975
C	4.65896	1.28620	0.38434
O	3.96942	1.69951	1.27509
C	6.00176	1.81632	0.00627
H	6.01384	2.09142	-1.04884
H	6.24618	2.67904	0.62004
H	6.75539	1.03994	0.14562
C	-4.97229	-1.43383	0.09875
H	-4.67866	-1.91413	-0.83795
H	-5.48012	-2.15754	0.73357
H	-5.65296	-0.62041	-0.15717
O	0.70654	-0.13431	-0.51589
C	1.93889	0.38338	-0.83926
C	3.06207	-0.36480	-0.14522
H	2.01875	1.43885	-0.53423
H	2.12872	0.36604	-1.93075
H	2.88260	-0.41957	0.93152
H	3.16242	-1.38111	-0.53235
C	-0.04279	-1.90193	-0.40694
O	0.59204	-2.34367	0.73438
C	1.57631	-3.25325	0.45324
C	1.57020	-3.55770	-1.01971
C	0.50945	-2.64349	-1.59827
H	2.57287	-3.40116	-1.41890
H	1.34822	-4.61852	-1.14512
H	0.89315	-1.93403	-2.33034
H	-0.31903	-3.17962	-2.06291
O	2.27935	-3.68974	1.30250
O	-1.17534	-1.44020	-0.31699

Int4

Ti	-1.80039	1.08581	0.01059
C	-2.75281	3.19199	-0.60895
C	-3.53407	2.19552	-1.20081
C	-1.45443	3.11905	-1.16940
H	-3.07201	3.88191	0.15637
C	-2.73450	1.52617	-2.15900
H	-4.55210	1.94597	-0.94315
C	-1.46942	2.11973	-2.15852
H	-0.61170	3.74164	-0.90844
H	-3.03529	0.66994	-2.74249
H	-0.61365	1.78935	-2.72605
C	-0.27322	1.37000	1.80360
C	-1.03105	0.22084	2.11023
C	-1.13928	2.47277	1.79148
H	0.77873	1.37972	1.56152
C	-2.36056	0.62109	2.30483
H	-0.66529	-0.79205	2.14067
C	-2.44429	2.00510	2.08840
H	-0.86383	3.49672	1.59063
H	-3.19211	-0.03367	2.51785
H	-3.33865	2.60503	2.15737
O	-3.15971	-0.34845	-0.13654
C	-3.08774	-1.61591	0.15490
O	-2.06540	-2.21991	0.41404
O	5.11622	0.05080	-2.44214
C	5.39348	-0.79214	-3.45148
O	4.58026	-1.16385	-4.25084
C	6.83415	-1.18029	-3.42880
H	7.07932	-1.64442	-2.47277
H	7.04533	-1.87026	-4.24126
H	7.45893	-0.29136	-3.52438
C	-4.43438	-2.28935	0.15349
H	-4.96706	-2.07453	-0.77347
H	-4.32915	-3.36390	0.28615
H	-5.03638	-1.88239	0.96953
O	1.66875	0.13264	-1.41791
C	2.93966	-0.45209	-1.55102
C	3.77695	0.52103	-2.34195
H	2.89205	-1.41076	-2.08566
H	3.40002	-0.63098	-0.57174
H	3.35034	0.67090	-3.33559
H	3.82749	1.48085	-1.82651
C	0.66868	-0.65167	-0.83583
O	1.14757	-1.03530	0.47733
C	1.16026	-2.36746	0.66405
C	0.81886	-3.07135	-0.61808
C	0.37905	-1.97702	-1.56615
H	1.71155	-3.60689	-0.95190
H	0.04796	-3.81347	-0.41446
H	0.88731	-1.99815	-2.52989
H	-0.69336	-2.01514	-1.74374
O	1.43624	-2.85209	1.72028
O	-0.40831	0.11327	-0.73962

TS3

Ti	-1.45582	0.97179	0.23696
C	-2.53286	2.76583	-0.86018
C	-2.81499	1.64523	-1.64722
C	-1.13227	2.98610	-0.89623
H	-3.26771	3.35136	-0.33038
C	-1.59948	1.15256	-2.16174
H	-3.79241	1.20664	-1.76332
C	-0.57316	2.00607	-1.73278
H	-0.58621	3.76179	-0.38104
H	-1.47523	0.25189	-2.74381
H	0.47874	1.87929	-1.92464
C	-0.82866	0.69066	2.52283
C	-2.17364	0.33003	2.42023
C	-0.71689	2.07212	2.23174
H	-0.00769	0.02838	2.75524
C	-2.90512	1.47228	2.02509
H	-2.57149	-0.66714	2.52996
C	-2.00005	2.54983	1.95261
H	0.20944	2.62689	2.20727
H	-3.95970	1.49941	1.79595
H	-2.24682	3.56974	1.70287
O	-2.84330	-0.44371	-0.03398
C	-4.11909	-0.63814	0.01637
O	-4.96585	0.23646	0.09383
O	3.45975	-0.26137	-4.40127
C	4.32778	-1.27663	-4.58212
O	4.11215	-2.39859	-4.22021
C	5.55223	-0.80013	-5.28600
H	5.99259	0.03950	-4.74748
H	6.27144	-1.61027	-5.36908
H	5.28585	-0.43992	-6.28074
C	-4.49002	-2.09878	-0.02193
H	-4.14888	-2.57839	0.89853
H	-5.56757	-2.21977	-0.11160
H	-3.98375	-2.59883	-0.84804
O	1.06075	-0.75097	-1.76832
C	2.37497	-0.59146	-2.28441
C	2.22293	-0.58240	-3.78525
H	3.02957	-1.40786	-1.96733
H	2.78993	0.36148	-1.94067
H	1.85589	-1.54885	-4.13694
H	1.51781	0.19629	-4.08188
C	0.81708	-0.89786	-0.47769
O	1.00595	1.24170	0.25209
C	1.99150	1.15732	1.06394
C	2.79777	-0.13089	0.89953
C	1.91575	-1.29829	0.46470
H	3.57846	0.07072	0.16031
H	3.31328	-0.36859	1.83006
H	2.51261	-2.09669	0.01532
H	1.40896	-1.72260	1.33249
O	2.33936	1.99018	1.88664
O	-0.35914	-0.87595	-0.13213

Int5

Ti	-1.50827	1.42262	0.41910
C	-3.07258	2.94511	-0.48777
C	-2.93956	1.90407	-1.41399
C	-1.82511	3.61170	-0.39551
H	-3.96475	3.18828	0.06820
C	-1.61577	1.92902	-1.90830
H	-3.69741	1.17246	-1.65042
C	-0.94395	2.99857	-1.30142
H	-1.59650	4.45820	0.23379
H	-1.18098	1.21118	-2.58725
H	0.09669	3.24885	-1.43235
C	-1.04911	0.64291	2.62386
C	-2.36698	0.26693	2.33690
C	-0.98535	2.05556	2.63773
H	-0.21438	-0.02418	2.78137
C	-3.12051	1.43471	2.12833
H	-2.73637	-0.73944	2.22034
C	-2.26749	2.54223	2.34966
H	-0.08641	2.63495	2.78643
H	-4.16619	1.46787	1.86263
H	-2.55275	3.58104	2.29113
O	-1.82684	-0.38405	-0.25162
C	-2.80331	-1.21995	-0.45055
O	-3.97122	-0.97330	-0.22636
O	1.11028	-6.92306	-1.90959
C	0.23282	-7.91974	-2.11317
O	-0.93529	-7.82504	-1.86209
C	0.91575	-9.11924	-2.67922
H	1.69385	-9.46085	-1.99543
H	0.19297	-9.91378	-2.84332
H	1.40410	-8.86071	-3.61957
C	-2.33461	-2.54478	-0.98759
H	-1.62148	-2.99733	-0.29441
H	-3.17507	-3.21723	-1.14406
H	-1.80121	-2.39481	-1.92864
O	1.19031	-3.57777	-0.68028
C	1.72750	-4.76693	-1.24252
C	0.57593	-5.72398	-1.36715
H	2.51141	-5.17183	-0.59625
H	2.17726	-4.55813	-2.21700
H	0.11672	-5.91811	-0.39346
H	-0.20196	-5.32307	-2.02366
C	2.04436	-2.55339	-0.52438
O	0.38977	1.24127	0.23585
C	1.52455	1.02033	0.84530
C	2.25338	-0.19775	0.32456
C	1.33659	-1.37161	0.05900
H	2.75277	0.09298	-0.60544
H	3.04376	-0.45416	1.03073
H	0.82754	-1.70189	0.97159
H	0.52273	-1.09543	-0.61961
O	1.98010	1.72851	1.71278
O	3.20196	-2.60964	-0.83082

$Cp_2Zr(OCH(Me)CH_2Cl)_2$

Zr	-0.04472	0.63011	-0.02216
C	0.25871	2.54196	-1.67905
C	-0.96591	1.90738	-1.99693
C	1.29694	1.64110	-1.95389
H	0.37142	3.54093	-1.28445
C	-0.66828	0.62717	-2.50403
H	-1.95172	2.34021	-1.89863
C	0.72184	0.45038	-2.45746
H	2.35125	1.81908	-1.79457
H	-1.38927	-0.11544	-2.81031
H	1.25935	-0.44514	-2.73473
C	0.43352	1.43495	2.35609
C	-0.78636	0.74672	2.42252
C	0.25002	2.57781	1.55363
H	1.36934	1.10668	2.78212
C	-1.74613	1.48591	1.69042
H	-0.95968	-0.19360	2.92611
C	-1.11046	2.61823	1.16285
H	1.00578	3.31033	1.30709
H	-2.78464	1.21757	1.55383
H	-1.57335	3.38232	0.55592
O	-1.26381	-0.93681	-0.06907
C	-2.43571	-1.53372	0.35862
C	-2.26203	-3.03331	0.42722
Cl	5.03678	-2.29953	-0.17516
C	-3.52694	-1.11938	-0.61300
H	-3.36948	-1.57732	-1.59118
Cl	-5.15803	-1.61487	-0.04686
H	-3.54560	-0.03414	-0.72112
O	1.66341	-0.31602	0.32958
C	3.01123	-0.45227	0.05131
C	3.36030	-1.90155	0.33477
C	3.82874	0.51711	0.87568
H	3.20811	-0.26677	-1.02052
H	3.28567	-2.11503	1.40198
H	2.69424	-2.56412	-0.21531
H	3.68330	0.31330	1.94074
H	3.50229	1.54077	0.67592
H	4.89322	0.44207	0.64909
H	-3.17415	-3.52387	0.77059
H	-1.45279	-3.28286	1.11467
H	-2.00491	-3.42168	-0.56217
H	-2.72171	-1.16135	1.35912

$Cp_2Zr(OCH_2CMeHCl)_2$

Zr	0.00539	-0.76620	-0.03558
C	-0.04071	-2.23502	2.05102
C	-1.08753	-1.29217	2.18361
C	1.17614	-1.53968	2.10337
H	-0.16139	-3.30028	1.92016
C	-0.50505	-0.02207	2.35327
H	-2.14674	-1.50619	2.17907
C	0.88854	-0.16547	2.28126
H	2.16059	-1.97440	2.00174
H	-1.04485	0.90838	2.44373
H	1.61309	0.63557	2.31968
C	0.21208	-2.29963	-2.08016
C	-0.73811	-1.32186	-2.41684
C	-0.31234	-3.07884	-1.03262
H	1.20110	-2.39265	-2.50250
C	-1.87551	-1.52049	-1.60120
H	-0.61497	-0.54049	-3.15329
C	-1.61525	-2.60141	-0.74727
H	0.18013	-3.91218	-0.55283
H	-2.77339	-0.91880	-1.60235
H	-2.28622	-2.99690	0.00137
O	-0.79937	1.00698	-0.38344
C	-1.71484	1.82343	-0.98307
H	-1.21504	2.71256	-1.40429
C	5.19754	1.29336	-0.49653
C	-2.76729	2.34708	-0.03227
O	1.86465	-0.36358	-0.61480
C	3.18801	-0.19263	-0.31662
C	3.71377	1.17054	-0.70551
H	3.80963	-0.92513	-0.86201
H	3.40033	-0.34464	0.75711
H	-2.22880	1.32736	-1.82669
H	5.45632	1.08762	0.54492
H	5.55249	2.29238	-0.74689
H	5.72104	0.57297	-1.13026
Cl	2.86901	2.44592	0.28231
H	3.42590	1.39384	-1.73435
Cl	-3.74308	0.94713	0.61316
C	-3.69639	3.33133	-0.68519
H	-2.28491	2.76689	0.85270
H	-4.18705	2.88007	-1.55084
H	-3.12893	4.20113	-1.02594
H	-4.46539	3.67291	0.00664