

Electronic Supplementary Information for

Cobalt-Oxygen Bond Homolysis in the Bench-stable
(Salen*)Cobalt(III) Acetate Complex: Insight into the
Organometallic Mediated Radical Polymerization of
Diverse Monomers

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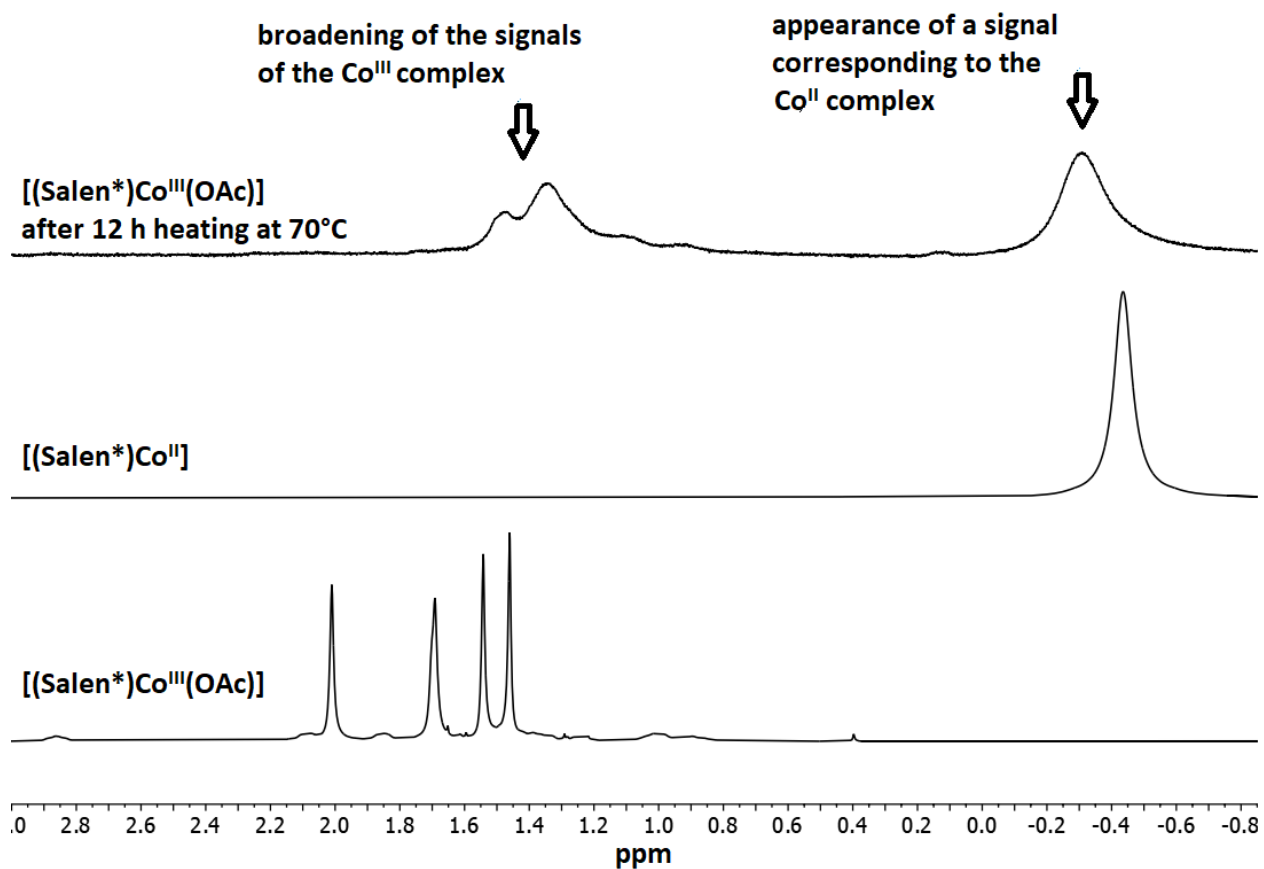


Figure S1. Stacking of the ^1H NMR (400 MHz, CDCl_3) spectra in the ^tBu region (0.8–3 ppm) of $[(\text{Salen}^*)\text{Co}^{\text{III}}(\text{OAc})]$ (**1**, bottom), $[(\text{Salen}^*)\text{Co}^{\text{II}}]$ (middle) and **1** after heating at 70°C for 12 h (top).

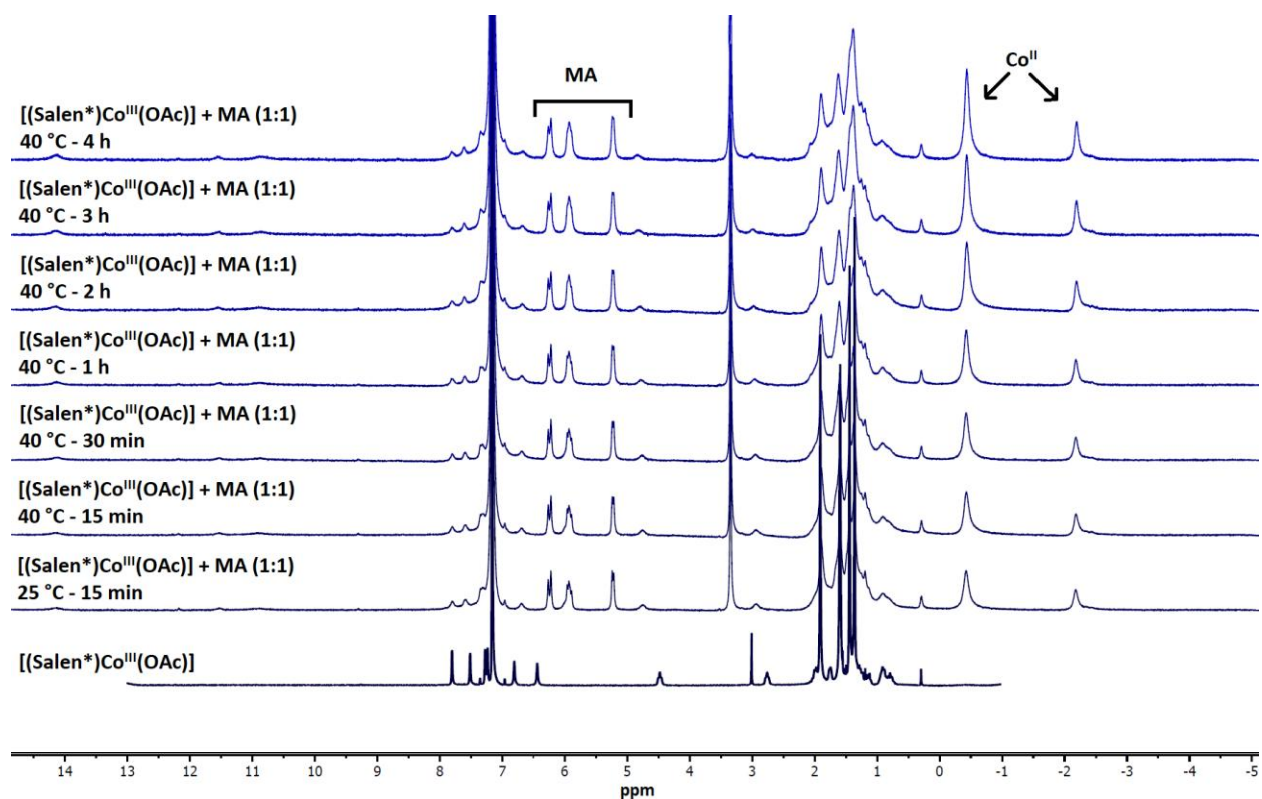


Figure S2. Evolution of the ^1H NMR (400 MHz, C_6D_6) spectra of a 1:1 mixture of [(Salen*)Co^{III}(OAc)] (**1**) and methyl acrylate (MA) over time. t_0 was recorded at 25 °C and the following spectra were recorded after heating at 40 °C upon the indicated duration. The ^1H NMR (400 MHz, C_6D_6) spectrum of [(Salen*)Co^{III}(OAc)] (**1**) is shown as reference (bottom).

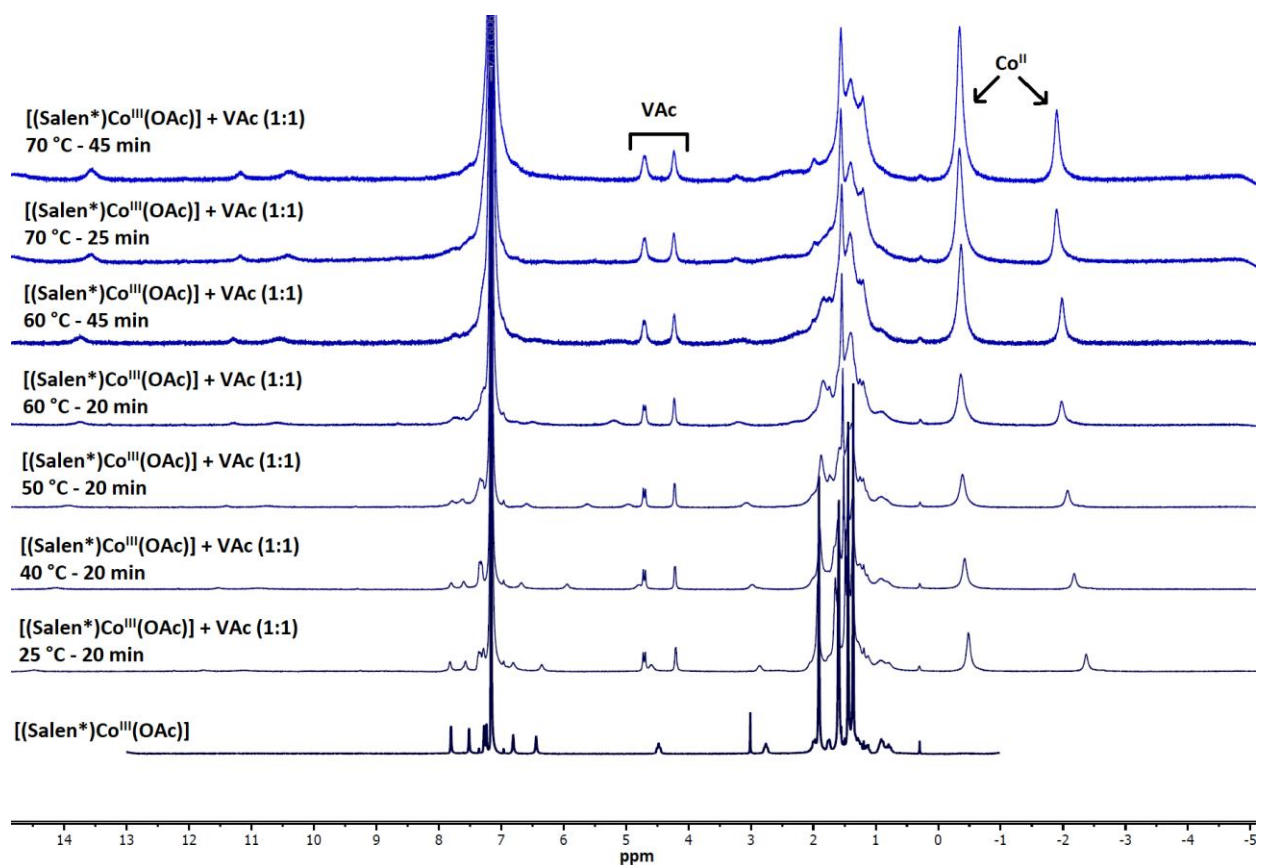


Figure S3. Evolution of the ^1H NMR (400 MHz, C_6D_6) spectra of a 1:1 mixture of $[(\text{Salen}^*)\text{Co}^{\text{III}}(\text{OAc})]$ (**1**) and vinyl acetate (VAc) recorded after treatment for the indicated duration and at the indicated temperature. The ^1H NMR (400 MHz, C_6D_6) spectrum of $[(\text{Salen}^*)\text{Co}^{\text{III}}(\text{OAc})]$ (**1**) is shown as reference (bottom).

Table S1. Results of the bulk polymerization of vinyl acetate (VAc) and methyl methacrylate (MMA) experiments initiated by complex **1**.

Entry	Monomer	[M]/[1]	Time (h)	Conv. ^a (%)	$M_{n, th}$ ^b (g/mol)	$M_{n, exp}$ ^c (g/mol)	\bar{D} ^d	Temp. (°C)
1	VAc	200	24 + 24	0	-	-	-	60 then 90
2	MMA	200	2.5	38	7600	5000	1.44	60
3	MMA	200	4.5	58	11700	3200	1.50	60
4	MMA	200	6	69	14000	2500	1.59	60
5 ^e	MMA	200	2	18	4200	3400	1.39	60
6 ^e	MMA	200	7	16	3700	3200	1.39	60
7 ^e	MMA	200	10	20	4700	3100	1.39	60
8 ^e	MMA	200	22	21	4900	3000	1.47	60
9	MMA	200	4	74	14800	1700	1.15	70
10	MMA	200	24	22	4400	4700	1.12	40
11	MMA	200	48	66	13200	2700	1.12	40

^a Determined by gravimetry and/or from ¹H NMR analysis. ^b Calculated according to $M_n(th) = ([Monomer]_0/[**1**]) \times M_{Monomer} \times conversion$, where $M_{Monomer}$ is the molecular weight of monomer. ^c Determined from GPC analysis by using PMMA standards. ^d Determined from GPC analysis. ^e Polymerization run treated with excess TEMPO after 2 h reaction.

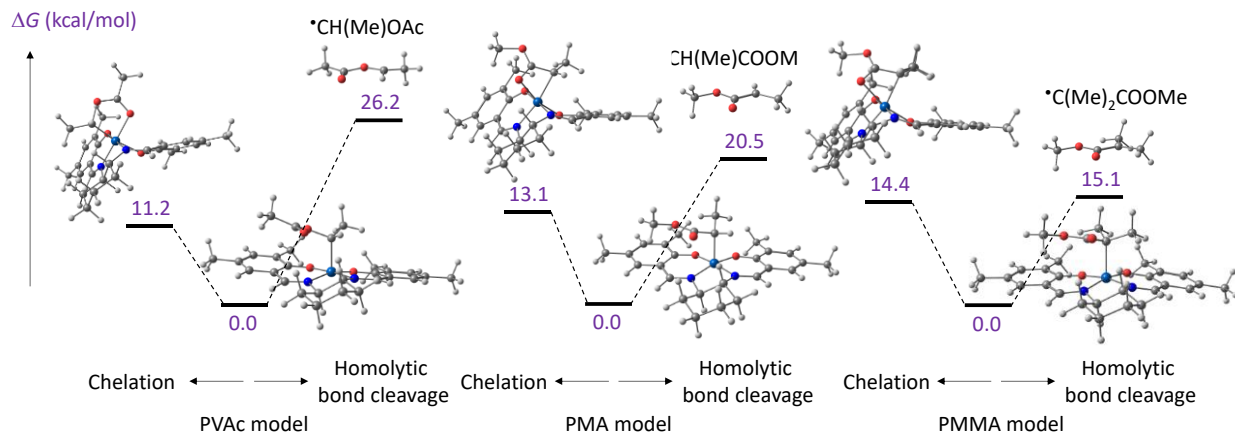


Figure S4. Gibbs energy profiles for the activation versus chelation of the $[(\text{Salen}^*)\text{Co}(\text{PVAc})]$, $[(\text{Salen}^*)\text{Co}(\text{PMA})]$ and $[(\text{Salen}^*)\text{Co}(\text{PMMA})]$ unimer models.

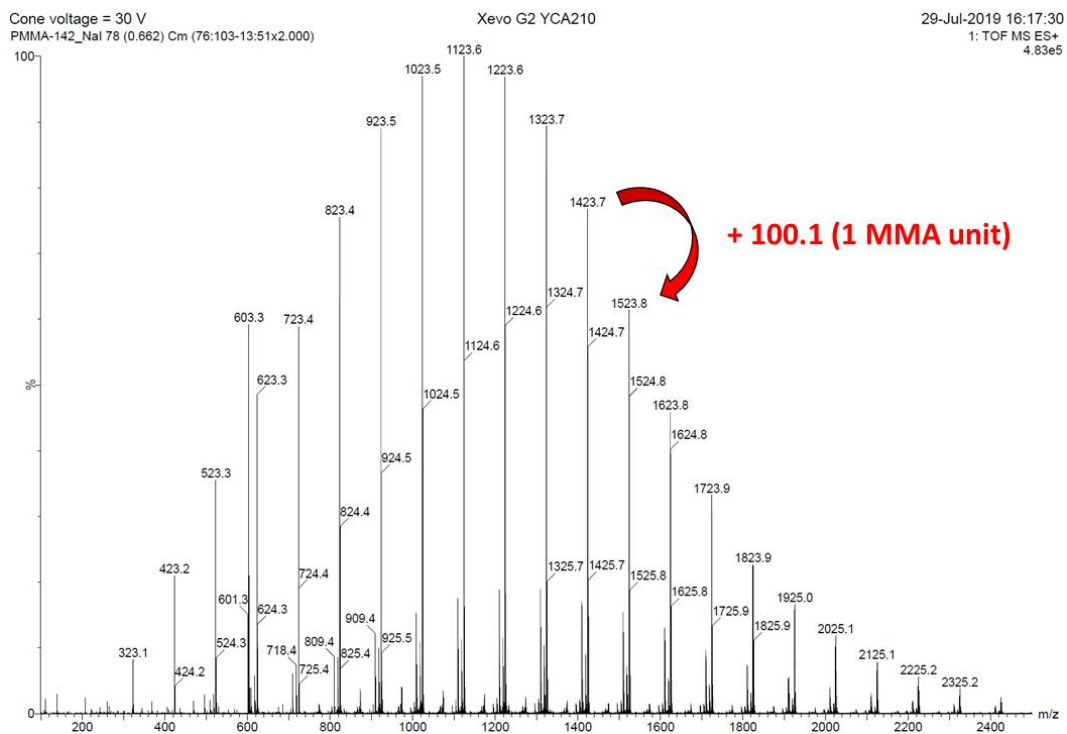


Figure S5. MALDI-ToF mass spectrum of the PMMA sample from the bulk polymerization of MMA (MMA/1 = 200/1) at 60 °C after 2.5 h (Table S1 – Entry 2) using a Dithranol/NaI (3/1) matrix.

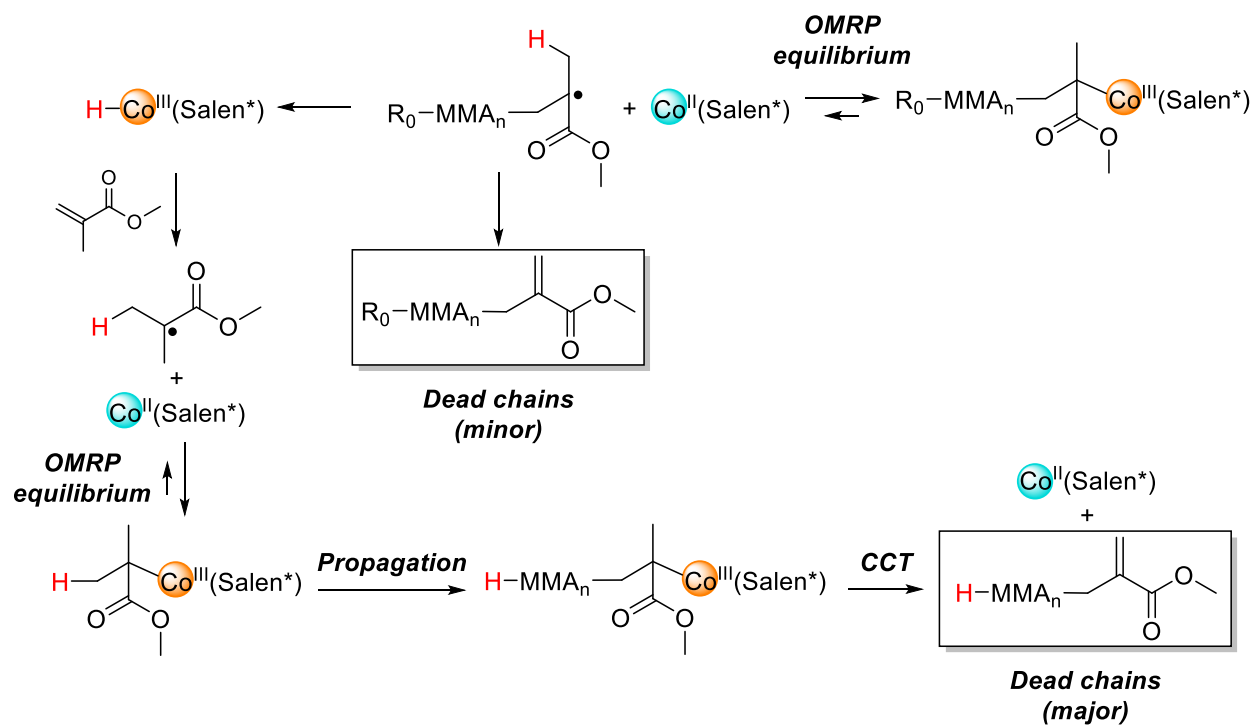


Figure S7. Mechanism of the $[(\text{Salen}^*)\text{Co}^{\text{II}}]$ -catalyzed chain transfer (CCT) in MMA polymerization and structure of the dead chains.

Table S2. Results of the bulk polymerization of methyl acrylate (MA) experiments initiated by complex **1**.

Entry	[M]/[1]	Time (h)	Conv. ^a (%)	$M_{n,th}$ ^b (g/mol)	$M_{n,exp}$ ^c (g/mol)	$M_{n,th}/M_{n,exp}$	\bar{D} ^d	Temp. (°C)
1	100	20	0	0	0	-	n/a	60
2	200	3	7	1200	7400	0.16	1.17	70
3	200	4	8	1400	7600	0.18	1.26	70
4	200	5	11	1900	10250	0.19	1.12	70
5	200	8	25	4300	15900	0.27	1.27	70
6	200	10	32	5500	18300	0.30	1.31	70
7	200	25	64	11000	39000	0.28	1.23	70
average						0.23±0.05		
8 ^e	200	5	11	2600	7600	0.34	1.26	70
9 ^e	200	8	10	2300	7500	0.31	1.29	70
10 ^e	200	21	14	3100	7300	0.42	1.28	70
11	100	3	15	1300	6000	0.22	1.21	70
12	100	5	32	2800	9900	0.28	1.27	70
13	100	7	51	4400	16000	0.28	1.27	70
14	100	9	69	5900	23000	0.26	1.43	70
15	100	11	87	7500	32000	0.23	1.65	70
average						0.25±0.02		
16	200	3	6	1000	5500	0.19	1.34	80
17	200	6	13	2200	11000	0.20	1.49	80
18	200	10.5	35	6000	17000	0.35	1.42	80
19	200	13	60	10300	20000	0.52	1.71	80
20	200	16	68	11700	24000	0.49	1.85	80
21	200	19	77	13300	29000	0.46	2.05	80
average						0.37±0.12		

^a Determined by gravimetry and/or from ¹H NMR analysis. ^b Calculated according to $M_n(th) = ([Monomer]_0/[1]) \times M_{Monomer} \times conversion$, where $M_{Monomer}$ is the molecular weight of monomer. ^c Determined from GPC analysis by using PMMA standards. ^d Determined from GPC analysis. ^e Polymerization run treated with excess TEMPO after 2 h reaction.

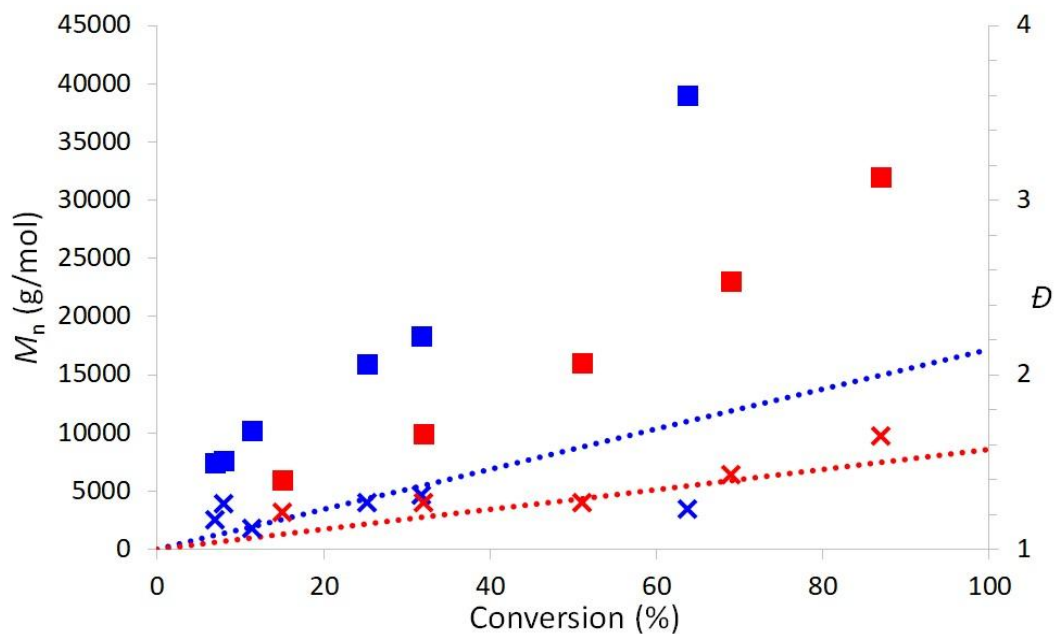


Figure S8. Dependence of PMA molar masses (M_n , squares) and dispersity (D , crosses) on monomer conversion for the bulk polymerization of MA at 70 °C initiated by complex 1 with initial [1]/[MA] ratio of 1/200 (blue) and 1/100 (red). The dotted lines represent the corresponding theoretical M_n values.

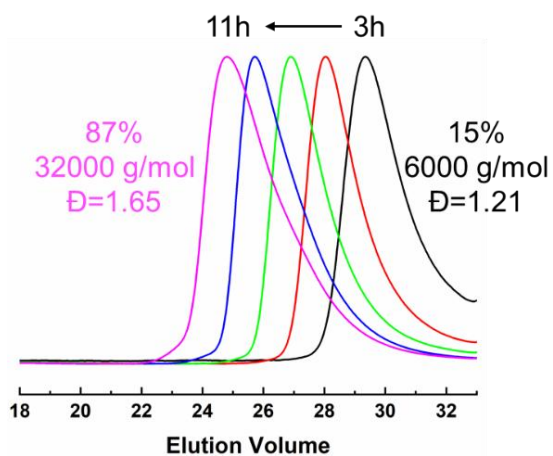


Figure S9. Evolution of the SEC chromatograms for the bulk polymerization of MA at 70°C initiated by complex 1 (initial ratio: [1]/[MA] = 1/100).

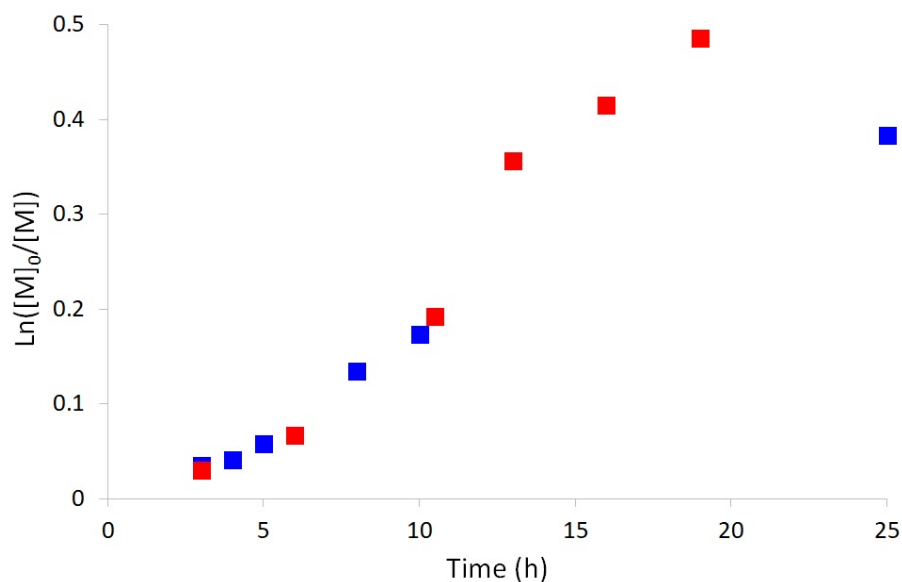


Figure S10. Time dependence of $\ln([M]_0/[M])$ for the bulk polymerization of MA at 70 °C (blue squares) and 80 °C (red squares) initiated by complex **1** (initial ratio: $[1]/[MA] = 1/200$). $[M]_0$ and $[M]$ are the MA concentration at times 0 and t, respectively.

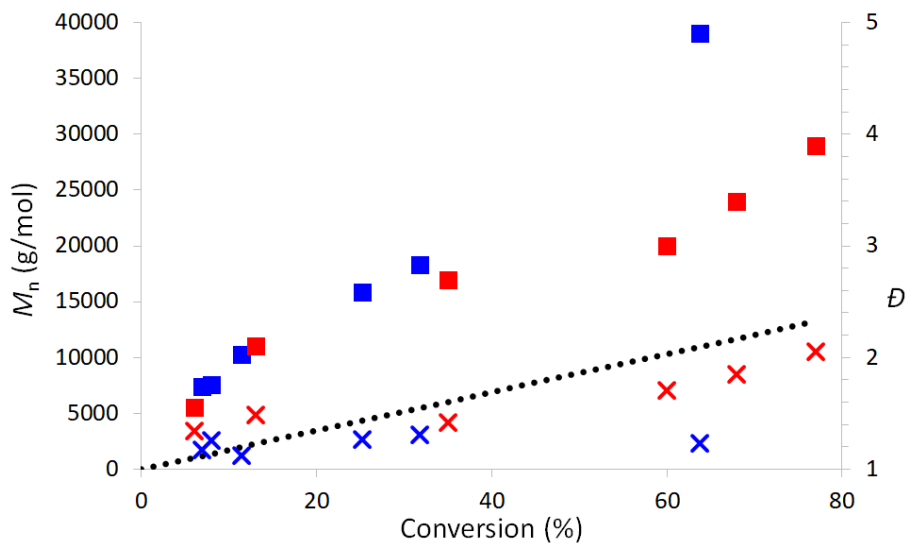


Figure S11. Dependence of PMA molar masses (M_n , squares) and dispersity (D , crosses) on monomer conversion for the bulk polymerization of MA at 70 °C (blue) and 80 °C (red) initiated by complex **1** with initial $[1]/[MA]$ ratio of 1/200. The dotted black line represents the theoretical M_n values.

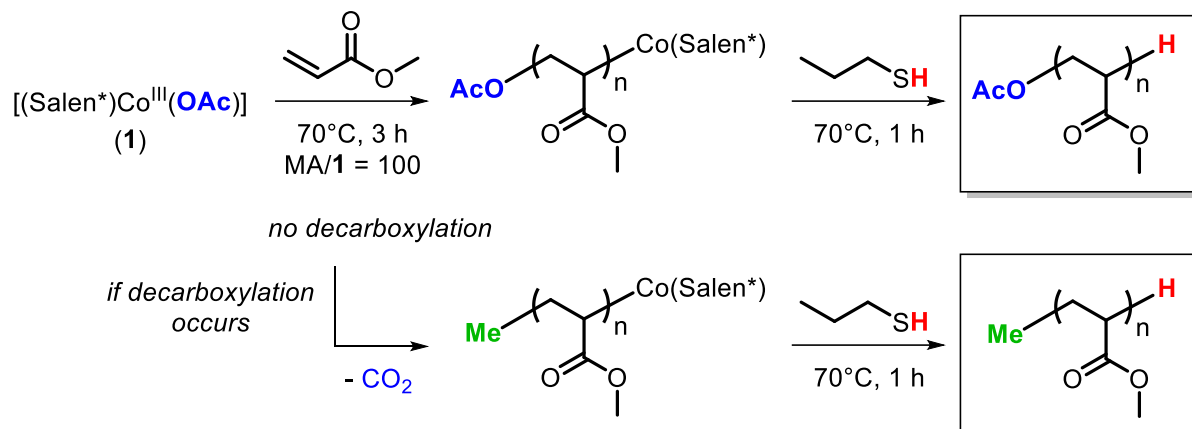


Figure S12. 1-propanethiol quenching of an OMRP of MA, and expected formula for the PMA sample (w/wo decarboxylation).

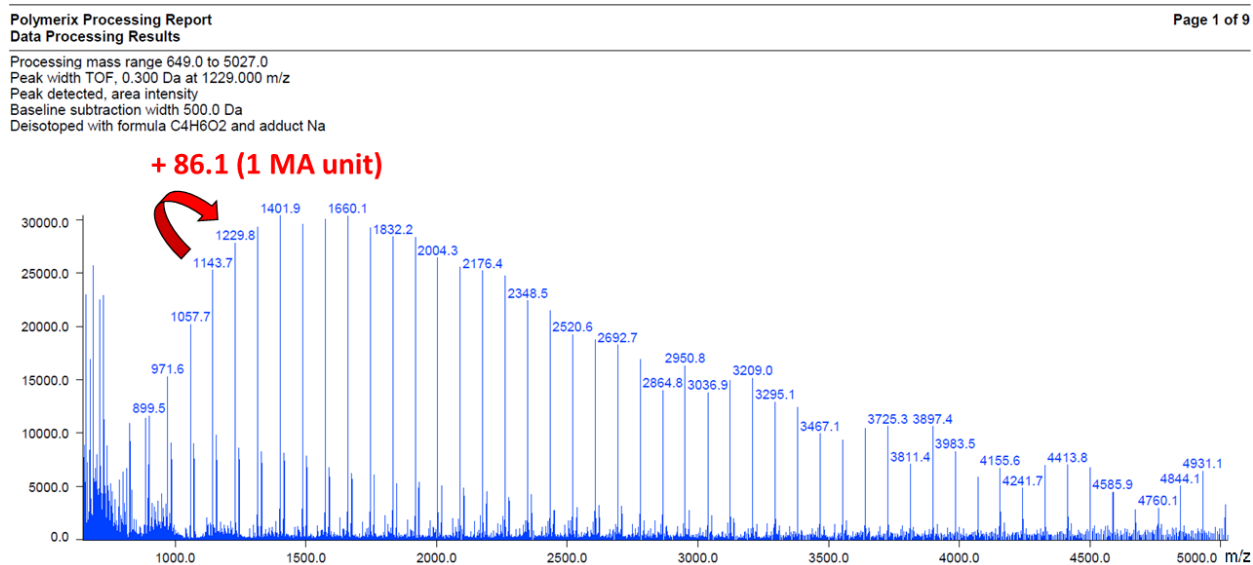
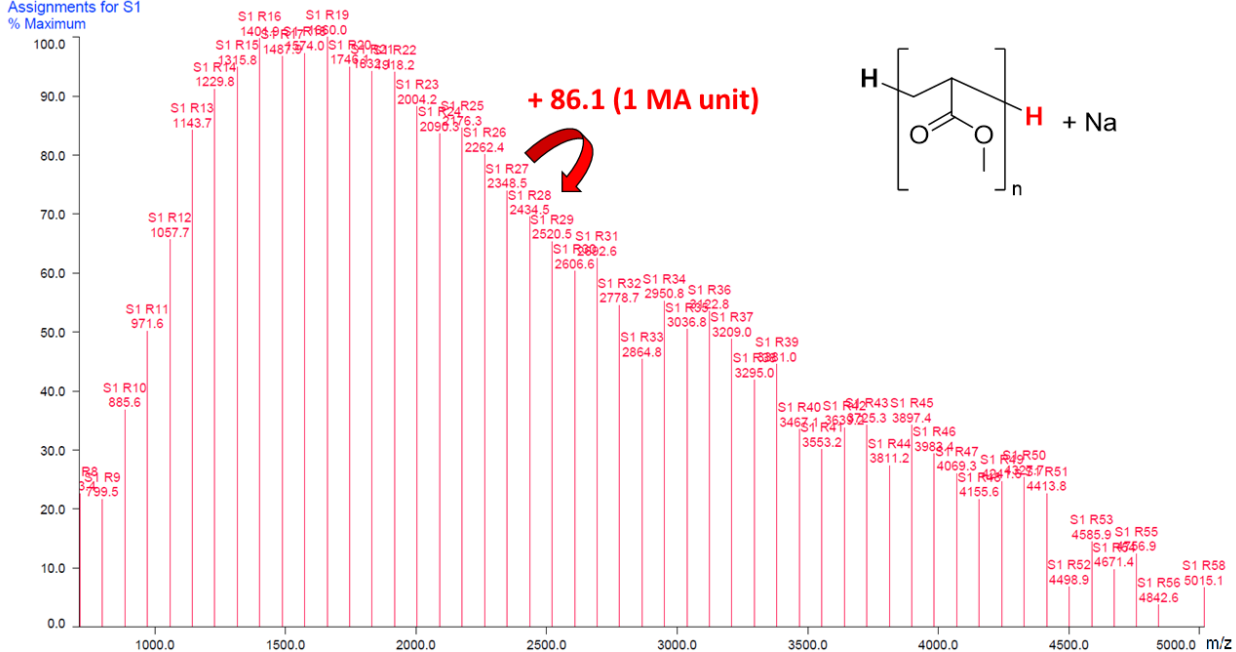


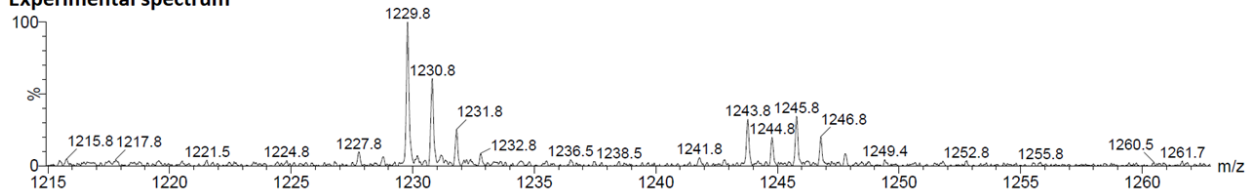
Figure S13. MALDI-ToF mass spectrum of the PMA sample isolated from the bulk polymerization of MA quenched with 1-propanethiol (MA/1 = 100, 70 °C, 3 h, 15% conv., $M_n = 6100\text{ g mol}^{-1}$, $D = 1.25$) using a Dithranol/NaI (3/1) matrix.

Assignments for S1
% Maximum



MALDI Micro

Experimental spectrum



Simulation for C56H86O28Na

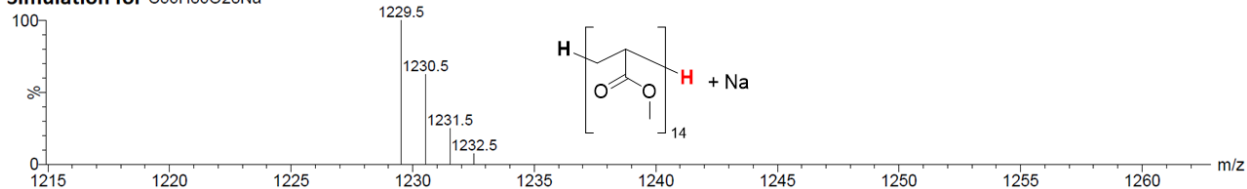


Figure S14. Top. MALDI-ToF mass spectrum of the most abundant homopolymer identified using the Polymerix software, from the PMA sample isolated from the bulk polymerization of MA quenched with 1-propanethiol (MA/1 = 100, 70 °C, 3 h, 15% conv., $M_n = 6100 \text{ g mol}^{-1}$, $D = 1.25$) using a Dithranol/NaI (3/1) matrix. Bottom. Comparison between the experimental spectrum and the simulated isotopic distribution for $n = 14$ MA units.

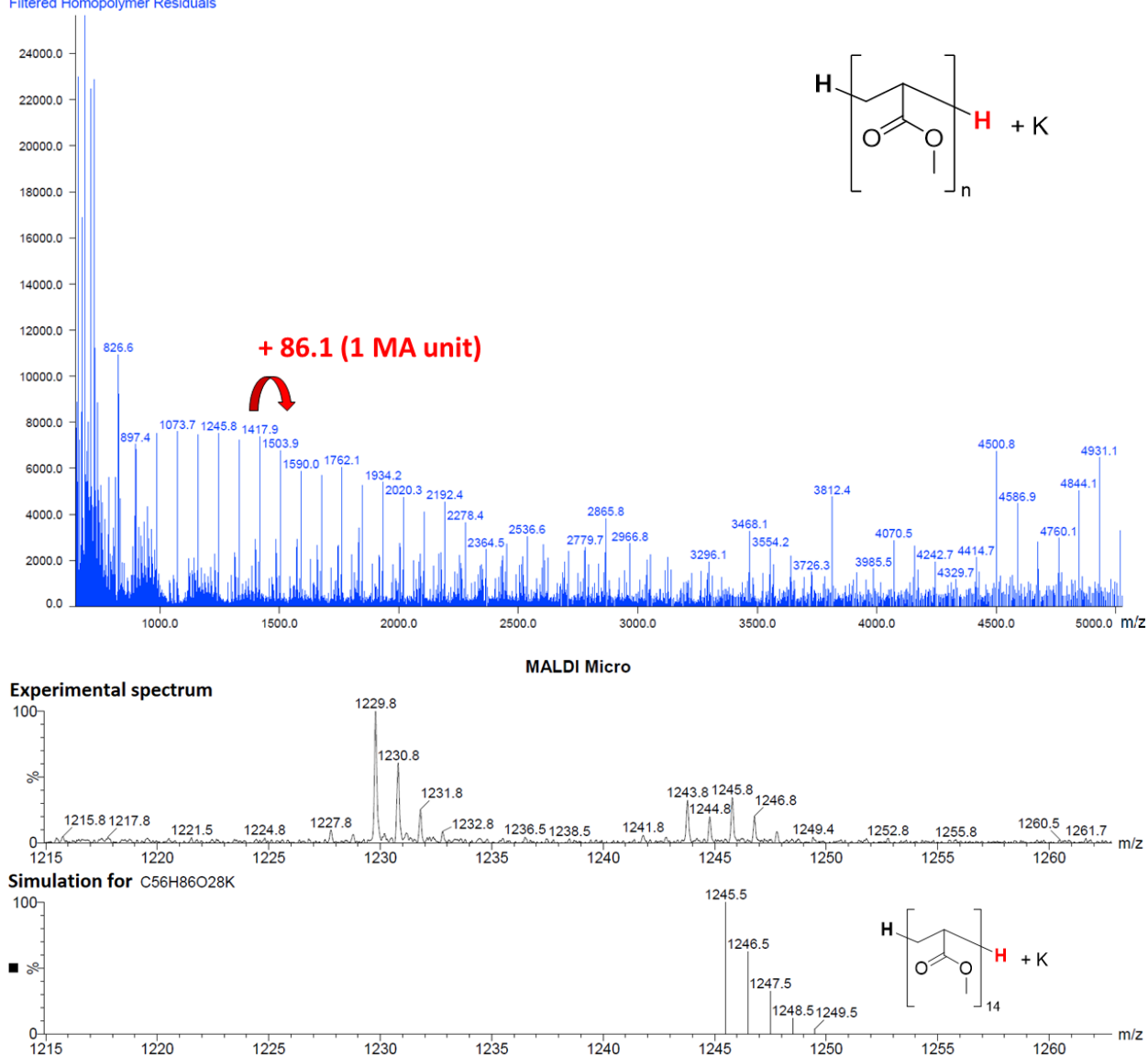


Figure S15. Top. MALDI-ToF mass spectrum of the third homopolymer identified using the Polymerix software, from the PMA sample isolated from the bulk polymerization of MA quenched with 1-propanethiol (MA/1 = 100, 70 °C, 3 h, 15% conv., $M_n = 6100 \text{ g mol}^{-1}$, $D = 1.25$) using a Dithranol/NaI (3/1) matrix. Bottom. Comparison between the experimental spectrum and the simulated isotopic distribution for $n = 14$ MA units.

Assignments for S2
% Maximum

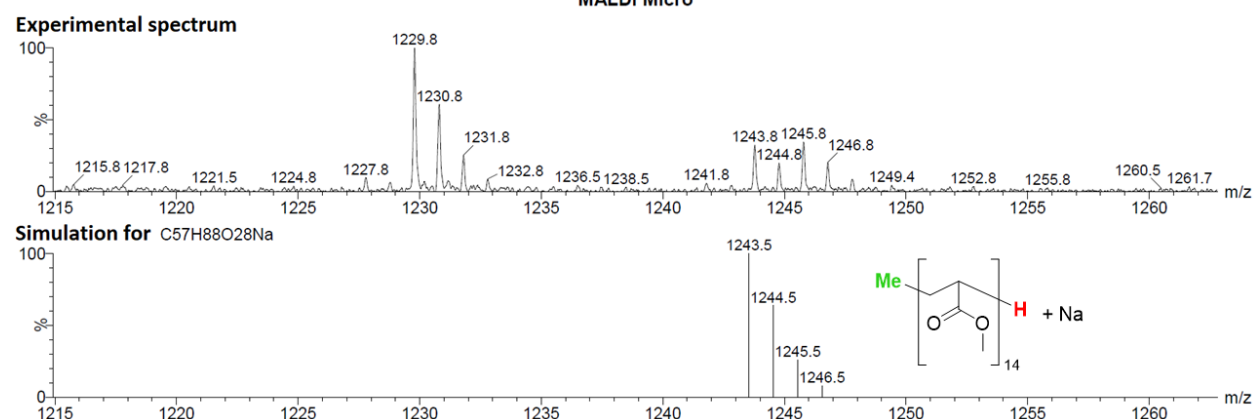
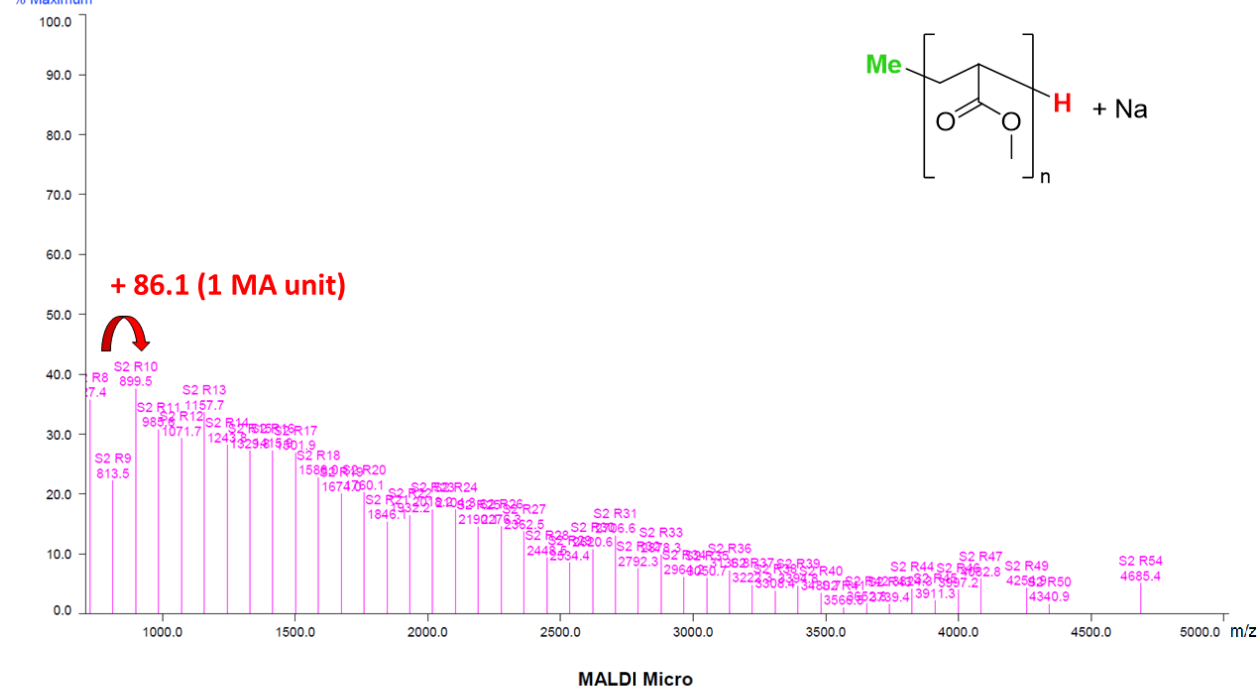


Figure S16. Top. MALDI-ToF mass spectrum of the second homopolymer identified using the Polymerix software, from the PMA sample isolated from the bulk polymerization of MA quenched with 1-propanethiol ($MA/1 = 100$, $70\text{ }^\circ\text{C}$, 3 h , 15% conv., $M_n = 6100\text{ g mol}^{-1}$, $D = 1.25$) using a Dithranol/NaI (3/1) matrix. Bottom. Comparison between the experimental spectrum and the simulated isotopic distribution for $n = 14$ MA units.

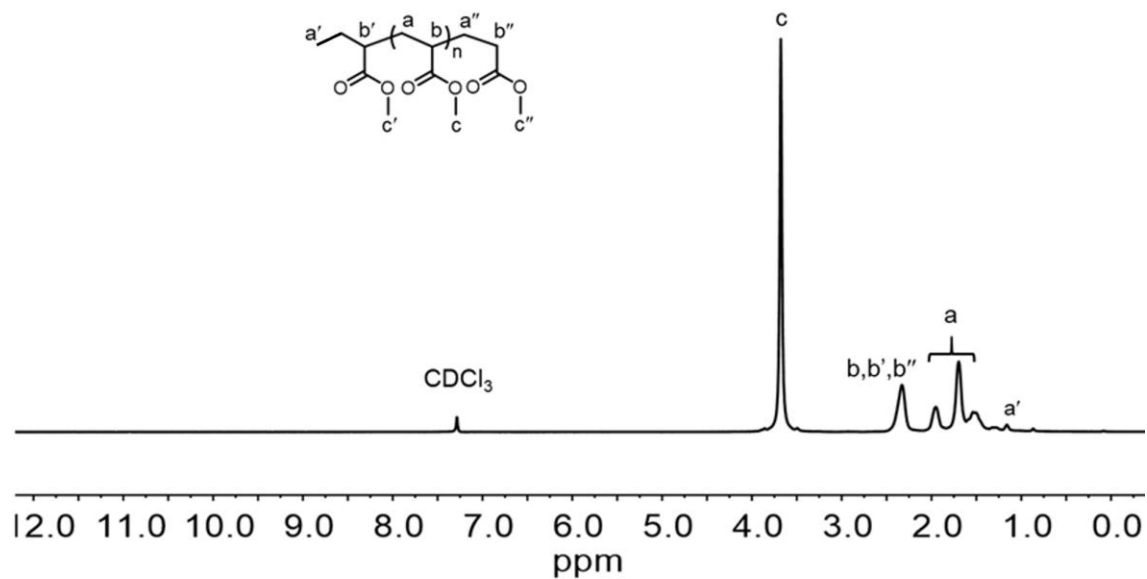


Figure S17. ^1H NMR spectrum (400 MHz, CDCl_3) of the PMA sample isolated from the bulk polymerization of MA quenched with 1-propanethiol ($\text{MA}/\mathbf{1} = 100$, $70\text{ }^\circ\text{C}$, 3 h, 15% conv., $M_n = 6100\text{ g mol}^{-1}$, $D = 1.25$). The signal of low intensity at $\delta 1.15$ ppm (a') can be attributed to the Me group of the α chain end.

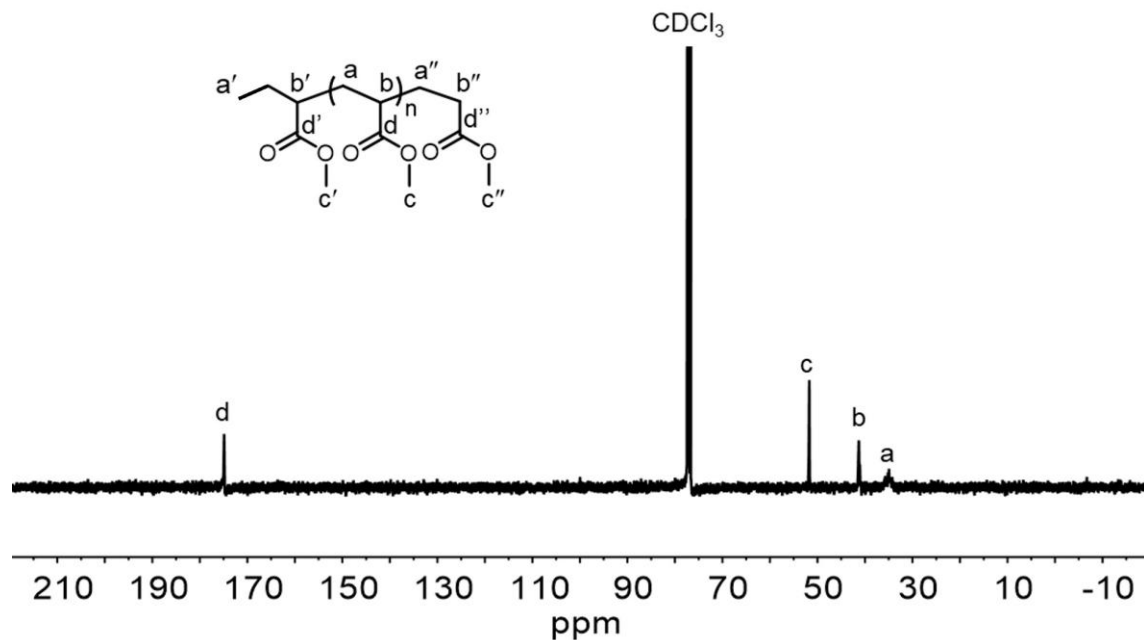


Figure S18. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100 MHz, CDCl_3) of the PMA sample isolated from the bulk polymerization of MA quenched with 1-propanethiol (MA/1 = 100, 70 °C, 3 h, 15% conv., $M_n = 6100 \text{ g mol}^{-1}$, $D = 1.25$). No signal of the chain ends could be observed.

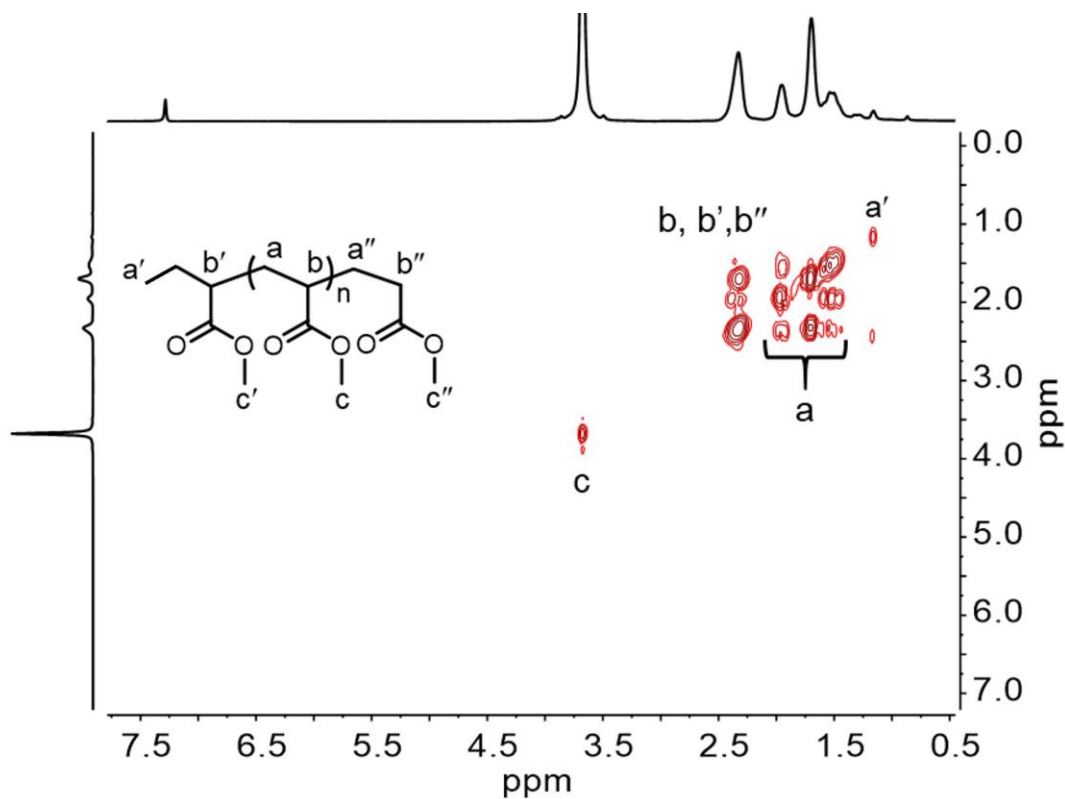


Figure S19. ^1H - ^1H COSY NMR spectrum (400 MHz, CDCl_3) of the PMA sample isolated from the bulk polymerization of MA quenched with 1-propanethiol ($\text{MA}/\mathbf{1} = 100$, $70\text{ }^\circ\text{C}$, 3 h, 15% conv., $M_n = 6100\text{ g mol}^{-1}$, $D = 1.25$). The signal at δ 1.15 ppm (a'), which presents a correlation with one C-H group at δ 2.30 ppm (b'), can be attributed to the Me group of the α chain end.

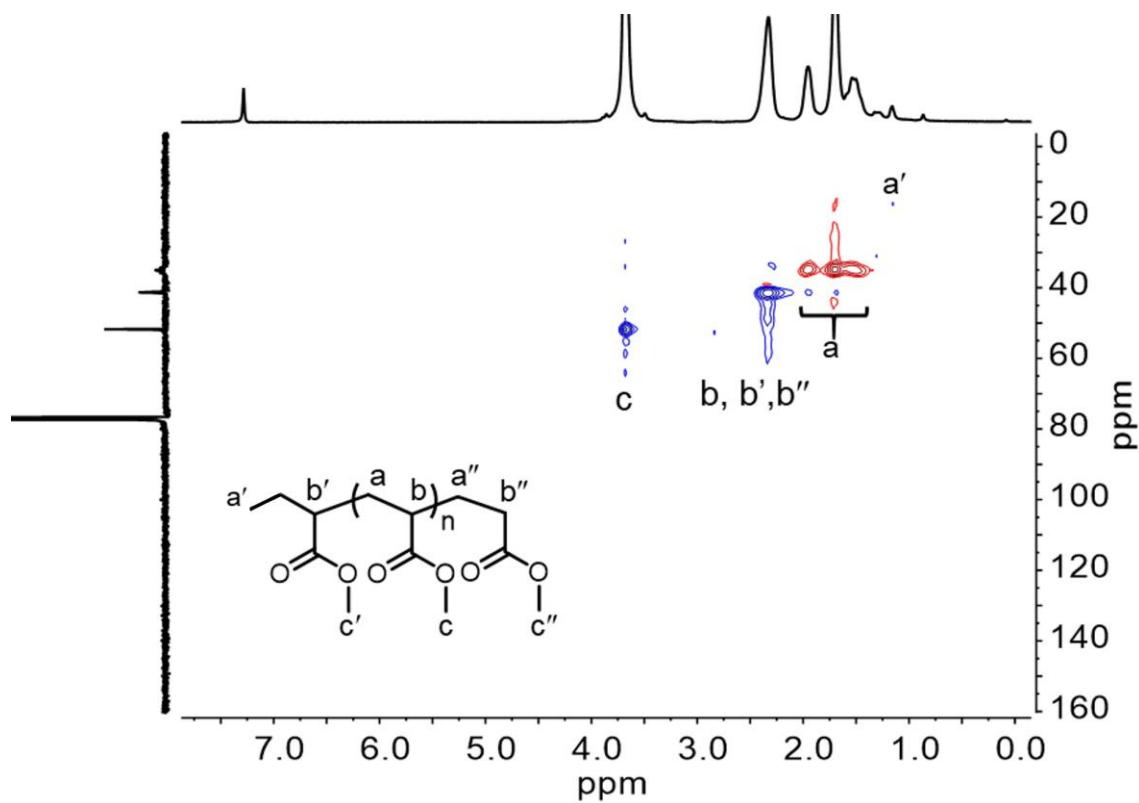


Figure S20. ^{13}C - ^1H HSQC NMR spectrum (CDCl_3) of the PMA sample isolated from the bulk polymerization of MA quenched with 1-propanethiol ($\text{MA}/1 = 100$, $70\text{ }^\circ\text{C}$, 3 h, 15% conv., $M_n = 6100\text{ g mol}^{-1}$, $D = 1.25$). The signal at $\delta 1.15\text{ ppm}$ (a'), which presents a correlation with a C atom at $\delta 16.0\text{ ppm}$, can be attributed to the Me group of the α chain end.

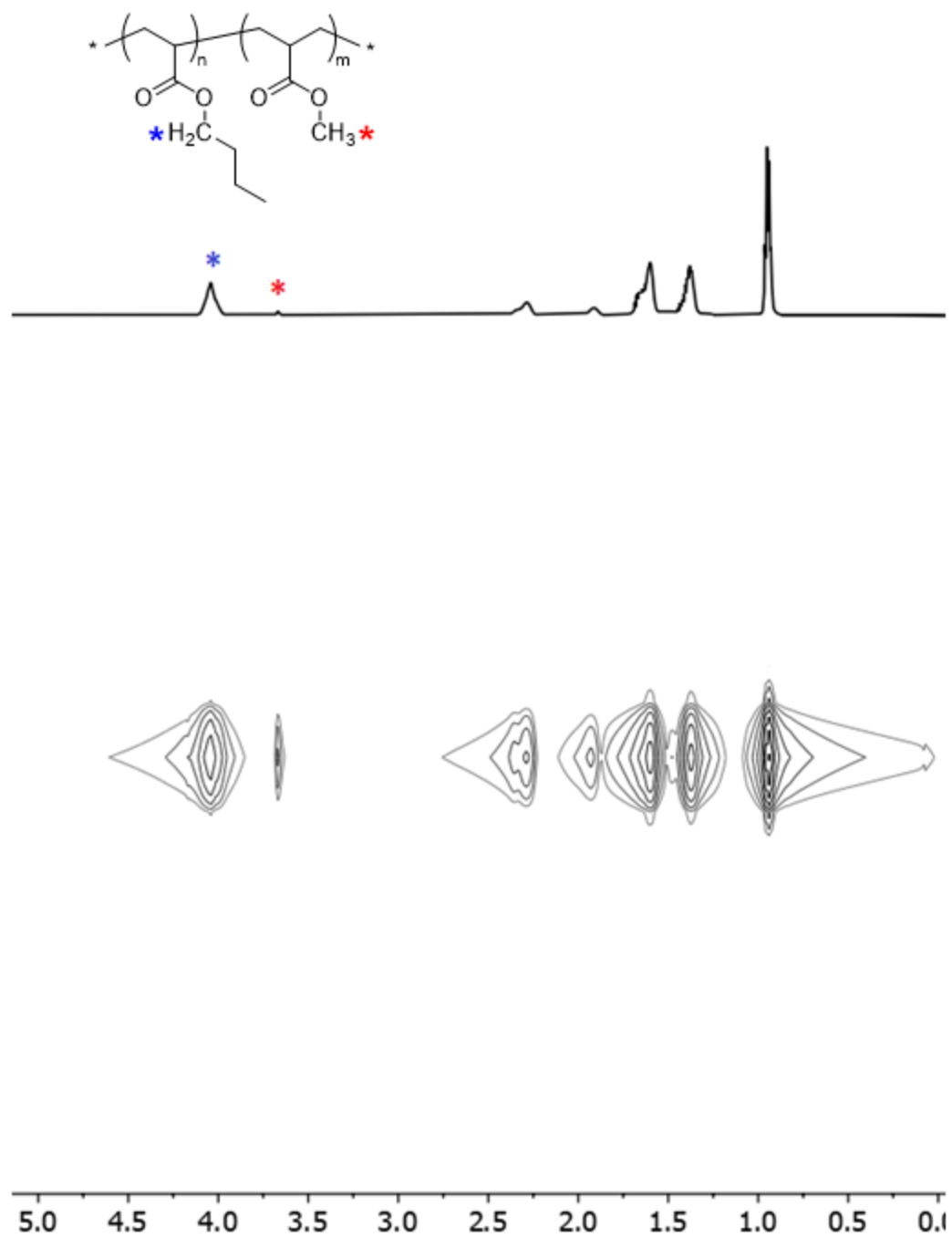


Figure S21. ¹H DOSY (600 MHz, CDCl₃) spectrum of the PMA-*b*-PBA block copolymer synthesized *via* OMRP using complex **1**.

Table S3. Cartesian coordinates (Å), energies and 1M-corrected Gibbs energies (hartrees) for all geometry-optimized molecules.

A. Radicals

CH₃COO• (AcO•)

E = -228.258298539

G = -228.238341

8	-0.807782000	1.040679000	0.001732000
6	-0.104322000	-0.000167000	-0.008501000
8	-0.809088000	-1.040016000	0.001719000
6	1.384508000	-0.000676000	-0.002810000
1	1.731616000	0.017827000	1.035971000
1	1.761183000	-0.907705000	-0.482500000
1	1.761051000	0.889631000	-0.513212000

CH₃CH•OOCCH₃ (H-VAc•)

E = -306.822891579

G = -306.757705

6	1.320165000	0.387361000	-0.125060000
1	1.152079000	1.449537000	0.011404000
6	2.607250000	-0.310799000	0.057527000
1	2.669764000	-1.199539000	-0.583198000
1	3.438332000	0.355639000	-0.190908000
1	2.752148000	-0.654554000	1.096463000
6	-1.024587000	0.162422000	0.009824000
6	-2.089755000	-0.893402000	0.014918000
1	-3.054217000	-0.431764000	0.226489000
1	-2.123925000	-1.379314000	-0.966330000
1	-1.861423000	-1.664880000	0.755464000
8	0.213258000	-0.421195000	-0.048329000
8	-1.194658000	1.352619000	0.036748000

CH₃CH•COOCH₃ (H-MA•)

E = -306.826016255

G = -306.758961

6	2.519286000	0.011893000	-0.000079000
6	1.209205000	-0.669728000	0.000022000
1	2.387882000	1.096811000	-0.000123000
1	3.114717000	-0.276078000	-0.878866000
1	3.114795000	-0.275986000	0.878688000
1	1.140785000	-1.753989000	0.000031000
6	-0.023582000	0.086597000	0.000139000
8	-1.110058000	-0.728492000	0.000072000
8	-0.104328000	1.302594000	0.000037000
6	-2.368114000	-0.048642000	-0.000113000
1	-3.127446000	-0.831592000	-0.001534000
1	-2.468871000	0.582610000	0.889082000
1	-2.467548000	0.584691000	-0.887959000

CH₃C•(CH₃)COOCH₃ (H-MMA•)

E = -346.114008362

G = -346.025751

6	2.173335000	-0.894487000	0.005371000
6	1.087881000	0.118462000	-0.014420000
1	1.767745000	-1.907575000	0.027030000
1	2.823868000	-0.749911000	0.880840000
1	2.820709000	-0.787558000	-0.877649000
6	-0.285907000	-0.352043000	-0.004901000
8	-1.192033000	0.663097000	-0.001273000
8	-0.621638000	-1.525177000	-0.000654000
6	-2.557625000	0.243942000	0.003934000
1	-3.148544000	1.160871000	0.011016000
1	-2.785067000	-0.352468000	-0.885895000
1	-2.775814000	-0.360511000	0.890558000
6	1.440030000	1.562558000	-0.001645000
1	1.856243000	1.846062000	0.978294000
1	2.225438000	1.775812000	-0.739626000
1	0.578501000	2.201334000	-0.199178000

B. Initiator complex (1)

[(Salen*)Co^{III}(OAc)] (κ²)

E = -1564.73451419

G = -1564.358032

27	-0.061957000	0.188106000	0.640361000
7	-1.592289000	1.218455000	0.243414000
7	0.817297000	1.393446000	-0.508530000
8	-0.518170000	-1.018556000	-0.7111474000
8	1.461427000	-0.841187000	1.019988000
6	-1.177353000	2.600490000	0.099877000
1	-0.741269000	2.894437000	1.063676000
6	-0.025085000	2.522408000	-0.921644000
1	-0.479395000	2.257245000	-1.890824000
6	0.667971000	3.877359000	-1.032399000
1	1.466765000	3.849866000	-1.781751000
1	1.138334000	4.107646000	-0.066819000
6	-0.352372000	4.957867000	-1.408672000
1	0.141074000	5.935868000	-1.443463000
1	-0.724898000	4.759778000	-2.424266000
6	-1.536377000	4.997212000	-0.440318000
1	-2.264383000	5.749916000	-0.763638000
1	-1.183389000	5.307044000	0.553323000
6	-2.213429000	3.627596000	-0.326237000
1	-3.035482000	3.661122000	0.398888000
1	-2.643779000	3.347412000	-1.298774000
6	-2.711802000	0.723839000	-0.166386000
1	-3.543147000	1.401400000	-0.381080000
6	-2.892057000	-0.667055000	-0.437759000
6	-1.744124000	-1.459674000	-0.741342000
6	-1.954764000	-2.801959000	-1.172352000
6	-3.243917000	-3.287139000	-1.259956000
1	-3.384969000	-4.322514000	-1.570768000
6	-4.388287000	-2.513014000	-0.963445000

6	-4.188823000	-1.207058000	-0.572350000
1	-5.044340000	-0.571143000	-0.347180000
6	-0.746107000	-3.627300000	-1.490673000
1	-1.016332000	-4.661994000	-1.721434000
1	-0.045871000	-3.612186000	-0.648082000
1	-0.200736000	-3.205569000	-2.343315000
6	-5.760948000	-3.116227000	-1.076957000
1	-6.540907000	-2.379039000	-0.862089000
1	-5.888793000	-3.949604000	-0.374581000
1	-5.942423000	-3.511667000	-2.084070000
6	2.007413000	1.210852000	-0.981778000
1	2.392670000	1.947768000	-1.692414000
6	2.885195000	0.138684000	-0.661330000
6	2.557203000	-0.825517000	0.340481000
6	3.525396000	-1.838971000	0.631964000
6	4.716007000	-1.859274000	-0.059484000
1	5.434156000	-2.646429000	0.172056000
6	5.053828000	-0.912178000	-1.055796000
6	4.132798000	0.070258000	-1.330379000
1	4.356084000	0.821930000	-2.087188000
6	3.177634000	-2.844195000	1.686136000
1	3.969276000	-3.589730000	1.806102000
1	2.238692000	-3.352456000	1.438206000
1	3.006205000	-2.349608000	2.649692000
6	6.374720000	-1.002768000	-1.768388000
1	6.497275000	-0.188017000	-2.488866000
1	6.469084000	-1.948695000	-2.316829000
1	7.213999000	-0.953521000	-1.063179000
8	0.175121000	1.147191000	2.361901000
6	-0.481423000	0.206234000	2.914289000
8	-0.946683000	-0.698493000	2.159709000
6	-0.659181000	0.152481000	4.396445000
1	-0.699884000	1.162429000	4.810136000
1	0.207388000	-0.361924000	4.826104000
1	-1.559495000	-0.411301000	4.648250000

[(Salen*)Co^{III}(OAc)] (κ⁻¹)

E = -1564.71248798

G = -1564.340114

27	-0.036853000	0.108915000	-0.481181000
8	1.202200000	-1.169711000	-1.002562000
8	-1.322104000	-1.171818000	-0.801029000
7	1.246548000	1.496315000	-0.581421000
7	-1.302517000	1.467838000	-0.154170000
6	2.447828000	-1.140955000	-0.650193000
6	3.136482000	-2.386951000	-0.550593000
6	4.476765000	-2.384716000	-0.227362000
6	5.216800000	-1.202095000	0.012464000
6	4.548705000	-0.000787000	-0.067919000
6	3.169943000	0.058188000	-0.377454000
6	2.524053000	1.325029000	-0.455681000
6	0.613069000	2.813291000	-0.663407000
6	1.469945000	4.017684000	-0.296434000
6	0.635307000	5.298428000	-0.369553000
6	-0.604212000	5.205756000	0.517942000
6	-1.464287000	3.991912000	0.158929000
6	-0.633366000	2.715688000	0.223782000

6	-2.581091000	1.298129000	-0.005048000
6	-3.273019000	0.064699000	-0.143601000
6	-4.666371000	0.021730000	0.104826000
6	-5.372983000	-1.156701000	0.034968000
6	-4.657693000	-2.338037000	-0.281786000
6	-3.305139000	-2.355936000	-0.542048000
6	-2.578237000	-1.127718000	-0.500710000
1	4.988909000	-3.342989000	-0.139847000
1	5.082431000	0.930017000	0.121869000
1	3.170263000	2.204725000	-0.409523000
1	0.259641000	2.931166000	-1.700896000
1	1.862468000	3.883565000	0.721846000
1	2.330702000	4.096279000	-0.970610000
1	0.325869000	5.470107000	-1.410559000
1	1.249730000	6.158566000	-0.080297000
1	-1.202173000	6.120592000	0.437077000
1	-0.291890000	5.126744000	1.569075000
1	-2.315371000	3.933629000	0.846526000
1	-1.873163000	4.103094000	-0.855782000
1	-0.275887000	2.554393000	1.253877000
1	-3.190268000	2.162952000	0.268073000
1	-5.178389000	0.946528000	0.368697000
1	-5.201887000	-3.282182000	-0.304803000
6	6.678932000	-1.284934000	0.352787000
1	7.110666000	-0.292139000	0.513242000
1	6.842853000	-1.872369000	1.264911000
1	7.247409000	-1.770859000	-0.450009000
6	2.334902000	-3.632771000	-0.761901000
1	1.459975000	-3.615769000	-0.101489000
1	1.945310000	-3.675701000	-1.785694000
1	2.930950000	-4.529921000	-0.569946000
6	-2.526894000	-3.601038000	-0.828817000
1	-1.670085000	-3.655693000	-0.147332000
1	-3.148067000	-4.495400000	-0.723963000
1	-2.108144000	-3.573775000	-1.841685000
6	-6.851088000	-1.222381000	0.300461000
1	-7.394352000	-1.607226000	-0.571608000
1	-7.074648000	-1.891425000	1.140791000
1	-7.260520000	-0.236244000	0.540177000
8	0.287142000	-0.055979000	1.328737000
6	0.287443000	-1.222491000	1.944223000
8	0.001160000	-2.310787000	1.492549000
6	0.762005000	-1.046974000	3.381204000
1	0.446991000	-0.088160000	3.798762000
1	0.386402000	-1.875302000	3.984621000
1	1.857102000	-1.076929000	3.379492000

C. Moderating complex

[(Salen*)Co^{II}]

E = -1336.40802803

G = -1336.061799

27	-0.000015000	-0.094647000	0.000029000
8	-1.278201000	-1.438128000	-0.077310000
8	1.278212000	-1.438101000	0.077565000
7	-1.261772000	1.265770000	0.222573000
7	1.261729000	1.265765000	-0.222650000

6	-2.568610000	-1.328710000	-0.052460000			
6	-3.341625000	-2.523446000	-0.193172000	27	-0.040377000	0.135646000 0.571603000
6	-4.716393000	-2.442464000	-0.170917000	7	-1.522478000	1.314671000 0.442167000
6	-5.421116000	-1.223787000	-0.014751000	7	0.828703000	1.401428000 -0.502832000
6	-4.680825000	-0.073581000	0.118814000	8	-0.785954000	-0.861802000 -0.971203000
6	-3.263399000	-0.092868000	0.102713000	8	1.387582000	-1.098502000 0.612646000
6	-2.557807000	1.131366000	0.242812000	6	-1.042559000	2.679748000 0.318262000
6	-0.620005000	2.566999000	0.448341000	1	-0.509485000	2.937193000 1.243667000
6	-1.467792000	3.815843000	0.234358000	6	0.013602000	2.588412000 -0.798773000
6	-0.617498000	5.070950000	0.448547000	1	-0.535621000	2.376886000 -1.730481000
6	0.617473000	5.070957000	-0.448345000	6	0.763638000	3.911079000 -0.931020000
6	1.467773000	3.815849000	-0.234180000	1	1.488822000	3.873849000 -1.751183000
6	0.619983000	2.567029000	-0.448287000	1	1.332613000	4.087226000 -0.007237000
6	2.557772000	1.131371000	-0.242881000	6	-0.224962000	5.055535000 -1.177146000
6	3.263384000	-0.092852000	-0.102818000	1	0.316009000	6.007367000 -1.229582000
6	4.680804000	-0.073558000	-0.119132000	1	-0.700042000	4.911260000 -2.158235000
6	5.421124000	-1.223746000	0.014445000	6	-1.310693000	5.119332000 -0.101440000
6	4.716433000	-2.442403000	0.170893000	1	-2.022817000	5.920592000 -0.329643000
6	3.341665000	-2.523397000	0.193350000	1	-0.851686000	5.373493000 0.864841000
6	2.568613000	-1.328687000	0.052565000	6	-2.048270000	3.783504000 0.024949000
1	-5.290866000	-3.362895000	-0.277173000	1	-2.800892000	3.831629000 0.821203000
1	-5.185922000	0.884333000	0.241232000	1	-2.578661000	3.567178000 -0.913372000
1	-3.171066000	2.024334000	0.379350000	6	-2.718002000	0.952541000 0.083713000
1	-0.257736000	2.557790000	1.489402000	1	-3.501596000	1.715850000 0.051829000
1	-2.318850000	3.829409000	0.924597000	6	-3.062148000	-0.347700000 -0.379580000
1	-1.876542000	3.806089000	-0.786421000	6	-2.036227000	-1.157635000 -0.977710000
1	-1.223590000	5.965446000	0.265013000	6	-2.460021000	-2.342164000 -1.668652000
1	-0.301640000	5.117105000	1.500759000	6	-3.793678000	-2.681971000 -1.687140000
1	1.223555000	5.965461000	-0.264828000	1	-4.085770000	-3.603587000 -2.192201000
1	0.301611000	5.117113000	-1.500563000	6	-4.808479000	-1.894543000 -1.088028000
1	2.318867000	3.829468000	-0.924372000	6	-4.421569000	-0.731227000 -0.465461000
1	1.876458000	3.806034000	0.786623000	1	-5.173510000	-0.082720000 -0.015531000
1	0.257708000	2.557937000	-1.489346000	6	-1.394103000	-3.176851000 -2.308567000
1	3.171011000	2.024355000	-0.379372000	1	-1.811355000	-4.072789000 -2.778598000
1	5.185877000	0.884352000	-0.241695000	1	-0.644194000	-3.472480000 -1.565693000
1	5.290929000	-3.362811000	0.277241000	1	-0.851117000	-2.596983000 -3.064485000
6	-6.924640000	-1.219441000	0.000616000	6	-6.244946000	-2.333949000 -1.155948000
1	-7.320811000	-0.207995000	0.134305000	1	-6.910129000	-1.597929000 -0.692937000
1	-7.334446000	-1.617396000	-0.936288000	1	-6.396757000	-3.289925000 -0.637960000
1	-7.317018000	-1.841996000	0.814520000	1	-6.573870000	-2.474843000 -2.193516000
6	-2.602311000	-3.815179000	-0.359295000	6	1.979269000	1.216767000 -1.064588000
1	-3.289892000	-4.661888000	-0.443929000	1	2.352958000	1.999134000 -1.730257000
1	-1.963809000	-3.781812000	-1.249711000	6	2.833324000	0.087428000 -0.903478000
1	-1.926291000	-3.983521000	0.486641000	6	2.483525000	-1.010335000 -0.060928000
6	2.602420000	-3.815139000	0.359764000	6	3.421962000	-2.083172000 0.061264000
1	1.963898000	-3.781606000	1.250155000	6	4.609023000	-2.032049000 -0.635803000
1	1.926454000	-3.983737000	-0.486164000	1	5.306495000	-2.863667000 -0.531289000
1	3.290060000	-4.661780000	0.444627000	6	4.966117000	-0.955293000 -1.481020000
6	6.924642000	-1.219419000	-0.001304000	6	4.070327000	0.082673000 -1.593053000
1	7.316781000	-1.841459000	-0.815720000	1	4.308825000	0.933249000 -2.231504000
1	7.320798000	-0.207896000	-0.134461000	6	3.048979000	-3.224489000 0.956841000
1	7.334692000	-1.617985000	0.935230000	1	3.825936000	-3.994463000 0.971580000
				1	2.103793000	-3.674260000 0.630920000
				1	2.880583000	-2.869634000 1.981285000
				6	6.278352000	-0.971258000 -2.215073000
				1	6.413527000	-0.063584000 -2.811631000
				1	6.345469000	-1.829499000 -2.895680000
				1	7.125168000	-1.042708000 -1.520727000

D. Dormant PVAc unimer model

[(Salen*)Co^{III}(CHMeOOCCH₃)] (κ^1 -C)

E = -1643.26733628

G = -1642.861308

6	0.586409000	0.862963000	2.261080000
1	-0.108570000	1.623730000	2.646097000
6	2.010113000	1.334868000	2.365893000
1	2.133426000	2.231547000	1.750473000
1	2.279147000	1.584929000	3.400845000
1	2.703292000	0.576314000	1.996092000
8	0.431360000	-0.252496000	3.245263000
6	-0.410689000	-1.165495000	2.857288000
8	-0.948294000	-1.144027000	1.743817000
6	-0.664857000	-2.265898000	3.831163000
1	-0.593633000	-1.905944000	4.858946000
1	0.103148000	-3.031978000	3.676046000
1	-1.641079000	-2.709867000	3.632852000

[(Salen*)Co^{III}(CHMeOOCCH₃)] (κ^2 -C,O)

E = -1643.25677323

G = -1642.843385

27	-0.263407000	-0.134024000	-0.314058000
8	0.900119000	-1.578571000	-0.552116000
8	-1.626390000	-1.411319000	-0.420168000
7	1.032924000	1.149122000	-0.763300000
7	-1.462020000	1.307461000	-0.194380000
6	2.189626000	-1.528638000	-0.597333000
6	2.912286000	-2.751517000	-0.428843000
6	4.287848000	-2.739238000	-0.496192000
6	5.043862000	-1.566330000	-0.739815000
6	4.352223000	-0.389017000	-0.907139000
6	2.939504000	-0.336143000	-0.822735000
6	2.292904000	0.922432000	-0.971356000
6	0.453297000	2.480385000	-1.000738000
6	1.385754000	3.674287000	-0.825151000
6	0.611969000	4.978623000	-1.033698000
6	-0.600566000	5.069358000	-0.109531000
6	-1.529043000	3.863892000	-0.281089000
6	-0.743944000	2.579331000	-0.056210000
6	-2.754446000	1.235381000	-0.107025000
6	-3.524376000	0.036909000	-0.135223000
6	-4.931785000	0.127609000	-0.011677000
6	-5.735544000	-0.988865000	-0.039347000
6	-5.103683000	-2.244635000	-0.200153000
6	-3.739473000	-2.393533000	-0.328946000
6	-2.902509000	-1.235380000	-0.297311000
6	0.020789000	-0.149093000	1.608690000
1	4.821793000	-3.679185000	-0.355061000
1	4.895796000	0.537385000	-1.091418000
1	2.929073000	1.758115000	-1.268678000
1	0.057696000	2.475209000	-2.030284000
1	1.813490000	3.630825000	0.184896000
1	2.214376000	3.630360000	-1.541116000
1	0.275271000	5.036656000	-2.079322000
1	1.278648000	5.833461000	-0.872166000
1	-1.155569000	5.995976000	-0.296463000
1	-0.257043000	5.109942000	0.933494000
1	-2.357842000	3.941298000	0.432070000
1	-1.966054000	3.859914000	-1.290648000
1	-0.324562000	2.590205000	0.960605000
1	-3.319322000	2.164439000	-0.004192000

1	-5.379662000	1.113539000	0.110947000
1	-5.725929000	-3.139633000	-0.219619000
6	6.544018000	-1.635649000	-0.810962000
1	6.982045000	-0.649560000	-0.994235000
1	6.971306000	-2.022816000	0.122670000
1	6.874519000	-2.302434000	-1.617262000
6	2.119965000	-3.993494000	-0.161530000
1	1.543451000	-3.885519000	0.764855000
1	1.384618000	-4.162044000	-0.955960000
1	2.766705000	-4.871763000	-0.076783000
6	-3.075338000	-3.725561000	-0.495322000
1	-2.335752000	-3.887829000	0.296902000
1	-3.803928000	-4.541473000	-0.478829000
1	-2.516953000	-3.764043000	-1.437815000
6	-7.230642000	-0.907593000	0.097915000
1	-7.735639000	-1.343817000	-0.772990000
1	-7.580710000	-1.455369000	0.982001000
1	-7.568193000	0.129078000	0.193543000
1	-0.371173000	0.790053000	2.011042000
6	-0.628373000	-1.367830000	2.211076000
1	-0.368447000	-1.431025000	3.276702000
1	-1.714042000	-1.302620000	2.114603000
1	-0.290028000	-2.270212000	1.698365000
8	1.413809000	-0.228577000	1.910597000
6	2.110943000	0.894178000	2.154319000
8	1.648526000	2.012943000	2.105461000
6	3.530227000	0.555967000	2.508003000
1	3.965060000	-0.077931000	1.729980000
1	3.543944000	-0.011261000	3.444339000
1	4.107259000	1.473791000	2.622917000

E. Dormant PMA unimer model

[(Salen*)Co^{III}(CHMeCOOCH₃)] (κ^1 -C)

E = -1643.2585421

G = -1642.853489

27	-0.257966000	-0.122292000	-0.253890000
8	0.932551000	-1.541083000	-0.501515000
8	-1.586883000	-1.432235000	-0.278229000
7	1.034623000	1.173458000	-0.704686000
7	-1.491095000	1.298195000	-0.242553000
6	2.220181000	-1.490799000	-0.591997000
6	2.946107000	-2.719174000	-0.500886000
6	4.320103000	-2.697897000	-0.600355000
6	5.067868000	-1.512931000	-0.806961000
6	4.369784000	-0.332833000	-0.916790000
6	2.959613000	-0.291648000	-0.807483000
6	2.297563000	0.959223000	-0.923092000
6	0.449089000	2.501804000	-0.954907000
6	1.351032000	3.704384000	-0.692378000
6	0.585008000	4.999239000	-0.973258000
6	-0.710209000	5.078220000	-0.167615000
6	-1.600203000	3.853207000	-0.403338000
6	-0.810438000	2.588062000	-0.095024000
6	-2.784655000	1.199575000	-0.210739000
6	-3.527556000	-0.014706000	-0.201552000
6	-4.941434000	0.048897000	-0.164053000

6	-5.717951000	-1.086753000	-0.157826000	8	1.345471000	-1.081817000	0.416178000
6	-5.051070000	-2.334533000	-0.192571000	6	-1.000010000	2.712272000	0.389453000
6	-3.679108000	-2.457964000	-0.229163000	1	-0.415526000	2.816007000	1.312677000
6	-2.871206000	-1.278764000	-0.231442000	6	0.001519000	2.699125000	-0.787566000
6	-0.107234000	-0.096425000	1.722457000	1	-0.598857000	2.594557000	-1.706829000
1	4.859482000	-3.641705000	-0.517704000	6	0.782549000	4.009768000	-0.832355000
1	4.905862000	0.601765000	-1.080815000	1	1.454265000	4.033604000	-1.697959000
1	2.920163000	1.805330000	-1.220642000	1	1.412830000	4.069276000	0.066052000
1	0.128524000	2.509383000	-2.010379000	6	-0.171893000	5.205210000	-0.897406000
1	1.679336000	3.661757000	0.354752000	1	0.402523000	6.138705000	-0.883567000
1	2.245386000	3.674998000	-1.324545000	1	-0.709464000	5.183331000	-1.856590000
1	0.348182000	5.051342000	-2.046182000	6	-1.188785000	5.189841000	0.245014000
1	1.222883000	5.862651000	-0.751862000	1	-1.878852000	6.036302000	0.151689000
1	-1.261057000	5.992185000	-0.418319000	1	-0.663983000	5.314976000	1.202705000
1	-0.466637000	5.138082000	0.902173000	6	-1.972688000	3.875033000	0.268122000
1	-2.484945000	3.923709000	0.239585000	1	-2.683452000	3.862190000	1.103415000
1	-1.953462000	3.829443000	-1.444962000	1	-2.555211000	3.784886000	-0.660360000
1	-0.471696000	2.630037000	0.950384000	6	-2.759239000	1.071733000	0.075552000
1	-3.372117000	2.119813000	-0.182895000	1	-3.507316000	1.868493000	0.050037000
1	-5.416140000	1.029401000	-0.138714000	6	-3.173222000	-0.235526000	-0.329612000
1	-5.652308000	-3.243921000	-0.189153000	6	-2.196168000	-1.137201000	-0.850193000
6	6.566784000	-1.573454000	-0.907576000	6	-2.655893000	-2.368759000	-1.408224000
1	6.998015000	-0.579685000	-1.063816000	6	-4.006248000	-2.651793000	-1.400678000
1	7.012661000	-1.991552000	0.003782000	1	-4.335368000	-3.607323000	-1.809663000
1	6.885188000	-2.209898000	-1.742740000	6	-4.982846000	-1.767944000	-0.886959000
6	2.163476000	-3.979172000	-0.293091000	6	-4.545679000	-0.565801000	-0.375722000
1	1.572726000	-3.922442000	0.628016000	1	-5.267108000	0.151593000	0.014541000
1	1.439606000	-4.120686000	-1.103704000	6	-1.625092000	-3.310115000	-1.950492000
1	2.819119000	-4.853429000	-0.242297000	1	-2.073101000	-4.255205000	-2.271321000
6	-2.979358000	-3.781727000	-0.273520000	1	-0.858219000	-3.508147000	-1.193055000
1	-2.293381000	-3.887380000	0.574606000	1	-1.097617000	-2.861149000	-2.800408000
1	-3.691999000	-4.611616000	-0.260918000	6	-6.437245000	-2.149338000	-0.911716000
1	-2.356401000	-3.858340000	-1.172103000	1	-7.068192000	-1.345142000	-0.520419000
6	-7.220055000	-1.034146000	-0.115683000	1	-6.625510000	-3.044472000	-0.305392000
1	-7.661246000	-1.530581000	-0.989080000	1	-6.775130000	-2.373052000	-1.931249000
1	-7.612350000	-1.540063000	0.775463000	6	1.970665000	1.350921000	-1.131736000
1	-7.584033000	-0.002215000	-0.100078000	1	2.395253000	2.185923000	-1.698758000
1	-0.997573000	0.453177000	2.040577000	6	2.820564000	0.207022000	-1.003588000
6	-0.088386000	-1.510286000	2.267316000	6	2.455735000	-0.936103000	-0.232539000
1	-0.069940000	-1.484861000	3.367002000	6	3.396931000	-2.009895000	-0.146202000
1	-0.976242000	-2.052145000	1.941881000	6	4.608204000	-1.912236000	-0.797758000
1	0.790550000	-2.052010000	1.920246000	1	5.307485000	-2.745060000	-0.718144000
6	1.084805000	0.725565000	2.067582000	6	4.983025000	-0.787476000	-1.566040000
8	1.084317000	1.921208000	2.305542000	6	4.079346000	0.247777000	-1.649077000
8	2.215720000	-0.005402000	2.084097000	1	4.330786000	1.134871000	-2.230517000
6	3.423928000	0.717630000	2.319603000	6	2.998122000	-3.212647000	0.653543000
1	3.518127000	1.547912000	1.612696000	1	3.812517000	-3.940320000	0.717875000
1	3.442685000	1.117183000	3.338597000	1	2.124353000	-3.699421000	0.202984000
1	4.228893000	-0.000783000	2.163757000	1	2.689402000	-2.925262000	1.665084000
				6	6.318993000	-0.747997000	-2.255408000
				1	6.458971000	0.190052000	-2.801843000
				1	6.422437000	-1.570098000	-2.974899000
				1	7.143902000	-0.841336000	-1.537687000
				8	0.566439000	0.857139000	2.236592000
				6	0.267712000	-0.315492000	2.603697000
				6	-0.887681000	-0.933873000	2.013307000
				8	1.107461000	-1.049547000	3.320447000
				1	-1.813354000	-0.386736000	2.188986000
27	-0.111856000	0.129385000	0.453184000				
7	-1.542874000	1.363540000	0.398971000				
7	0.786985000	1.473755000	-0.636388000				
8	-0.920837000	-0.897233000	-0.885719000				

[(Salen*)Co^{III}(CHMeCOOCH₃)] (κ^2 -C,O)

E = -1643.24230828

G = -1642.832641

6	-0.984827000	-2.429374000	1.948230000
1	-1.127734000	-2.880284000	2.939434000
1	-1.829737000	-2.721230000	1.317303000
1	-0.067994000	-2.834753000	1.512008000
6	2.440427000	-0.525664000	3.452338000
1	2.434413000	0.416955000	4.006145000
1	2.998171000	-1.286800000	3.998396000
1	2.869831000	-0.367523000	2.459403000

F. Dormant PMMA unimer model

[(Salen*)Co^{III}(CMe₂COOCH₃)] (κ^1 -C)

E = -1682.53401533

G = -1682.111532

27	-0.218951000	-0.141390000	-0.207972000
8	0.952133000	-1.567841000	-0.505937000
8	-1.549588000	-1.453933000	-0.150222000
7	1.074446000	1.139418000	-0.724393000
7	-1.453427000	1.276244000	-0.311840000
6	2.237451000	-1.534548000	-0.630385000
6	2.951683000	-2.770338000	-0.550929000
6	4.322860000	-2.764070000	-0.688964000
6	5.076087000	-1.588770000	-0.926989000
6	4.387497000	-0.401843000	-1.028162000
6	2.982268000	-0.345446000	-0.876451000
6	2.324119000	0.906640000	-0.996152000
6	0.498223000	2.463366000	-1.019764000
6	1.392432000	3.670316000	-0.747048000
6	0.639434000	4.958209000	-1.089366000
6	-0.688184000	5.057836000	-0.339400000
6	-1.567896000	3.824885000	-0.574129000
6	-0.785698000	2.573261000	-0.201636000
6	-2.742571000	1.172919000	-0.410057000
6	-3.484311000	-0.042105000	-0.378624000
6	-4.895252000	0.016617000	-0.482120000
6	-5.673273000	-1.117163000	-0.442289000
6	-5.011144000	-2.358608000	-0.290003000
6	-3.642582000	-2.477586000	-0.182620000
6	-2.831973000	-1.300911000	-0.230716000
6	-0.017045000	-0.140196000	1.803312000
1	4.854944000	-3.712595000	-0.613689000
1	4.928071000	0.525236000	-1.218142000
1	2.937102000	1.738127000	-1.350912000
1	0.213185000	2.452957000	-2.085320000
1	1.675038000	3.650590000	0.313966000
1	2.313301000	3.626795000	-1.338801000
1	0.446923000	4.984209000	-2.172108000
1	1.268183000	5.827055000	-0.863101000
1	-1.228362000	5.963449000	-0.638751000
1	-0.488121000	5.149157000	0.737120000
1	-2.475687000	3.907496000	0.034775000
1	-1.882411000	3.773197000	-1.627119000
1	-0.474368000	2.657497000	0.849531000
1	-3.328646000	2.089231000	-0.508019000
1	-5.366712000	0.992643000	-0.594429000
1	-5.613434000	-3.266649000	-0.254797000
6	6.570933000	-1.665692000	-1.068767000

1	7.007499000	-0.678215000	-1.248310000
1	7.037607000	-2.077926000	-0.165234000
1	6.859492000	-2.314889000	-1.904924000
6	2.161271000	-4.020927000	-0.316191000
1	1.574723000	-3.942640000	0.605633000
1	1.433379000	-4.172193000	-1.121685000
1	2.811071000	-4.898776000	-0.253647000
6	-2.948277000	-3.794862000	-0.020231000
1	-2.395139000	-3.827226000	0.925964000
1	-3.658448000	-4.626688000	-0.041573000
1	-2.201498000	-3.937279000	-0.809273000
6	-7.172011000	-1.069675000	-0.551894000
1	-7.526353000	-1.637848000	-1.421197000
1	-7.651165000	-1.503796000	0.334616000
1	-7.533561000	-0.041996000	-0.655983000
6	0.275184000	-1.572295000	2.229012000
1	0.262276000	-1.627786000	3.328296000
1	-0.494571000	-2.236371000	1.833122000
1	1.245451000	-1.918383000	1.881613000
6	1.116540000	0.807071000	2.049241000
8	1.012912000	1.999417000	2.281703000
8	2.317661000	0.199334000	1.987920000
6	3.453326000	1.052270000	2.122823000
1	3.421297000	1.855519000	1.379206000
1	3.485641000	1.499626000	3.121210000
1	4.319501000	0.413311000	1.949208000
6	-1.297895000	0.358615000	2.447835000
1	-2.154092000	-0.229147000	2.108542000
1	-1.221942000	0.241096000	3.538695000
1	-1.487725000	1.413465000	2.250652000

[(Salen*)Co^{III}(CMe₂COOCH₃)] (κ^2 -C,O)

E = -1682.51641988

G = -1682.088521

27	-0.085435000	0.151956000	0.443554000
7	-1.538674000	1.353608000	0.249440000
7	0.810939000	1.469648000	-0.719001000
8	-0.825657000	-0.999590000	-0.825836000
8	1.420783000	-1.010497000	0.455738000
6	-1.012432000	2.709751000	0.240620000
1	-0.468935000	2.833593000	1.185851000
6	0.033631000	2.696850000	-0.894792000
1	-0.530700000	2.603599000	-1.838221000
6	0.818742000	4.006419000	-0.896485000
1	1.533811000	4.032965000	-1.726383000
1	1.402309000	4.061076000	0.032932000
6	-0.131986000	5.201762000	-1.005730000
1	0.439587000	6.135932000	-0.958546000
1	-0.618980000	5.183111000	-1.991717000
6	-1.208093000	5.182886000	0.082053000
1	-1.895419000	6.026568000	-0.049197000
1	-0.735252000	5.311597000	1.065929000
6	-1.987278000	3.864534000	0.066517000
1	-2.740558000	3.846542000	0.863511000
1	-2.519261000	3.773305000	-0.891471000
6	-2.712748000	1.053069000	-0.197721000
1	-3.445832000	1.852157000	-0.335045000

6	-3.106841000	-0.268969000	-0.568148000	1	4.291343000	1.048510000	-2.433265000
6	-2.100783000	-1.226340000	-0.892444000	6	3.085231000	-3.126477000	0.746028000
6	-2.524164000	-2.502834000	-1.372819000	1	3.908504000	-3.842044000	0.829967000
6	-3.873607000	-2.767573000	-1.486147000	1	2.204912000	-3.647875000	0.350167000
1	-4.178079000	-3.754199000	-1.836232000	1	2.802544000	-2.781012000	1.746882000
6	-4.879896000	-1.825812000	-1.170999000	6	6.282370000	-0.833032000	-2.428150000
6	-4.473573000	-0.584753000	-0.731626000	1	6.403532000	0.076879000	-3.024341000
1	-5.216035000	0.174795000	-0.488245000	1	6.355589000	-1.689492000	-3.110332000
6	-1.462001000	-3.501358000	-1.715818000	1	7.134076000	-0.895463000	-1.738981000
1	-1.893338000	-4.468929000	-1.988979000	8	0.620294000	1.000272000	2.183446000
1	-0.777618000	-3.633095000	-0.870281000	6	0.408027000	-0.174430000	2.589966000
1	-0.844536000	-3.140640000	-2.547022000	6	-0.779972000	-0.850912000	2.100250000
6	-6.331168000	-2.190132000	-1.320179000	8	1.313195000	-0.845429000	3.283312000
1	-6.982785000	-1.345289000	-1.076106000	6	-0.747063000	-2.354022000	2.024151000
1	-6.604138000	-3.022395000	-0.658994000	1	-0.823628000	-2.811712000	3.021032000
1	-6.561227000	-2.504150000	-2.345922000	1	-1.597489000	-2.703183000	1.428037000
6	1.977527000	1.327580000	-1.247341000	1	0.175254000	-2.690715000	1.548470000
1	2.383787000	2.139200000	-1.861176000	6	2.624519000	-0.254784000	3.338775000
6	2.832732000	0.190595000	-1.098358000	1	2.598802000	0.693901000	3.881445000
6	2.501208000	-0.904901000	-0.248507000	1	3.247408000	-0.979696000	3.862992000
6	3.448068000	-1.971350000	-0.136859000	1	2.991122000	-0.090294000	2.322319000
6	4.632577000	-1.911320000	-0.840197000	6	-2.079382000	-0.283597000	2.637033000
1	5.336732000	-2.737741000	-0.739349000	1	-2.918172000	-0.558300000	1.991399000
6	4.974184000	-0.833055000	-1.686439000	1	-2.278220000	-0.705432000	3.633766000
6	4.065077000	0.195446000	-1.793457000	1	-2.044584000	0.804844000	2.723728000