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Supporting Information

The Role of Local Chemical Hardness and van der Waals Interactions in the Anionic Polymerization of Alkyl Cyanoacrylates

Hayrensa Ablat,[a] Ian Povey,[a] Ruairí O'Kane.[b‖] Sabine Cahill,[b] Simon D. Elliott [a*]

[a]Tyndall National Institute, University College Cork, Lee Maltings, Prospect Row, Cork, T12 R5CP, Ireland

[b]Henkel, Adhesives Technologies R&D Acrylate Platform, Dublin, Ireland

[‖]Henkel, Adhesive Technologies, Aerospace, Bay Point, USA.

E-mail: simon.elliott@tyndall.ie

Table S 1 3D visualised HOMO and LUMO of the five CA monomers. methyl-CA, ethyl-CA, allyl-CA, 2-phenylethyl-CA and β-methoxy-CA.

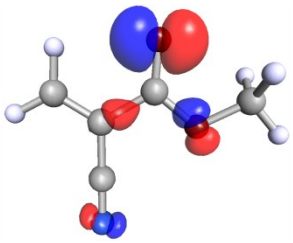
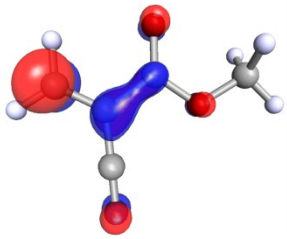
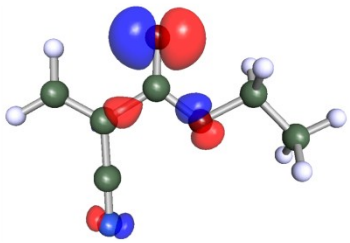
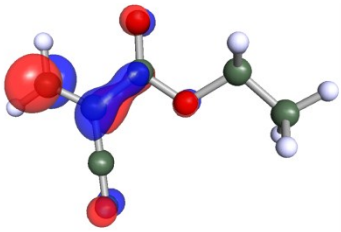
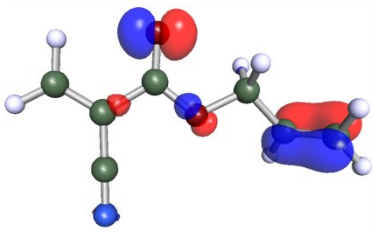
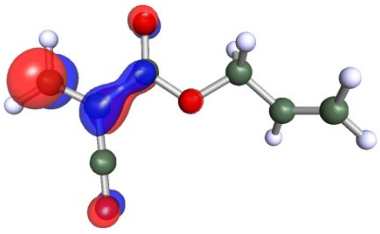
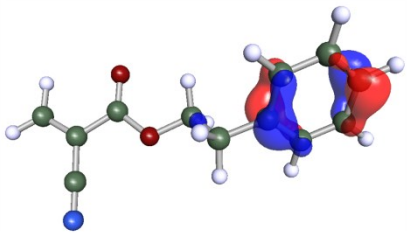
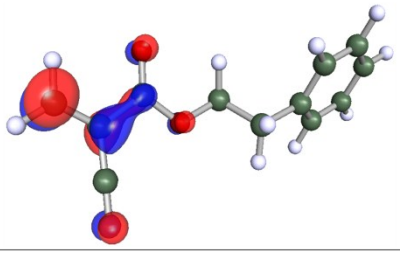
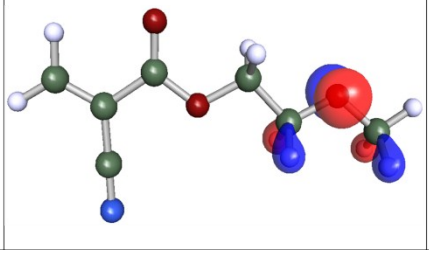
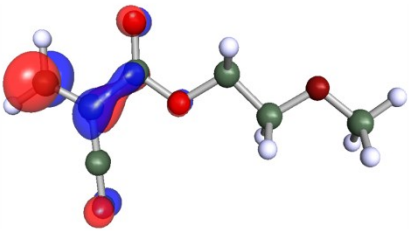
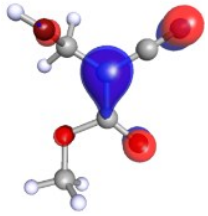
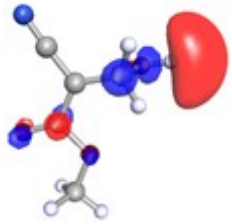
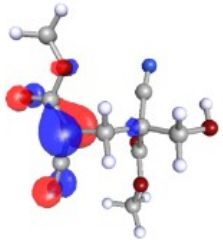
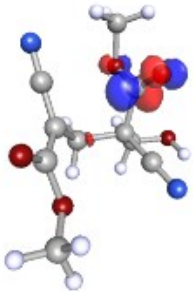
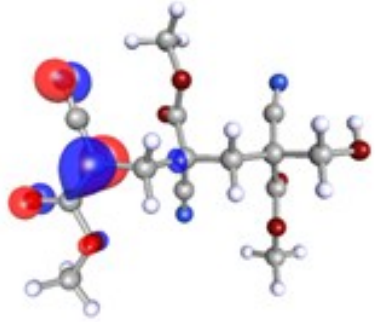
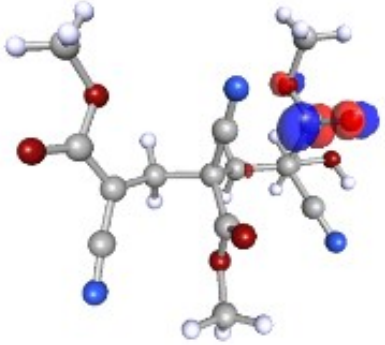
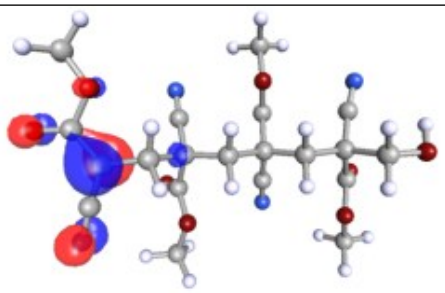
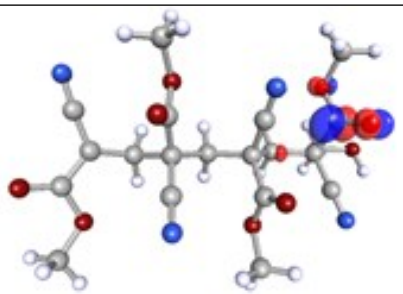
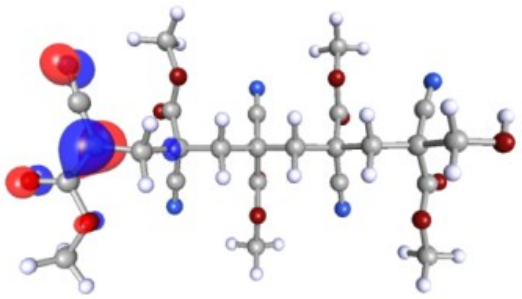
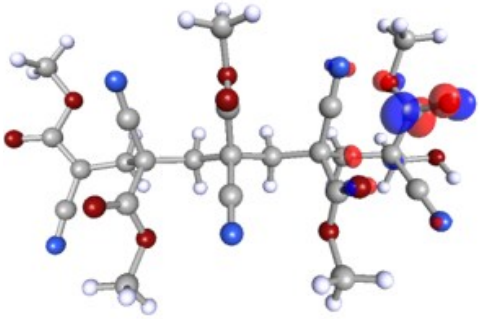
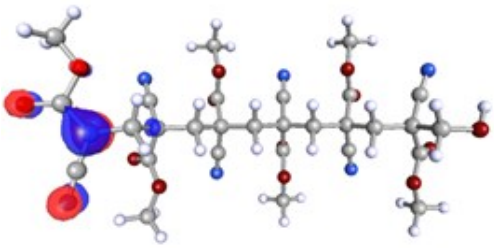
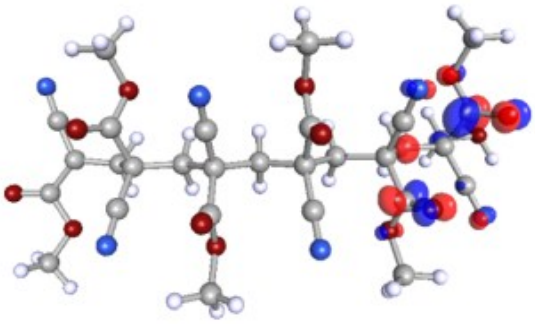
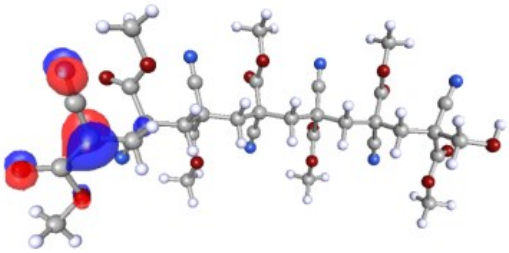
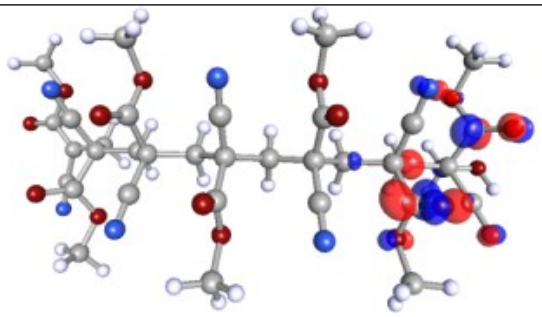
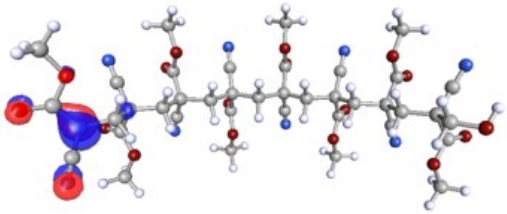
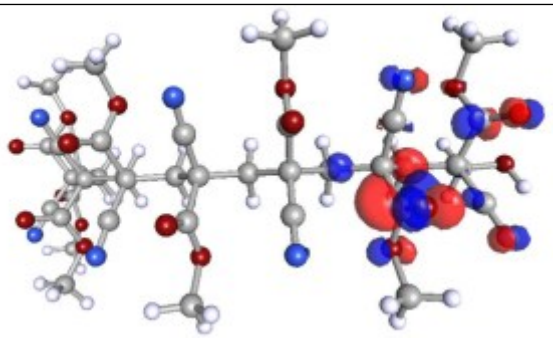
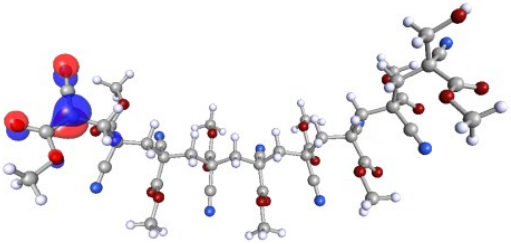
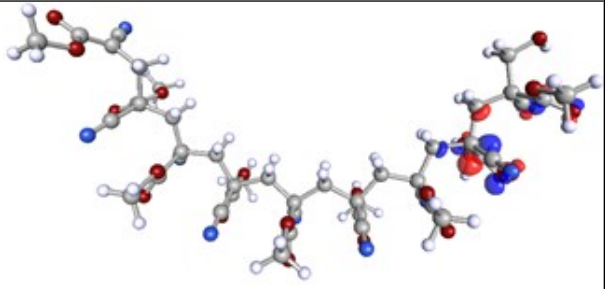
Cyanoacrylates	HOMO	LUMO
methyl-CA		
ethyl-CA		
allyl-CA		
2-phenylethyl-CA		
β-methoxy-CA		

Table S 2 Visualised HOMO and LUMO of poly(methyl-CA)$_n$ initiated by hydroxide anion, n from 1 to 13.

	HOMO	LUMO
1		
2		
3		
4		

5		
6		
7		
8		
9		

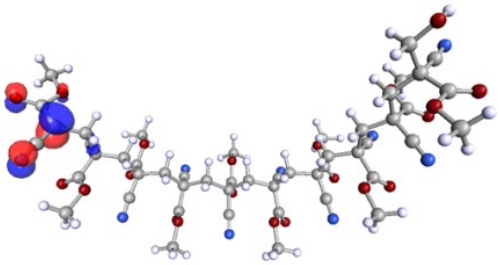
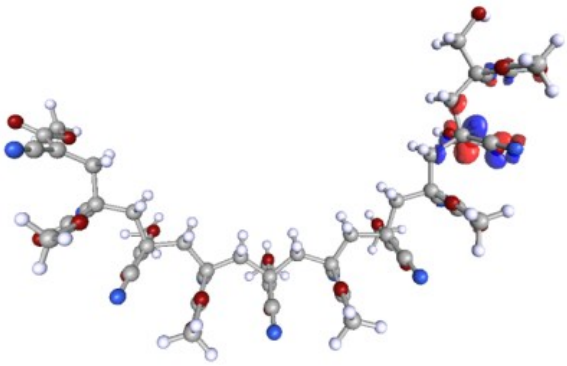
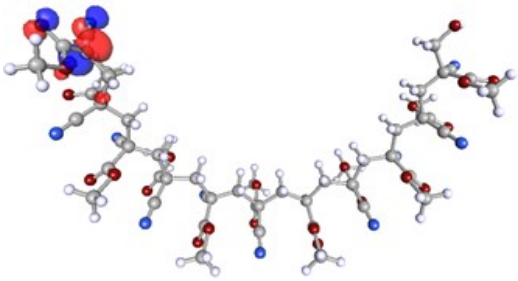
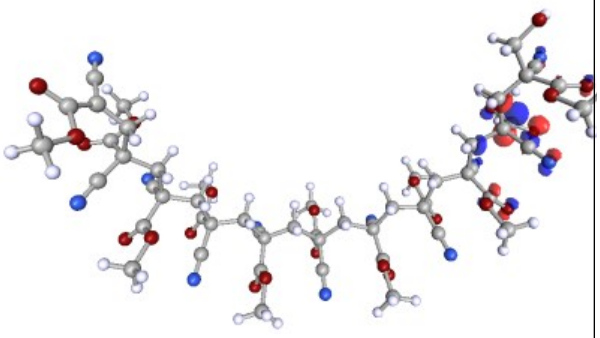
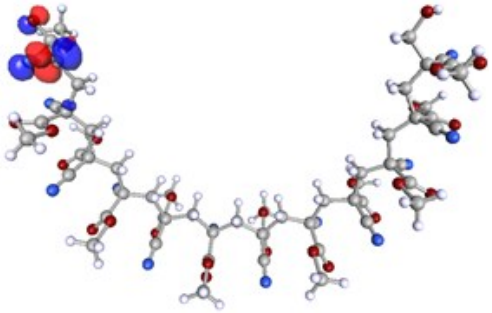
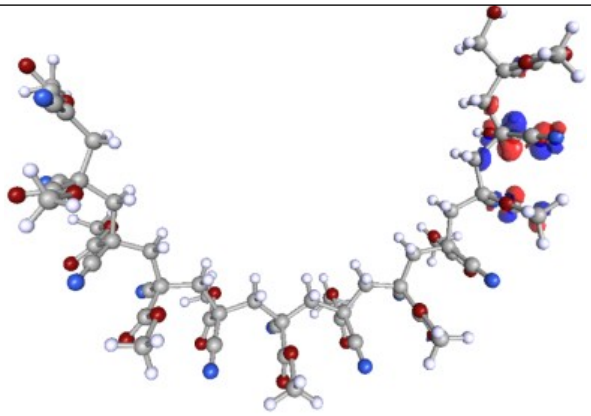
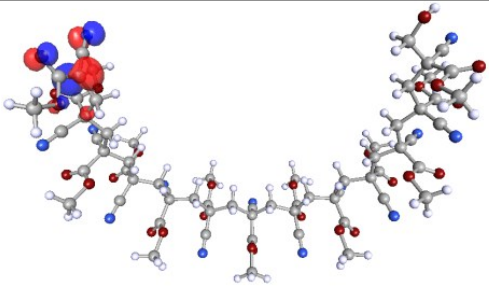
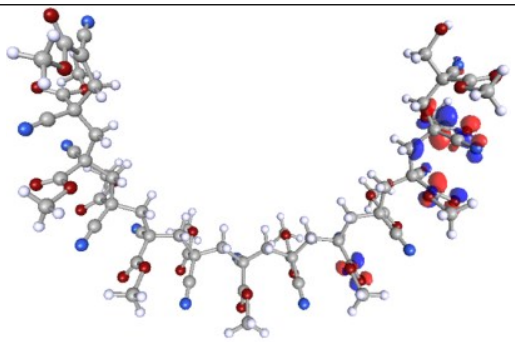
10		
11		
12		
13		

Table S 3 Natural Bond Orbital population analysis selected atoms (Fig. 7) of poly (alky-CA) for polymerization degrees up to 7 in units of electronic charge.

poly(methyl-CA)$_n$

	C(1)	C(2)	C(3)	O(4)	C(5)	N(6)	SUM
1	-0.106	-0.464	0.645	-0.644	0.283	-0.475	-0.762
2	-0.368	-0.466	0.649	-0.632	0.286	-0.486	-1.017
3	-0.357	-0.467	0.652	-0.627	0.285	-0.475	-0.987
4	-0.354	-0.466	0.654	-0.625	0.285	-0.474	-0.979
5	-0.354	-0.466	0.654	-0.624	0.285	-0.472	-0.978
6	-0.353	-0.466	0.654	-0.624	0.285	-0.472	-0.976
7	-0.353	-0.467	0.661	-0.623	0.285	-0.476	-0.972

poly(ethyl-CA)$_n$

	C(1)	C(2)	C(3)	O(4)	C(5)	N(6)	SUM
1	-0.106	-0.464	0.651	-0.644	0.284	-0.475	-0.754
2	-0.368	-0.467	0.655	-0.632	0.287	-0.491	-1.017
3	-0.356	-0.467	0.659	-0.627	0.286	-0.479	-0.985
4	-0.353	-0.467	0.660	-0.625	0.286	-0.477	-0.976
5	-0.353	-0.467	0.660	-0.624	0.285	-0.475	-0.974
6	-0.353	-0.467	0.660	-0.623	0.285	-0.476	-0.973
7	-0.353	-0.467	0.661	-0.623	0.285	-0.476	-0.972

poly(allyl-CA)$_n$

	C(1)	C(2)	C(3)	O(4)	C(5)	N(6)	SUM
1	-0.081	-0.451	0.632	-0.702	0.268	-0.470	-0.804
2	-0.369	-0.463	0.652	-0.625	0.289	-0.487	-1.004
3	-0.357	-0.460	0.657	-0.618	0.292	-0.480	-0.966
4	-0.356	-0.461	0.657	-0.618	0.288	-0.470	-0.960
5	-0.355	-0.461	0.657	-0.617	0.287	-0.468	-0.957
6	-0.355	-0.463	0.658	-0.615	0.285	-0.471	-0.961
7	-0.354	-0.462	0.658	-0.617	0.287	-0.469	-0.957

poly(2-phenylethyl-CA)$_n$

	C(1)	C(2)	C(3)	O(4)	C(5)	N(6)	SUM
1	-0.081	-0.448	0.628	-0.715	0.267	-0.469	-0.819
2	-0.367	-0.465	0.657	-0.622	0.300	-0.508	-1.006
3	-0.358	-0.463	0.656	-0.628	0.301	-0.492	-0.984
4	-0.352	-0.465	0.662	-0.613	0.298	-0.491	-0.962
5	-0.353	-0.464	0.661	-0.611	0.292	-0.481	-0.956
6	-0.355	-0.465	0.662	-0.614	0.298	-0.490	-0.964
7	-0.354	-0.465	0.661	-0.610	0.292	-0.482	-0.958

poly(β-methoxy-CA)$_n$

	C(1)	C(2)	C(3)	O(4)	C(5)	N(6)	SUM
1	-0.102	-0.483	0.641	-0.659	0.272	-0.472	-0.803
2	-0.366	-0.468	0.656	-0.623	0.291	-0.492	-1.003
3	-0.356	-0.467	0.659	-0.618	0.290	-0.480	-0.972
4	-0.351	-0.467	0.661	-0.616	0.291	-0.482	-0.965
5	-0.353	-0.466	0.661	-0.615	0.288	-0.477	-0.962
6	-0.352	-0.467	0.661	-0.614	0.287	-0.477	-0.961
7	-0.351	-0.467	0.661	-0.613	0.289	-0.480	-0.960

Optimized coordinates of all cyanoacrylate (CA) monomers and polymers from modelling at PBE/TZVPP level, xyz file format, units are Angstrom.

methylCA monomer

13

C	-2.2083069	0.0359318	-1.0281507
C	-1.1431710	-0.4561462	-0.3692371
C	0.0426432	0.4418380	-0.1250656
O	0.0982829	1.6020754	-0.4788623
O	1.0184125	-0.2156484	0.5320542
C	-1.1106213	-1.8049306	0.1037540
H	-2.1854186	1.0712209	-1.3681993
H	-3.0867930	-0.5747243	-1.2275066
N	-1.0967740	-2.9057669	0.4866192
C	2.2000065	0.5662813	0.8137458
H	2.6503832	0.9240125	-0.1204491
H	1.9439118	1.4280987	1.4424093
H	2.8774448	-0.1122422	1.3388882

poly(methyl-CA)$_1$

15

C	-1.0760052	0.3004652	0.0305914
C	-1.2642822	-1.1544949	0.2525656
H	-0.5041969	-1.7201966	-0.3116701
H	-2.2682160	-1.4603600	-0.0967874
C	0.1913775	0.8895424	-0.2384713
O	0.4772298	2.0761955	-0.4361359
O	1.2279915	-0.0849622	-0.2886472
C	2.5023965	0.4625961	-0.5816306
H	2.5287967	0.9448650	-1.5731755
C	-2.2073934	1.1331721	0.0992722
H	2.8044344	1.2198807	0.1597050
N	-3.1937930	1.7744977	0.1496005
O	-1.1489085	-1.5177928	1.6773495
H	-1.2756845	-2.4815387	1.7181392
H	3.2062533	-0.3818695	-0.5607056

poly(methyl-CA)$_2$

28

C	-0.0601705	-0.6569977	0.9061620
C	-0.2217601	-2.1069025	1.4463315
H	0.6033566	-2.7106622	1.0495189
H	-1.1747473	-2.5043892	1.0508851
C	1.3208479	-0.0819416	1.2502149
O	1.5245873	0.9624789	1.8297224
O	2.2863861	-0.9060517	0.7807859
C	3.6230035	-0.3614408	0.8089759
H	3.7088314	0.3939837	0.0142367

C	-1.0930619	0.1384883	1.5704917
H	3.8364706	0.0812024	1.7899710
N	-1.9599805	0.6269753	2.1761029
O	-0.1610803	-2.2160144	2.8627441
H	-0.8201037	-1.5953765	3.2227133
C	0.0218584	0.5529491	-1.4528746
C	-0.2544570	-0.6984785	-0.6761067
H	-1.2910831	-1.0199533	-0.8439764
H	0.4128020	-1.5121956	-1.0037216
C	-1.0056808	1.4395316	-1.8868806
O	-0.9085193	2.4752384	-2.5507709
O	-2.2847471	0.9909401	-1.4714767
C	-3.3439105	1.8645004	-1.8374414
H	-3.2024995	2.8711195	-1.4148153
C	1.3513191	0.8237549	-1.8054368
H	-3.4287091	1.9686698	-2.9310070
N	2.4926562	0.9744289	-2.0618381
H	4.2874204	-1.2083544	0.6073994
H	-4.2590288	1.4144972	-1.4299095

poly(methyl-CA)$_3$

41

C	-0.4428411	-0.6617198	2.2543402
C	-0.7828285	-2.0204420	2.9664712
H	-0.0342856	-2.7587568	2.6528854
H	-1.7769483	-2.3423488	2.6079526
C	0.9562076	-0.2059568	2.7314556
O	1.1732011	0.7581014	3.4280980
O	1.8886820	-1.0808794	2.2979494
C	3.2524477	-0.6965414	2.5816674
H	3.4901356	0.2184527	2.0242679
C	-1.4415868	0.2936261	2.7481497
H	3.3859046	-0.5306166	3.6578796
N	-2.2892758	0.9301513	3.2279052
O	-0.7233514	-1.9564742	4.3770951
H	-1.3501166	-1.2709507	4.6697460
C	-0.3066116	0.2272964	-0.2915745
C	-0.5381536	-0.9203584	0.7254019
H	-1.5408418	-1.3187224	0.5186293
H	0.1886682	-1.7131436	0.4980111
C	-1.3617893	1.3407678	-0.2041136
O	-1.1240047	2.5269897	-0.1811198
O	-2.6000657	0.7951553	-0.2112457
C	-3.6780692	1.7478184	-0.3507540
H	-3.5973539	2.5261074	0.4179778
C	1.0246718	0.8080671	-0.1273394
H	-3.6346772	2.1843577	-1.3583936
N	2.1124238	1.1942030	0.0213716
C	-0.4108430	0.4138618	-2.9569445
C	-0.4238199	-0.4629085	-1.7517419
H	0.4074916	-1.1792769	-1.7987058
H	-1.3680967	-1.0279264	-1.6872351
C	0.7429853	0.5949958	-3.7769166

O	0.8609886	1.2649453	-4.8052042
O	1.8483070	-0.1424384	-3.2887399
C	3.0405986	0.0520072	-4.0380213
H	2.9199385	-0.2632915	-5.0864207
C	-1.6196416	1.0173515	-3.3366399
H	3.3496135	1.1085094	-4.0376038
N	-2.6761249	1.4769185	-3.5848505
H	-4.5959333	1.1655494	-0.2211845
H	3.8670546	-1.5321344	2.2333979
H	3.8079402	-0.5603463	-3.5459037

poly(methyl-CA)$_4$

54

C	-0.2232876	-0.4225562	3.5955692
C	-0.5067929	-1.7481061	4.3965519
H	0.2995219	-2.4556855	4.1664409
H	-1.4636389	-2.1608405	4.0297434
C	1.1188936	0.1614433	4.0989493
O	1.2379427	1.1975297	4.7089128
O	2.1199823	-0.6908982	3.7968956
C	3.4424896	-0.2166842	4.1420832
H	3.6756028	0.6725724	3.5435523
C	-1.3111255	0.4892294	3.9663046
H	3.4917280	0.0236632	5.2110572
N	-2.2335507	1.0898438	4.3432012
O	-0.5040312	-1.5725305	5.7958764
H	-1.2113673	-0.9433499	6.0234237
C	-0.0055141	0.2692539	0.9809688
C	-0.2280290	-0.8094988	2.0919277
H	-1.1976579	-1.2777973	1.8742030
H	0.5508884	-1.5735367	1.9647950
C	-1.0774282	1.3878913	1.0839569
O	-0.8395509	2.5500660	1.3108867
O	-2.3033871	0.8513948	0.9203926
C	-3.3848201	1.8145468	0.9261079
H	-3.3972692	2.3552533	1.8802885
C	1.3187854	0.8831279	1.1408315
H	-3.2499545	2.5093754	0.0881646
N	2.3885861	1.3103555	1.2957531
C	0.0880073	0.1678857	-1.7362330
C	-0.1029828	-0.5255186	-0.3645393
H	0.6430654	-1.3305799	-0.3210111
H	-1.0983975	-0.9920271	-0.3714763
C	1.5130194	0.6864211	-1.9785964
O	1.7905521	1.7724115	-2.4333253
O	2.4084814	-0.2804741	-1.6690591
C	3.7679939	0.0098572	-2.0646584
H	3.8234498	0.0176273	-3.1621494
C	-0.8674869	1.2583780	-1.9152496
H	4.0853283	0.9737336	-1.6480690
N	-1.6868063	2.0781900	-2.0199723
C	0.0669028	-0.7146024	-4.2676757
C	-0.2080156	-0.9970745	-2.8324121

H	-1.2670243	-1.2539074	-2.6937629
H	0.4074901	-1.8380661	-2.4735790
C	-0.9542566	-0.3679869	-5.2037032
O	-0.8480070	-0.1451293	-6.4112001
O	-2.2263752	-0.3171900	-4.5881697
C	-3.2704720	0.0876756	-5.4645274
H	-3.0843133	1.0913331	-5.8761348
C	1.3829502	-0.8834168	-4.7252560
H	-3.3856505	-0.6079653	-6.3104983
N	2.5096860	-1.0565374	-5.0237893
H	4.1187182	-1.0392634	3.8920443
H	4.3683554	-0.8091546	-1.6555290
H	-4.2961300	1.2229718	0.7987626
H	-4.1850975	0.0983462	-4.8570681

poly(methyl-CA)$_5$

67

C	-0.4448247	0.7366722	4.7603820
C	-0.9744257	-0.3983827	5.7166387
H	-0.3135588	-1.2666386	5.6007646
H	-1.9902813	-0.6713504	5.3794948
C	0.9718007	1.1370492	5.2404285
O	1.2596038	2.2031775	5.7295220
O	1.8126455	0.0948554	5.0774865
C	3.1886605	0.3685469	5.4335810
H	3.5886795	1.1443030	4.7692907
C	-1.3546514	1.8694020	4.9614964
H	3.2504322	0.6989820	6.4774067
N	-2.1559051	2.6754587	5.2094465
O	-0.9408151	-0.0443109	7.0797200
H	-1.5343269	0.7155622	7.2135933
C	-0.0909947	1.0340395	2.0908852
C	-0.4941397	0.1557495	3.3224403
H	-1.5231671	-0.1803986	3.1362088
H	0.1561768	-0.7296063	3.3223789
C	-0.9954305	2.2941335	1.9919563
O	-0.5909630	3.4311273	2.0133852
O	-2.2842502	1.9117575	1.9064472
C	-3.2293732	3.0029913	1.7688017
H	-3.1531684	3.6689030	2.6366847
C	1.3047915	1.4675981	2.2313928
H	-3.0186706	3.5487129	0.8415602
N	2.4246831	1.7415309	2.3791979
C	0.0048609	0.5491580	-0.6035604
C	-0.2663882	0.0784392	0.8629805
H	0.3898447	-0.7861039	1.0311849
H	-1.3057486	-0.2748434	0.8981713
C	1.4658086	1.0478465	-0.7740595
O	1.7757039	2.1694601	-1.0955823
O	2.3188351	0.0455411	-0.4818234
C	3.7157346	0.3715868	-0.6812701
H	3.8809963	0.6073450	-1.7396489
C	-0.9047874	1.6447483	-0.9603857

H	3.9936452	1.2213950	-0.0460602
N	-1.6720749	2.4826815	-1.2047339
C	-0.1717906	-0.7094401	-3.0133100
C	-0.2853089	-0.7258842	-1.4692740
H	-1.3115030	-1.0453908	-1.2422396
H	0.3976473	-1.5049138	-1.1017533
C	-1.2204108	0.1727888	-3.7063710
O	-0.9926205	0.9457685	-4.6082956
O	-2.4471930	-0.0945046	-3.2002769
C	-3.5407279	0.5139417	-3.9238372
C	1.1661571	-0.3121783	-3.4440253
H	-3.5982388	0.0636178	-4.9244338
N	2.2627300	-0.0427405	-3.7252000
C	-0.5891778	-2.5604411	-4.9083745
C	-0.4481203	-2.2505814	-3.4600733
H	0.3852123	-2.8231734	-3.0306558
H	-1.3700514	-2.5057644	-2.9124410
C	0.4625474	-3.1282132	-5.6900471
O	0.4478494	-3.4541815	-6.8783920
O	1.6304269	-3.3316772	-4.9190168
C	2.7289238	-3.8372961	-5.6672753
H	2.5010686	-4.8176324	-6.1142713
C	-1.8468379	-2.3603641	-5.4987080
H	3.0107535	-3.1525758	-6.4815769
N	-2.9349230	-2.1693114	-5.9088275
H	3.7182521	-0.5773550	5.2887583
H	-4.2125324	2.5260658	1.7250745
H	4.2644729	-0.5300244	-0.3934544
H	-4.4379249	0.2759549	-3.3434148
H	-3.3932563	1.5990566	-3.9887821
H	3.5596188	-3.9306700	-4.9553087

poly(methyl-CA)$_6$

80

C	-0.4370958	0.9014493	5.8745330
C	-0.7563216	-0.3865188	6.7254949
H	0.0587615	-1.1030773	6.5632437
H	-1.6972494	-0.8178216	6.3395404
C	0.8684790	1.5241438	6.4280255
O	0.9391104	2.5896087	6.9920539
O	1.8929423	0.6706568	6.2264976
C	3.1847018	1.1642695	6.6562253
H	3.4616226	2.0347355	6.0489948
C	-1.5508267	1.8213865	6.1278011
H	3.1491132	1.4418984	7.7163206
N	-2.4976855	2.4389828	6.4019242
O	-0.8083440	-0.1415193	8.1108841
H	-1.5468334	0.4669469	8.2890994
C	-0.0862422	1.4759275	3.2510139
C	-0.3493226	0.4400211	4.3959092
H	-1.2957371	-0.0599557	4.1483631
H	0.4518078	-0.3101870	4.3507777

C	-1.1869757	2.5742239	3.2387109
O	-0.9784961	3.7524738	3.3948322
O	-2.3904059	1.9976514	3.0555560
C	-3.5029106	2.9277401	3.0050553
H	-3.5645186	3.4795579	3.9505363
C	1.2160408	2.1214237	3.4587489
H	-3.3614552	3.6167892	2.1641137
N	2.2724707	2.5674065	3.6471556
C	0.1581804	1.2531803	0.5363525
C	-0.0891660	0.6155120	1.9443023
H	0.6781214	-0.1606699	2.0658467
H	-1.0693113	0.1213644	1.9083206
C	1.5587566	1.9226753	0.4543362
O	1.7476485	3.0832229	0.1842738
O	2.5061223	1.0093945	0.7437820
C	3.8663564	1.5040544	0.6535895
H	4.0679933	1.8208684	-0.3764903
C	-0.8666460	2.2660368	0.2556800
H	4.0012876	2.3400518	1.3501757
N	-1.7296798	3.0208965	0.0661275
C	0.2282060	0.1889851	-1.9913002
C	0.0292495	0.0390110	-0.4474793
H	-0.9771382	-0.3795215	-0.3117216
H	0.7560445	-0.7092960	-0.1038780
C	-0.7773373	1.2075740	-2.5946074
O	-0.4653394	2.2275334	-3.1598805
O	-2.0365319	0.7849149	-2.3637977
C	-3.0646226	1.6194522	-2.9510392
H	-2.9883142	2.6386642	-2.5533690
C	1.5901504	0.6496749	-2.2872828
H	-2.9470664	1.6180539	-4.0415621
N	2.6896873	0.9778013	-2.4717988
C	0.1255457	-1.5975489	-4.0464181
C	-0.0043030	-1.2615895	-2.5409983
H	0.7011451	-1.9228213	-2.0196594
H	-1.0205920	-1.5443435	-2.2318859
C	1.5546790	-1.4745723	-4.5936723
O	1.8544850	-0.9510225	-5.6419365
C	-0.7815097	-0.7854749	-4.8531523
N	-1.5626590	-0.1497159	-5.4360899
C	-0.3109662	-3.1640471	-4.1525637
C	-0.1179788	-3.8749935	-5.4447335
C	-1.1783521	-4.1056036	-6.3735455
O	-1.1414240	-4.7048290	-7.4495740
C	1.1516264	-4.4111827	-5.7104430
N	2.2434265	-4.8329533	-5.8468645
H	-1.3710717	-3.1808791	-3.8653657
H	0.2789412	-3.6396817	-3.3520993
O	-2.3992486	-3.5631479	-5.9112298
C	-3.4747155	-3.7083850	-6.8304672
H	-3.2556269	-3.2118888	-7.7879213
H	-3.6908571	-4.7675089	-7.0409368
O	2.4177147	-2.1007955	-3.7595718
C	3.7595102	-2.2443594	-4.2781944
H	3.7402158	-2.9570571	-5.1145720

H	4.1462126	-1.2700794	-4.6011640
H	3.8803097	0.3370200	6.4894321
H	4.4984051	0.6553510	0.9300133
H	4.3494832	-2.6425536	-3.4463215
H	-4.3425453	-3.2329527	-6.3546867
H	-4.0115149	1.1545235	-2.6611319
H	-4.3896159	2.3054443	2.8557623

poly(methyl-CA)$_7$

93

C	-0.6932075	1.1089843	6.8650764
C	-1.0750678	-0.2463223	7.5750365
H	-0.2925192	-0.9781248	7.3373770
H	-2.0326796	-0.5906255	7.1454843
C	0.6293420	1.6144519	7.4930744
O	0.7336109	2.6043264	8.1764828
O	1.6238237	0.7515075	7.2006382
C	2.9266279	1.1406207	7.6997190
C	-1.7705394	2.0453642	7.2010336
H	2.8892185	1.2745674	8.7872754
N	-2.6931736	2.6757246	7.5241692
O	-1.1214470	-0.1473714	8.9780598
H	-1.8383450	0.4638113	9.2224036
C	-0.3041802	1.9430940	4.3201407
C	-0.6040616	0.7998720	5.3477113
H	-1.5607178	0.3538846	5.0428820
H	0.1781720	0.0375123	5.2310401
C	-1.3905467	3.0540768	4.3929434
O	-1.1652837	4.2138380	4.6374401
O	-2.6003888	2.5100254	4.1610570
C	-3.7024996	3.4543191	4.1908304
H	-3.7569308	3.9234780	5.1802815
C	1.0019845	2.5445248	4.6167457
H	-3.5537641	4.2114417	3.4121141
N	2.0614286	2.9506409	4.8679732
C	-0.0302248	2.0035463	1.5997374
C	-0.2878299	1.2214568	2.9321148
H	0.4832052	0.4408224	2.9830890
H	-1.2640618	0.7279991	2.8332441
C	1.3475451	2.7250693	1.6237652
O	1.4953248	3.9173720	1.5166726
O	2.3249626	1.8143177	1.7970495
C	3.6663498	2.3672294	1.8087629
H	3.8665930	2.8527961	0.8464175
C	-1.0820679	3.0061926	1.3917336
H	3.7603899	3.0860418	2.6312716
N	-1.9628277	3.7499639	1.2454299
C	0.0831566	1.2194226	-1.0212537
C	-0.0925106	0.8908338	0.4987983
H	-1.0698667	0.3988110	0.5904552
H	0.6828381	0.1593713	0.7632241
C	-1.0259935	2.1830941	-1.5294103
O	-0.8172445	3.2458248	-2.0605733

O	-2.2344725	1.6458479	-1.2723437
C	-3.3563654	2.4341106	-1.7454710
H	-3.3362505	3.4234686	-1.2731984
C	1.3927745	1.8388872	-1.2575847
H	-3.3005023	2.5235816	-2.8367183
N	2.4597845	2.2782508	-1.3950698
C	0.0806421	-0.3654424	-3.2633084
C	-0.0013846	-0.1865994	-1.7118570
H	0.8096393	-0.7982509	-1.2937616
H	-0.9558530	-0.6259482	-1.3918165
C	1.4074239	0.2107012	-3.8294685
O	1.4783379	1.1208948	-4.6191359
C	-1.0403941	0.3221492	-3.9154075
N	-1.9658655	0.8477241	-4.3822693
C	-0.0204586	-1.9175477	-3.4648976
C	-0.0276535	-2.5617414	-4.8722362
C	-1.2846414	-2.2510021	-5.6966175
O	-1.2900762	-1.9497463	-6.8679010
C	1.1634985	-2.1931336	-5.6324095
N	2.1574594	-1.9079829	-6.1663026
H	-0.9455055	-2.2491294	-2.9740272
H	0.8262012	-2.3509945	-2.9136404
O	-2.3880731	-2.4346422	-4.9337385
C	-3.6364840	-2.3901260	-5.6615209
H	-3.7078828	-1.4563449	-6.2325924
H	-3.6899175	-3.2634843	-6.3263810
O	2.4507904	-0.4439663	-3.2816545
C	3.7445229	-0.0431807	-3.7953517
H	3.7853639	-0.2590276	-4.8699797
H	3.9046240	1.0253722	-3.6074752
C	-0.0118474	-4.1667795	-4.5831407
C	-0.2197435	-5.1028687	-5.7196099
C	0.8510982	-5.7843242	-6.3748739
O	2.1032375	-5.4380918	-5.8179240
O	0.7934086	-6.6000670	-7.2965259
C	3.2097279	-6.0397350	-6.4787351
H	3.2501518	-5.7509755	-7.5399444
H	3.1654934	-7.1389696	-6.4292707
H	0.9602473	-4.3563495	-4.1079738
H	-0.8041760	-4.2885282	-3.8264989
C	-1.5416573	-5.3837745	-6.0986485
N	-2.6797349	-5.5660788	-6.3437559
H	4.1049451	-5.6736848	-5.9590269
H	-4.4181644	-2.4409692	-4.8966890
H	4.4710579	-0.6513306	-3.2484804
H	-4.2464417	1.8731726	-1.4466744
H	4.3281922	1.5096655	1.9587805
H	-4.5962849	2.8572109	3.9902723
H	3.5970814	0.3205756	7.4278026
H	3.2375341	2.0754183	7.2175356

ethyl-CA monomer
16

C	-2.8580275	0.2498160	-1.3764189
C	-1.8090415	-0.2786449	-0.7201427
C	-0.5973311	0.5831454	-0.4631343
O	-0.5093088	1.7427380	-0.8142672
O	0.3524995	-0.1053401	0.1960273
C	-1.8166265	-1.6323307	-0.2602514
H	-2.8041397	1.2873216	-1.7059239
H	-3.7534955	-0.3330503	-1.5829433
N	-1.8332804	-2.7373821	0.1109363
C	1.5725456	0.6331722	0.4964746
C	2.5062483	-0.3045605	1.2275188
H	1.9960652	0.9954668	-0.4510221
H	1.3017745	1.5119698	1.0988274
H	3.4384276	0.2236043	1.4697976
H	2.7555715	-1.1769243	0.6098900
H	2.0581186	-0.6590013	2.1646317

poly(ethyl-CA)$_1$
18

C	-1.7140174	0.5065474	0.1142797
C	-1.9201455	-0.9476570	0.3257507
H	-1.1757536	-1.5199677	-0.2526002
H	-2.9325664	-1.2352101	-0.0140427
C	-0.4401421	1.0821918	-0.1516761
O	-0.1399267	2.2665179	-0.3406287
O	0.5844141	0.0924864	-0.2084608
C	1.8780010	0.6105512	-0.4878285
H	1.8925457	1.1021167	-1.4770021
C	2.8586101	-0.5501578	-0.4396744
H	2.5978206	-1.3162193	-1.1843794
H	2.8500953	-1.0259178	0.5513064
C	-2.8348881	1.3526560	0.1919496
H	2.1443636	1.3891935	0.2470861
H	3.8810074	-0.1991635	-0.6483018
N	-3.8131314	2.0056019	0.2500902
O	-1.7921955	-1.3251269	1.7455180
H	-1.9240912	-2.2884426	1.7786140

poly(ethyl-CA)$_2$
34

C	-0.0629884	-0.6732951	0.9755269
C	-0.1661651	-2.1204715	1.5390368
H	0.6823465	-2.6957601	1.1490372
H	-1.1026873	-2.5618954	1.1505090
C	1.2999419	-0.0447067	1.3040742
O	1.4702881	0.9983551	1.8979184
O	2.2877360	-0.8162073	0.8013606
C	3.6157066	-0.2262027	0.8291546
H	3.5495868	0.7706323	0.3731429
C	4.5289748	-1.1315915	0.0323291

H	4.1975089	-1.1648349	-1.0133977
H	4.5477882	-2.1501585	0.4457530
C	-1.1193349	0.0912089	1.6388473
H	3.9281197	-0.1213408	1.8792352
H	5.5525700	-0.7306351	0.0560641
N	-1.9994750	0.5536046	2.2462068
O	-0.0990596	-2.2067245	2.9564247
H	-0.7786821	-1.6046332	3.3096845
C	0.0264170	0.4770365	-1.4167605
C	-0.2659752	-0.7491219	-0.6043272
H	-1.3068564	-1.0654469	-0.7579254
H	0.3900108	-1.5765926	-0.9183935
C	-0.9801048	1.4113352	-1.7986336
O	-0.8716512	2.4353762	-2.4783671
O	-2.2487369	1.0289064	-1.2959828
C	-3.2954459	1.9628728	-1.5538162
H	-3.0042419	2.9605338	-1.1865461
C	-4.5432815	1.4582060	-0.8495849
H	-4.3669083	1.3657868	0.2308648
H	-4.8395476	0.4709880	-1.2332260
C	1.3416919	0.6727380	-1.8606757
H	-3.4564745	2.0627081	-2.6410954
H	-5.3799688	2.1548558	-1.0107402
N	2.4688982	0.7644745	-2.1956975

poly(ethyl-CA)$_3$
50

C	-0.6689148	-0.5493301	2.3715774
C	-1.0394745	-1.9005743	3.0827883
H	-0.3080552	-2.6552815	2.7674424
H	-2.0408594	-2.1996789	2.7246200
C	0.7405838	-0.1271918	2.8524247
O	0.9725723	0.8189497	3.5695605
O	1.6558361	-1.0041211	2.3932351
C	3.0419047	-0.6527133	2.6697190
H	3.2059036	0.3660548	2.2933886
C	3.9162702	-1.6639857	1.9624010
H	3.7507821	-1.6275178	0.8778474
H	3.7197299	-2.6848979	2.3179806
C	-1.6475025	0.4282220	2.8616099
H	3.1880236	-0.6553686	3.7596161
H	4.9728763	-1.4308994	2.1547202
N	-2.4842506	1.0859136	3.3320764
O	-0.9773147	-1.8405361	4.4934372
H	-1.5843953	-1.1383944	4.7880050
C	-0.5162942	0.3347094	-0.1764645
C	-0.7706248	-0.8061454	0.8431115
H	-1.7822196	-1.1819438	0.6371019
H	-0.0623380	-1.6153105	0.6151328
C	-1.5525038	1.4682277	-0.0904346
O	-1.2895649	2.6491605	-0.0456987
O	-2.7981078	0.9478568	-0.1299125
C	-3.8715605	1.9218569	-0.2635440

H	-3.8914023	2.5361229	0.6484375
C	-5.1553863	1.1512262	-0.4771414
H	-5.3632562	0.4738814	0.3632499
H	-5.0980182	0.5724914	-1.4080333
C	0.8243038	0.8937354	-0.0109617
H	-3.6372436	2.5568725	-1.1286562
H	-5.9935103	1.8571680	-0.5646864
N	1.9183692	1.2622631	0.1364221
C	-0.6491400	0.5125618	-2.8434535
C	-0.6430653	-0.3587827	-1.6331913
H	0.1901417	-1.0730137	-1.6844300
H	-1.5839167	-0.9278038	-1.5610569
C	0.5069035	0.7330875	-3.6509179
O	0.6131060	1.4039135	-4.6797362
O	1.6311725	0.0399611	-3.1405126
C	2.8504695	0.2951638	-3.8353896
H	2.7844091	-0.0814688	-4.8707405
C	3.9675554	-0.3886273	-3.0657476
H	3.7997272	-1.4742049	-3.0087613
H	4.0256617	0.0049396	-2.0413999
C	-1.8754443	1.0689762	-3.2385363
H	3.0192204	1.3817717	-3.9055023
H	4.9343778	-0.2163380	-3.5622631
N	-2.9455365	1.4890424	-3.4987332

poly(ethyl-CA)$_4$
66

C	-0.2224729	-0.3817066	3.7035519
C	-0.4806245	-1.7199512	4.4917398
H	0.3390153	-2.4095834	4.2540745
H	-1.4295941	-2.1476424	4.1212811
C	1.1114794	0.2195039	4.2122215
O	1.2075920	1.2431573	4.8480330
O	2.1275780	-0.5989458	3.8783163
C	3.4588948	-0.1076626	4.2169752
H	3.5714696	0.8852598	3.7615840
C	4.4620263	-1.0989940	3.6723615
H	4.3818426	-1.1744886	2.5801624
H	4.3200336	-2.0968481	4.1092350
C	-1.3266349	0.5062395	4.0832832
H	3.5168533	-0.0028377	5.3097008
H	5.4781961	-0.7595956	3.9161004
N	-2.2615961	1.0854565	4.4629140
O	-0.4803706	-1.5591108	5.8928954
H	-1.1946867	-0.9401882	6.1266922
C	-0.0141734	0.3332623	1.0928992
C	-0.2251669	-0.7550693	2.1967714
H	-1.1908750	-1.2301304	1.9759362
H	0.5599849	-1.5114784	2.0624166
C	-1.0936275	1.4450151	1.2081134
O	-0.8575166	2.6045144	1.4539156
O	-2.3140511	0.9070455	1.0275040
C	-3.4170664	1.8638157	1.0350729

H	-3.4632473	2.3154374	2.0360141
C	-4.6761107	1.1061793	0.6794442
H	-4.8845350	0.3102505	1.4075038
H	-4.5959392	0.6633441	-0.3219453
C	1.3067408	0.9556309	1.2478057
H	-3.1805194	2.6426831	0.2980678
H	-5.5284709	1.7997157	0.6786396
N	2.3754591	1.3895475	1.3917549
C	0.0746975	0.2426714	-1.6264630
C	-0.1093248	-0.4554559	-0.2561568
H	0.6432696	-1.2547039	-0.2175129
H	-1.1007052	-0.9304471	-0.2631087
C	1.4944165	0.7805552	-1.8648750
O	1.7568002	1.8773413	-2.3038378
O	2.3984629	-0.1812727	-1.5759471
C	3.7695324	0.1273935	-1.9532406
H	3.7698449	0.3827040	-3.0217279
C	4.6001357	-1.1075798	-1.6831820
H	4.2493540	-1.9430588	-2.3026977
H	4.5593592	-1.3973024	-0.6231213
C	-0.8941664	1.3216209	-1.8038607
H	4.0983320	0.9974800	-1.3667555
H	5.6488254	-0.9061435	-1.9439641
N	-1.7254859	2.1293894	-1.9088819
C	0.1178219	-0.6643820	-4.1531922
C	-0.2054909	-0.9261956	-2.7234294
H	-1.2710899	-1.1690862	-2.6114378
H	0.3880951	-1.7726557	-2.3423037
C	-0.8623598	-0.2741525	-5.1160995
O	-0.7155431	-0.0628859	-6.3213589
O	-2.1422658	-0.1547649	-4.5271122
C	-3.1563128	0.3350708	-5.4037896
H	-2.8213371	1.2746742	-5.8717377
C	-4.4126316	0.5470589	-4.5767174
H	-4.2248865	1.2687718	-3.7697510
H	-4.7499046	-0.3966708	-4.1233978
C	1.4355246	-0.8975086	-4.5764258
H	-3.3282283	-0.3827083	-6.2241635
H	-5.2254387	0.9332159	-5.2099971
N	2.5608125	-1.1227981	-4.8447898

poly(ethyl-CA)$_5$
82

C	-0.6071337	0.8207196	4.8308211
C	-1.1498698	-0.3278920	5.7627192
H	-0.4866757	-1.1939692	5.6437158
H	-2.1606727	-0.5968362	5.4073181
C	0.8048041	1.2117896	5.3357493
O	1.0819019	2.2701401	5.8490093
O	1.6477269	0.1762768	5.1588951
C	3.0356057	0.4362747	5.5294129
H	3.3695125	1.3181537	4.9664699

C	3.8383854	-0.7977024	5.1859798
H	3.7970878	-1.0048444	4.1087027
H	3.4742600	-1.6791164	5.7308682
C	-1.5195327	1.9504766	5.0366615
H	3.0633699	0.6740077	6.6020424
H	4.8896776	-0.6357569	5.4608520
N	-2.3257519	2.7514448	5.2854621
O	-1.1363084	0.0058352	7.1314713
H	-1.7266275	0.7680279	7.2664663
C	-0.2104719	1.1505587	2.1697194
C	-0.6406818	0.2612120	3.3841446
H	-1.6705443	-0.0607620	3.1780784
H	-0.0006082	-0.6316423	3.3812173
C	-1.0944513	2.4273048	2.0802711
O	-0.6679683	3.5558923	2.1362001
O	-2.3842811	2.0679944	1.9563713
C	-3.3272443	3.1775114	1.8140619
H	-3.2890466	3.7659446	2.7413284
C	-4.6924126	2.5826124	1.5570132
H	-5.0131290	1.9397235	2.3878826
H	-4.6972447	1.9972019	0.6282598
C	1.1907991	1.5591998	2.3285667
H	-2.9809439	3.7989663	0.9781306
H	-5.4257379	3.3938847	1.4514296
N	2.3143705	1.8110638	2.4867062
C	-0.0961724	0.6977783	-0.5303949
C	-0.3873715	0.2138889	0.9278914
H	0.2556821	-0.6615959	1.0908226
H	-1.4314795	-0.1261330	0.9493847
C	1.3708435	1.1875609	-0.6817725
O	1.6874820	2.3124121	-0.9875193
O	2.2128401	0.1758527	-0.3989688
C	3.6279316	0.4833006	-0.5843568
H	3.7522319	0.8457402	-1.6135014
C	4.4044347	-0.7890273	-0.3310899
H	4.1118967	-1.5740682	-1.0406789
H	4.2491295	-1.1569543	0.6927982
C	-0.9950228	1.8019244	-0.8883151
H	3.8918309	1.2871587	0.1169507
H	5.4772871	-0.5920106	-0.4639450
N	-1.7573119	2.6431792	-1.1376231
C	-0.2548587	-0.5422937	-2.9533191
C	-0.3887705	-0.5665216	-1.4109045
H	-1.4218854	-0.8750976	-1.2004820
H	0.2788979	-1.3570925	-1.0398656
C	-1.2797964	0.3634035	-3.6541084
O	-1.0211480	1.1504079	-4.5361428
O	-2.5182604	0.0963470	-3.1840929
C	-3.6043214	0.7368235	-3.9111593
H	-3.4710753	1.8256362	-3.8384154
C	-4.9012131	0.2657569	-3.2914082
H	-4.9610288	0.5366739	-2.2273625
H	-5.0003535	-0.8226204	-3.3946885
C	1.0951365	-0.1643549	-3.3638538
H	-3.5256068	0.4254529	-4.9621265

H	-5.7466901	0.7358104	-3.8133247
N	2.2004640	0.0850755	-3.6293168
C	-0.7186260	-2.3741586	-4.8601019
C	-0.5502313	-2.0765377	-3.4114360
H	0.2833903	-2.6600885	-2.9970454
H	-1.4666933	-2.3303065	-2.8548123
C	0.3286184	-2.9040955	-5.6743535
O	0.2946853	-3.2123832	-6.8668901
O	1.5177502	-3.0834099	-4.9301405
C	2.6413363	-3.5109540	-5.6993476
H	2.4673343	-4.5272715	-6.0931652
C	3.8598058	-3.4668347	-4.7934169
H	3.7336350	-4.1365217	-3.9299595
H	4.0225852	-2.4472921	-4.4175430
C	-1.9946490	-2.1964191	-5.4170299
H	2.7666122	-2.8513460	-6.5726334
H	4.7571392	-3.7843835	-5.3454872
N	-3.0965780	-2.0241068	-5.7977465

poly(ethyl-CA)$_6$
98

C	-0.4379181	0.9410779	5.9487938
C	-0.8025386	-0.3539594	6.7697688
H	-0.0118759	-1.0938842	6.5919887
H	-1.7567901	-0.7443170	6.3728490
C	0.8882053	1.5051580	6.5196861
O	0.9872297	2.5496453	7.1190299
O	1.8853017	0.6311069	6.2854603
C	3.2085008	1.0670727	6.7242286
H	3.4242197	2.0222934	6.2268545
C	4.1951465	-0.0125556	6.3427142
H	4.2166928	-0.1592961	5.2549310
H	3.9510165	-0.9688536	6.8244122
C	-1.5204402	1.8921396	6.2213834
H	3.1680410	1.2387372	7.8087845
H	5.2022478	0.2852358	6.6650380
N	-2.4470430	2.5344801	6.5081654
O	-0.8492280	-0.1401732	8.1607322
H	-1.5605519	0.4964229	8.3509896
C	-0.0638145	1.5579098	3.3374768
C	-0.3643576	0.5090843	4.4608027
H	-1.3276391	0.0486055	4.2018719
H	0.4093591	-0.2684468	4.4006735
C	-1.1279905	2.6933130	3.3416396
O	-0.8735306	3.8618217	3.5081280
O	-2.3488342	2.1613117	3.1558559
C	-3.4460744	3.1293473	3.1105495
H	-3.4772825	3.6401885	4.0826361
C	-4.7153798	2.3645742	2.8154195
H	-4.9266831	1.6220236	3.5965331
H	-4.6533950	1.8550991	1.8447650
C	1.2592522	2.1548558	3.5587633

H	-3.2072053	3.8607993	2.3273884
H	-5.5591080	3.0670651	2.7769574
N	2.3311992	2.5585528	3.7557527
C	0.1604364	1.3755260	0.6153061
C	-0.0896180	0.7213299	2.0154352
H	0.6644048	-0.0703387	2.1201064
H	-1.0782671	0.2444590	1.9767271
C	1.5613353	2.0482738	0.5452601
O	1.7428958	3.2191848	0.3144130
O	2.5098952	1.1271898	0.7928342
C	3.8854598	1.6167758	0.7067389
H	4.0134320	2.0646169	-0.2874235
C	4.8020322	0.4347275	0.9231281
H	4.6481099	-0.3299447	0.1504773
H	4.6449814	-0.0193309	1.9112670
C	-0.8658116	2.3892773	0.3433436
H	4.0093749	2.3950547	1.4722366
H	5.8462535	0.7712158	0.8645981
N	-1.7314826	3.1418634	0.1567676
C	0.2254347	0.3377560	-1.9236860
C	0.0339434	0.1718123	-0.3808133
H	-0.9696108	-0.2537993	-0.2462959
H	0.7658205	-0.5759690	-0.0472539
C	-0.7974683	1.3455450	-2.5180201
O	-0.4973641	2.3663951	-3.0894310
O	-2.0480590	0.9090328	-2.2774221
C	-3.1079630	1.7284092	-2.8585676
H	-3.0533773	2.7242349	-2.3970765
C	-4.4209616	1.0305353	-2.5853592
H	-4.6014226	0.9224266	-1.5066684
H	-4.4407634	0.0370932	-3.0522596
C	1.5799825	0.8177000	-2.2229595
H	-2.9021771	1.8159110	-3.9336656
H	-5.2423850	1.6235584	-3.0108442
N	2.6755891	1.1567719	-2.4115577
C	0.1233363	-1.4388841	-3.9916586
C	0.0135135	-1.1128786	-2.4820901
H	0.7425479	-1.7619939	-1.9780651
H	-0.9903323	-1.4208431	-2.1566904
C	1.5358784	-1.2531309	-4.5679690
O	1.7931199	-0.6829622	-5.6037058
C	-0.8331120	-0.6600607	-4.7741434
N	-1.6546747	-0.0575954	-5.3369014
C	-0.2541973	-3.0191942	-4.0940539
C	-0.0369340	-3.7278129	-5.3848732
C	-1.0841452	-3.9748425	-6.3247125
O	-1.0268013	-4.5728466	-7.4006130
C	1.2433236	-4.2454426	-5.6359030
N	2.3431782	-4.6496793	-5.7600674
H	-1.3116587	-3.0762242	-3.8015145
H	0.3554246	-3.4729118	-3.2961057
O	-2.3155858	-3.4468159	-5.8728552
C	-3.3890186	-3.5626961	-6.8064341
C	-4.5853489	-2.8323691	-6.2211453
H	-3.0891722	-3.1287124	-7.7738108

H	-3.6159638	-4.6261157	-6.9936939
H	-4.3441125	-1.7742911	-6.0489444
H	-4.8881971	-3.2776742	-5.2620638
H	-5.4409154	-2.8882288	-6.9107874
O	2.4341437	-1.8811039	-3.7778471
C	3.7838721	-1.9565693	-4.3172532
C	4.5961276	-2.8227515	-3.3803435
H	4.6205917	-2.4043845	-2.3636284
H	4.1802579	-3.8380409	-3.3473810
H	5.6295945	-2.8888646	-3.7489448
H	3.7167505	-2.4049012	-5.3178066
H	4.1771279	-0.9329070	-4.3983521

poly(ethyl-CA)$_7$
114

C	-0.8635610	1.2047043	6.9178540
C	-1.3149971	-0.1415458	7.6030256
H	-0.5597687	-0.9026694	7.3692178
H	-2.2785837	-0.4400926	7.1528375
C	0.4701874	1.6438898	7.5747304
O	0.6000722	2.6195238	8.2753013
O	1.4313278	0.7470604	7.2828139
C	2.7571800	1.0671337	7.8062364
H	3.0417805	2.0505799	7.4084483
C	3.7008173	-0.0265603	7.3614315
H	3.7585731	-0.0762562	6.2661836
H	3.3883165	-1.0072699	7.7442291
C	-1.9052126	2.1819080	7.2501246
H	2.6822958	1.1413853	8.8998557
H	4.7082519	0.1846658	7.7451375
N	-2.8058172	2.8455803	7.5689809
O	-1.3822147	-0.0588290	9.0065534
H	-2.0707249	0.5860115	9.2461693
C	-0.3895303	2.0484657	4.3893109
C	-0.7646460	0.9109693	5.3980987
H	-1.7380303	0.5193052	5.0722953
H	-0.0216599	0.1098217	5.2839826
C	-1.4131016	3.2189438	4.4638302
O	-1.1192575	4.3608798	4.7230825
O	-2.6471704	2.7483125	4.2138055
C	-3.7109512	3.7550513	4.2348338
H	-3.7327451	4.1911190	5.2427969
C	-5.0030307	3.0595600	3.8753193
H	-5.2468339	2.2689453	4.5974340
H	-4.9510893	2.6220686	2.8695219
C	0.9457629	2.5703577	4.7063088
H	-3.4401466	4.5351772	3.5113953
H	-5.8213994	3.7923004	3.8846516
N	2.0255836	2.9085278	4.9709816
C	-0.0990227	2.1245966	1.6684736
C	-0.3957818	1.3424771	2.9930278
H	0.3411185	0.5290617	3.0401276
H	-1.3911967	0.8912944	2.8836520

C	1.2966621	2.8123163	1.7160347
O	1.4676773	4.0047693	1.6424587
O	2.2510951	1.8764656	1.8661582
C	3.6207636	2.3913225	1.8959701
H	3.7786781	2.9587430	0.9693230
C	4.5500268	1.2051281	2.0094829
H	4.4422801	0.5327725	1.1480974
H	4.3629747	0.6367769	2.9307419
C	-1.1224953	3.1543497	1.4510840
H	3.7000422	3.0733712	2.7532925
H	5.5890337	1.5610524	2.0342781
N	-1.9827339	3.9196944	1.2937937
C	0.0134732	1.3507232	-0.9550953
C	-0.1751998	1.0186678	0.5622534
H	-1.1616658	0.5436782	0.6454495
H	0.5853643	0.2723808	0.8280970
C	-1.0860138	2.3234270	-1.4703534
O	-0.8606494	3.3769411	-2.0144169
O	-2.2985738	1.8029741	-1.2086596
C	-3.4293200	2.5957653	-1.6912598
H	-3.3955928	3.5669923	-1.1787169
C	-4.6898841	1.8190333	-1.3887670
H	-4.8068929	1.6471264	-0.3097746
H	-4.6892566	0.8512538	-1.9070962
C	1.3298599	1.9591957	-1.1823825
H	-3.2870587	2.7508799	-2.7686237
H	-5.5599572	2.3912385	-1.7388539
N	2.4031070	2.3855739	-1.3127091
C	-0.0166620	-0.2298369	-3.2027740
C	-0.0734200	-0.0535870	-1.6495712
H	0.7485466	-0.6604672	-1.2457551
H	-1.0189950	-0.5015975	-1.3151623
C	1.2792775	0.3906273	-3.7958373
O	1.2993337	1.3241159	-4.5620783
C	-1.1740580	0.4188123	-3.8309291
N	-2.1299426	0.9048329	-4.2795468
C	-0.0755753	-1.7837780	-3.4023251
C	-0.1107311	-2.4283237	-4.8092490
C	-1.4081820	-2.1598862	-5.5871403
O	-1.4640111	-1.8438183	-6.7537292
C	1.0375463	-2.0156586	-5.6117845
N	2.0010892	-1.6950117	-6.1803652
H	-0.9732263	-2.1445158	-2.8820055
H	0.8016014	-2.1910399	-2.8797162
O	-2.4739347	-2.4030941	-4.7921316
C	-3.7626401	-2.3926366	-5.4685791
C	-4.8044503	-2.8244929	-4.4605916
H	-3.9384762	-1.3779584	-5.8541053
H	-3.7027158	-3.0991829	-6.3075993
H	-4.8304994	-2.1496741	-3.5926361
H	-4.6009169	-3.8482530	-4.1209594
H	-5.7964755	-2.8130427	-4.9338488
O	2.3525437	-0.2544644	-3.3027004
C	3.6359873	0.1821922	-3.8454995
C	4.7012826	-0.7267771	-3.2758285

H	4.7362911	-0.6652247	-2.1791719
H	4.5246759	-1.7697209	-3.5698372
H	5.6829102	-0.4239483	-3.6658670
H	3.5706890	0.1087733	-4.9392141
H	3.7806348	1.2338116	-3.5614489
C	-0.0279757	-4.0310789	-4.5211955
C	-0.2953053	-4.9800976	-5.6354979
C	0.7418383	-5.6028283	-6.3958139
O	2.0194067	-5.1837034	-5.9602095
O	0.6387236	-6.4193881	-7.3126355
C	3.1061620	-5.6807138	-6.7410713
C	4.3769015	-5.0299191	-6.2226463
H	2.9394554	-5.4428919	-7.8039613
H	3.1548698	-6.7804996	-6.6668830
H	4.3125418	-3.9364784	-6.3095343
H	5.2461327	-5.3765417	-6.8014021
H	4.5458977	-5.2826368	-5.1655314
H	0.9805971	-4.1905686	-4.1155903
H	-0.7591251	-4.1748053	-3.7094110
C	-1.6311641	-5.3314078	-5.8842382
N	-2.7769917	-5.5726836	-6.0182574

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17

C	-3.2869242	0.0306159	-1.2641533
C	-2.1563609	-0.4267313	-0.6955046
C	-0.9429038	0.4684967	-0.6603078
O	-0.9145154	1.5851397	-1.1377025
O	0.0847505	-0.1359699	-0.0338589
C	-2.0787742	-1.7365862	-0.1279001
H	-3.2958363	1.0362697	-1.6841702
H	-4.1869502	-0.5791213	-1.3132118
N	-2.0269279	-2.8079777	0.3283399
C	1.3142689	0.6501601	0.0441456
C	2.3704351	-0.2076229	0.6532979
H	1.5742308	0.9639271	-0.9791383
H	1.1215057	1.5550906	0.6373458
H	2.5625541	-1.1616069	0.1545117
C	3.0830642	0.1512128	1.7229094
H	3.8774797	-0.4819479	2.1172899
H	2.9009039	1.0966515	2.2381073

poly(allyl-CA)$_1$

19

C	-2.8941801	-0.2702096	-1.3779627
C	-1.7688795	-0.6895193	-0.4534952
C	-0.6949261	0.2052364	-0.3259870
O	-0.6223667	1.3410665	-0.8602753
O	0.3604982	-0.2544422	0.4927643
C	-1.8447461	-1.9146824	0.2195854
H	-2.5713420	-0.3478668	-2.4396462

H	-3.7506255	-0.9470427	-1.2452179
N	-1.9681569	-2.9602510	0.7501267
C	1.3926723	0.6931400	0.7578541
C	2.7273116	0.0757235	0.4956636
H	1.2299129	1.5671465	0.1006761
H	1.3224980	1.0309690	1.8084060
H	2.8330993	-0.3943863	-0.4876856
C	3.7577539	0.0754000	1.3487203
H	4.7219250	-0.3631751	1.0874749
H	3.6672412	0.5161600	2.3448800
O	-3.3692216	1.0652831	-1.1411999
H	-2.5284678	1.5714503	-1.0746816

poly(allyl-CA)$_2$

36

C	-0.0850830	-0.4531098	1.2034640
C	-0.3299936	-1.8085927	1.9300378
H	0.4544905	-2.5077414	1.6154793
H	-1.3081046	-2.1950221	1.5893994
C	1.3272284	0.0755695	1.5020783
O	1.5878307	1.1401598	2.0184160
O	2.2466144	-0.8255061	1.0843079
C	3.6311071	-0.3790089	1.1448744
H	3.6505774	0.6856346	0.8690131
C	4.4216617	-1.1945473	0.1781946
H	4.1014335	-1.1022243	-0.8639501
C	-1.0691391	0.4830950	1.7500487
H	3.9939464	-0.4872704	2.1786028
N	-1.8999532	1.1044577	2.2792892
O	-0.2630533	-1.7333651	3.3474804
H	-0.8864905	-1.0384679	3.6256999
C	0.0745568	0.4407217	-1.2810797
C	-0.2769286	-0.6878863	-0.3558253
H	-1.3294835	-0.9706249	-0.4918104
H	0.3439664	-1.5698208	-0.5783193
C	-0.8851339	1.3682604	-1.7683236
O	-0.7223992	2.3265661	-2.5280806
O	-2.1868885	1.0576235	-1.2697688
C	-3.2055059	2.0080185	-1.5796701
H	-3.5494441	2.4744403	-0.6402604
C	-4.3394933	1.3375498	-2.2851253
H	-4.0600579	0.7749467	-3.1824095
C	1.4030722	0.5398792	-1.7191840
H	-2.7532625	2.7847593	-2.2235544
N	2.5365349	0.5467043	-2.0427739
C	5.4753336	-1.9374825	0.5288006
H	5.7957525	-2.0177354	1.5710001
H	6.0617012	-2.4825074	-0.2121655
C	-5.6214511	1.3954430	-1.9074576
H	-5.9202058	1.9349429	-1.0051924
H	-6.4137362	0.9121411	-2.4812359

poly(allyl-CA)$_3$
53

C	-1.0287036	-1.0601411	2.1536753
C	-1.4060008	-2.5498246	2.4809727
H	-0.6038487	-3.1900656	2.0931241
H	-2.3421087	-2.7809377	1.9417910
C	0.2925549	-0.7260037	2.8886538
O	0.3945088	0.0419177	3.8171478
O	1.2936828	-1.4604299	2.3601576
C	2.6327255	-1.1271198	2.8451517
H	2.8856055	-0.1332538	2.4493546
C	3.5690985	-2.1818150	2.3606268
H	3.4054071	-3.1937113	2.7446190
C	-2.1089220	-0.2495581	2.7266782
H	2.5919937	-1.0770197	3.9436255
N	-3.0308937	0.2598760	3.2210787
O	-1.5094683	-2.8217046	3.8639010
H	-2.1912551	-2.2327152	4.2332040
C	-0.6244898	0.4042262	-0.0793331
C	-0.9334968	-0.9515105	0.6068605
H	-1.8893477	-1.2967311	0.1900792
H	-0.1560552	-1.6623419	0.2932804
C	-1.7342846	1.4531163	0.0999358
O	-1.5522825	2.6104649	0.4028290
O	-2.9326933	0.8986371	-0.1977973
C	-4.0419553	1.8401468	-0.3211491
H	-3.9301309	2.5973757	0.4694773
C	-5.3140382	1.0757809	-0.1788248
H	-5.4601427	0.5542891	0.7727002
C	0.6412382	0.9615131	0.3954104
H	-3.9472345	2.3228098	-1.3065688
N	1.6741506	1.3401313	0.7748048
C	4.5721239	-1.9381325	1.5133812
H	4.7347470	-0.9406131	1.1006949
H	5.2555224	-2.7262295	1.1953723
C	-6.2563473	1.0365923	-1.1251315
H	-6.1114683	1.5406127	-2.0828791
H	-7.1955885	0.5022297	-0.9746538
C	-0.4097571	1.2001210	-2.6213661
C	-0.5119889	0.0655546	-1.6578239
H	0.3628903	-0.5923729	-1.7467197
H	-1.4175357	-0.5281629	-1.8575138
C	0.8302641	1.6724556	-3.1354681
O	1.0383270	2.5911722	-3.9300359
O	1.9163423	0.9033947	-2.6237573
C	3.2145290	1.4280495	-2.8979072
H	3.1173443	2.1599700	-3.7208333
C	4.1333720	0.3140311	-3.2759204
H	3.7794393	-0.3253774	-4.0918455
C	-1.6061071	1.7822615	-3.0695205
H	3.5892957	1.9585899	-2.0041396
N	-2.6571698	2.2044456	-3.3939962
C	5.3214639	0.0732597	-2.7097718

H	5.6868860	0.6870143	-1.8826276
H	5.9698024	-0.7342675	-3.0530034

poly(allyl-CA)$_4$
70

C	-0.4552032	-1.8808449	3.2060315
C	-0.6861605	-3.4303355	3.3609215
H	0.1965670	-3.9405931	2.9560021
H	-1.5681978	-3.6986386	2.7524759
C	0.7886257	-1.4946966	4.0440338
O	0.7692496	-0.7902973	5.0257402
O	1.8775632	-2.1007318	3.5283716
C	3.1464277	-1.7345684	4.1598441
H	3.3388878	-0.6766118	3.9344151
C	4.2062365	-2.6267450	3.6089823
H	4.0792918	-3.6996209	3.7835360
C	-1.6456346	-1.2542891	3.7910069
H	3.0256277	-1.8526634	5.2473264
N	-2.6477875	-0.9057050	4.2685429
O	-0.8163974	-3.8485155	4.7015207
H	-1.5978758	-3.4092258	5.0811324
C	-0.0625719	-0.1633210	1.1412261
C	-0.3054669	-1.6104527	1.6843179
H	-1.2201565	-1.9710903	1.1940207
H	0.5309029	-2.2323651	1.3373196
C	-1.1999077	0.7881162	1.6078303
O	-1.0462107	1.7189490	2.3625454
O	-2.3665798	0.3836948	1.0703126
C	-3.5200768	1.2374808	1.3648505
H	-3.8529623	1.0195061	2.3897459
C	-4.5710012	0.9520500	0.3470254
H	-4.2928975	1.1433852	-0.6935831
C	1.2135337	0.3585565	1.6456565
H	-3.1744204	2.2798500	1.3067644
N	2.2500164	0.7157087	2.0319267
C	5.2790463	-2.1728894	2.9560535
H	5.4130780	-1.1071799	2.7601871
H	6.0563974	-2.8474757	2.5963058
C	-5.8021405	0.5373794	0.6575030
H	-6.0938870	0.3463781	1.6929268
H	-6.5614798	0.3869787	-0.1104884
C	0.2455265	0.8737200	-1.3516807
C	-0.0241060	-0.3289880	-0.4137389
H	0.7465436	-1.0764862	-0.6456861
H	-0.9973760	-0.7524104	-0.6984452
C	1.6784503	1.4248289	-1.2649744
O	1.9673201	2.5974888	-1.1993011
O	2.5635136	0.4030274	-1.3464241
C	3.9528383	0.8075269	-1.5361094
H	4.0494925	1.1716130	-2.5708797
C	4.8150931	-0.3792176	-1.2685581
H	4.7467044	-0.8123167	-0.2648860

C	-0.7008813	1.9619233	-1.1165597
H	4.1624041	1.6318789	-0.8374403
N	-1.5070723	2.7775283	-0.9203867
C	0.3488642	1.1637164	-4.0067128
C	0.0326932	0.2836309	-2.8465741
H	-1.0201089	-0.0258016	-2.8845678
H	0.6643842	-0.6188490	-2.8544833
C	-0.6490838	1.8728268	-4.7347131
O	-0.5130235	2.6178583	-5.7063120
O	-1.9471492	1.6065901	-4.2120076
C	-3.0123831	2.3409371	-4.8164510
H	-2.5721538	3.1894488	-5.3703295
C	-3.9455865	2.8069290	-3.7468221
H	-3.4703964	3.3400188	-2.9171508
C	1.6859511	1.2233689	-4.4302570
H	-3.5411579	1.7053230	-5.5501743
N	2.8289935	1.2013932	-4.7147433
C	5.6540987	-0.8950840	-2.1711669
H	5.7139633	-0.4840386	-3.1809612
H	6.3001078	-1.7414974	-1.9330718
C	-5.2702039	2.6168765	-3.7544751
H	-5.7599986	2.0672364	-4.5628963
H	-5.9106971	3.0098230	-2.9633897

poly(allyl-CA)$_5$

87

C	-1.0868168	-2.5926955	4.1210039
C	-1.5231978	-4.1029728	4.0174485
H	-0.7544264	-4.6325333	3.4407475
H	-2.4774943	-4.1377576	3.4621534
C	0.2399111	-2.5373720	4.9204761
O	0.3603240	-2.0573449	6.0225619
O	1.2101064	-3.1490998	4.2122642
C	2.5470198	-3.0917686	4.8092123
H	2.8879787	-2.0481694	4.7627003
C	3.4318158	-4.0094416	4.0365920
H	3.1569798	-5.0685847	4.0416862
C	-2.1426825	-1.9335670	4.8964147
H	2.4545913	-3.3897062	5.8642908
N	-3.0536686	-1.5388311	5.5030354
O	-1.6077729	-4.7488696	5.2666799
H	-2.2972506	-4.3081500	5.7937704
C	-0.6213345	-0.5694030	2.3821014
C	-0.9751211	-2.0673587	2.6653879
H	-1.9376210	-2.2539580	2.1701302
H	-0.2133819	-2.6848091	2.1704809
C	-1.6868906	0.3815857	2.9974888
O	-1.4429583	1.2591190	3.7900299
O	-2.9013321	0.0582262	2.5145439
C	-3.9940602	0.9298521	2.9642918
H	-3.9532266	0.9647350	4.0630488
C	-5.2738290	0.3496107	2.4675514
H	-5.5394881	-0.6404726	2.8500885

C	0.6881337	-0.2502876	2.9645402
H	-3.8068591	1.9332191	2.5588835
N	1.7483585	-0.0700498	3.4048679
C	4.5221595	-3.6002644	3.3836486
H	4.8046038	-2.5459591	3.3580160
H	5.1676502	-4.3007581	2.8535386
C	-6.0901652	0.9920231	1.6283047
H	-5.8333710	1.9766568	1.2323726
H	-7.0395822	0.5593700	1.3114979
C	-0.3115544	0.8738696	0.0729186
C	-0.5776326	-0.4746664	0.8194579
H	0.2011267	-1.1702223	0.4781096
H	-1.5462546	-0.8502308	0.4629993
C	1.0391997	1.5042564	0.5141928
O	1.1442995	2.5589092	1.0929679
O	2.0477941	0.6799383	0.1713459
C	3.3902872	1.1910115	0.4550550
H	3.4005500	2.2516266	0.1637372
C	4.3612033	0.3963454	-0.3495359
H	4.2200183	0.4253061	-1.4340575
C	-1.3870409	1.8336003	0.3502619
H	3.5669197	1.1072358	1.5367957
N	-2.2825826	2.5459467	0.5539838
C	-0.1136464	1.5185688	-2.5647093
C	-0.3060053	0.4706931	-1.4411009
H	-1.2617965	-0.0281761	-1.6507833
H	0.4933116	-0.2750220	-1.5530195
C	-1.2911055	2.4956560	-2.7183297
O	-1.1843461	3.6926602	-2.8544883
O	-2.4541366	1.8031110	-2.7520284
C	-3.6217015	2.5824618	-3.1527954
H	-3.5931015	3.5375927	-2.6065061
C	-4.8386119	1.7883342	-2.8184087
H	-4.9800756	1.5386279	-1.7614135
C	1.1211598	2.2797292	-2.3897714
H	-3.5307433	2.7758512	-4.2330099
N	2.1371527	2.8242588	-2.2324956
C	5.3854175	-0.2742933	0.1846535
H	5.5423421	-0.3051055	1.2656463
H	6.1090045	-0.7996750	-0.4393268
C	-5.7403580	1.4100576	-3.7286224
H	-5.5978631	1.6362042	-4.7872721
H	-6.6414264	0.8627594	-3.4476121
C	0.0429566	1.3589501	-5.2292211
C	-0.0191631	0.6405149	-3.9258423
H	0.8729392	0.0128925	-3.7991825
H	-0.9119222	-0.0026989	-3.8734581
C	1.2607679	1.5751796	-5.9358209
O	1.4373390	2.1429897	-7.0146228
O	2.3637917	1.0070156	-5.2359102
C	3.6455580	1.2439988	-5.8192430
H	3.9717678	0.3554026	-6.3901155
C	4.6184709	1.5639916	-4.7315983
H	4.3040426	2.3592454	-4.0482190
C	-1.1718436	1.7637261	-5.8049664

H	3.5469204	2.0791436	-6.5357121
N	-2.2393669	2.0545103	-6.2097716
C	5.7999407	0.9587757	-4.5624832
H	6.1223858	0.1488390	-5.2224777
H	6.4885094	1.2560897	-3.7700452

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104

C	-0.7448178	-3.3555535	4.9370412
C	-1.0679585	-4.8669831	4.6238249
H	-0.2283067	-5.2727119	4.0453317
H	-1.9802552	-4.8910020	4.0014092
C	0.5258432	-3.3198732	5.8233006
O	0.5463915	-2.9913448	6.9854707
O	1.5798580	-3.7571641	5.1058441
C	2.8669422	-3.7164978	5.8035244
H	2.9518387	-2.7246408	6.2719399
C	3.9397374	-3.9449331	4.7945245
H	3.9846346	-3.2244744	3.9725050
C	-1.8891503	-2.8625095	5.7098150
H	2.8636761	-4.4831011	6.5909128
N	-2.8628717	-2.5970602	6.2883303
O	-1.1856870	-5.6645197	5.7779280
H	-1.9460493	-5.3473473	6.2961127
C	-0.3065008	-1.1102927	3.4887467
C	-0.5857899	-2.6492727	3.5657197
H	-1.5076741	-2.8223840	2.9937927
H	0.2366406	-3.1597712	3.0466495
C	-1.4543414	-0.3093400	4.1697736
O	-1.3059628	0.4179085	5.1216159
O	-2.6141637	-0.5805285	3.5432168
C	-3.7869659	0.1295562	4.0693211
H	-4.0398527	-0.3111997	5.0436301
C	-4.8874971	-0.0107882	3.0746677
H	-4.6943701	0.4072432	2.0822690
C	0.9532216	-0.7943217	4.1730249
H	-3.4930463	1.1798946	4.2096229
N	1.9776234	-0.6023397	4.6871552
C	4.8368090	-4.9300057	4.8810795
H	4.8079609	-5.6561138	5.6965160
H	5.6369372	-5.0388457	4.1488226
C	-6.0684037	-0.5656925	3.3589731
H	-6.2756809	-0.9848164	4.3460015
H	-6.8699604	-0.6093055	2.6213064
C	0.0879708	0.6203996	1.4104073
C	-0.2052066	-0.8165019	1.9562909
H	0.5878394	-1.4611957	1.5544696
H	-1.1599637	-1.1405690	1.5211665
C	1.4662583	1.1452152	1.9046414
O	1.6251149	2.1644670	2.5305453
O	2.4282237	0.2794270	1.5312241
C	3.7907791	0.6782992	1.8972694

H	3.9321451	1.7092074	1.5396595
C	4.7327526	-0.2675563	1.2348445
H	4.6780777	-0.3135352	0.1431029
C	-0.9585232	1.5517718	1.8483866
H	3.8718365	0.6569287	2.9927514
N	-1.8395518	2.2325673	2.1814001
C	0.3282572	1.6182261	-1.1314973
C	0.0560395	0.4358977	-0.1455788
H	-0.9398538	0.0511808	-0.4035334
H	0.7914032	-0.3469832	-0.3747727
C	-0.6910821	2.7726702	-0.9242727
O	-0.3956622	3.8993567	-0.6070166
O	-1.9379289	2.3061244	-1.1325577
C	-2.9948385	3.3146732	-1.0361428
H	-3.0772412	3.6294005	0.0135410
C	-4.2522564	2.7016481	-1.5503536
H	-4.2239129	2.3546861	-2.5873721
C	1.6828887	2.1476488	-0.9332937
H	-2.6813612	4.1698902	-1.6535430
N	2.7780125	2.5006091	-0.7685289
C	5.6377451	-0.9912898	1.8992907
H	5.7091148	-0.9497948	2.9886443
H	6.3485493	-1.6327382	1.3776319
C	-5.3759624	2.6123196	-0.8335194
H	-5.4185281	2.9614945	0.2008590
H	-6.2933555	2.2052798	-1.2599408
C	0.3985652	1.7696314	-3.8519663
C	0.1905412	0.9601637	-2.5480806
H	0.9072202	0.1286323	-2.5886322
H	-0.8215194	0.5335633	-2.5900640
C	1.8377591	2.2780115	-4.0396597
O	2.1426636	3.4045745	-4.3556342
O	2.7039761	1.2549001	-3.8540134
C	4.0987397	1.5620766	-4.1492025
H	4.1164602	2.1834655	-5.0565331
C	4.8105124	0.2714311	-4.3743064
H	4.4419644	-0.3148975	-5.2210679
C	-0.5297418	2.8957900	-3.9308471
H	4.5138736	2.1328446	-3.3053161
N	-1.3256287	3.7441790	-3.9594823
C	0.3838501	1.1162859	-6.4447000
C	0.0781148	0.7166655	-5.0417009
H	-0.9898013	0.4826096	-4.9353582
H	0.6617680	-0.1739270	-4.7601760
C	-0.5966873	1.6482305	-7.3294837
O	-0.4666671	2.0022972	-8.5019855
O	-1.8673173	1.7204147	-6.6889823
C	-2.8829470	2.4130627	-7.4156675
H	-3.0502341	3.3983861	-6.9461903
C	-4.1395245	1.6061472	-7.4177110
H	-4.0354342	0.5823359	-7.7929776
C	1.6855148	0.8812813	-6.9156191
H	-2.5126684	2.5702839	-8.4451568
N	2.7972936	0.6388443	-7.2202289
C	5.8573169	-0.1318248	-3.6480671

H	6.2326579	0.4640638	-2.8120127
H	6.3863469	-1.0587619	-3.8737053
C	-5.3365982	2.0503567	-7.0184195
H	-5.4604091	3.0622278	-6.6248259
H	-6.2305481	1.4275615	-7.0761482

poly(allyl-CA)$_7$

121

C	-1.3917368	-4.2793985	5.4800171
C	-1.6435999	-5.7315643	4.9199481
H	-0.7539279	-6.0260530	4.3489758
H	-2.5097815	-5.6811798	4.2365342
C	-0.1976080	-4.3527687	6.4653430
O	-0.2781451	-4.1810912	7.6580435
O	0.9207451	-4.6788717	5.7864038
C	2.1443114	-4.7123289	6.5921794
H	2.3472019	-3.6905849	6.9413441
C	3.2423071	-5.2435109	5.7354717
H	3.0973050	-6.2480240	5.3266848
C	-2.6072670	-3.9270038	6.2205375
H	1.9502510	-5.3534987	7.4652006
N	-3.6295861	-3.7655686	6.7515184
O	-1.8125705	-6.6974298	5.9297912
H	-2.6228372	-6.4880267	6.4264825
C	-0.9043899	-1.8334855	4.4275744
C	-1.1443994	-3.3706673	4.2474543
H	-2.0126144	-3.4707693	3.5816417
H	-0.2681911	-3.7822594	3.7283092
C	-2.1202070	-1.1658615	5.1349730
O	-2.0595968	-0.5897116	6.1937370
O	-3.2238268	-1.3586667	4.3899097
C	-4.4536349	-0.7681329	4.9354175
H	-4.7378930	-1.3437950	5.8271005
C	-5.4926625	-0.8162705	3.8685232
H	-5.2671053	-0.2648164	2.9508241
C	0.2952233	-1.6056186	5.2423799
H	-4.2132229	0.2639943	5.2294001
N	1.2778477	-1.4731497	5.8485257
C	4.3706905	-4.5729817	5.4895903
H	4.5310263	-3.5682071	5.8860491
H	5.1741550	-5.0069741	4.8941604
C	-6.6610624	-1.4472085	4.0102453
H	-6.9008600	-1.9998659	4.9211587
H	-7.4201499	-1.4237163	3.2281003
C	-0.4123473	0.2086838	2.6807877
C	-0.7027757	-1.3020343	2.9709806
H	0.1340377	-1.8624565	2.5330940
H	-1.6154534	-1.5688757	2.4216232
C	0.9074977	0.6753819	3.3618852
O	0.9814871	1.5832778	4.1529508
O	1.9239845	-0.0955472	2.9315017
C	3.2405003	0.2641992	3.4724703

H	3.5021928	1.2581918	3.0854305
C	4.2087416	-0.7855206	3.0464836
H	3.9976821	-1.8047551	3.3849962
C	-1.5149444	1.0421560	3.1747139
H	3.1392121	0.3143636	4.5668391
N	-2.4325566	1.6538441	3.5410357
C	-0.0403154	1.6119971	0.3591037
C	-0.3172073	0.2719899	1.1182853
H	-1.2673095	-0.1097597	0.7216386
H	0.4777145	-0.4304199	0.8339339
C	-1.1485311	2.6655490	0.6435782
O	-0.9481529	3.7600682	1.1099204
O	-2.3451106	2.1508401	0.3003174
C	-3.4807868	3.0585108	0.4893729
H	-3.5728125	3.2759576	1.5621846
C	-4.6919250	2.3879785	-0.0623036
H	-4.6488688	2.1128879	-1.1203003
C	1.2574859	2.1651572	0.7641446
H	-3.2453563	3.9860228	-0.0540142
N	2.3148554	2.5310691	1.0780797
C	5.3024833	-0.5259613	2.3254537
H	5.5251364	0.4846391	1.9768745
H	6.0144629	-1.3095582	2.0651068
C	-5.7998389	2.1659730	0.6500112
H	-5.8598761	2.4401911	1.7056301
H	-6.6878479	1.7218749	0.1993345
C	0.2108187	2.2065666	-2.3058681
C	-0.0170659	1.1807517	-1.1482818
H	0.7731482	0.4255335	-1.2549844
H	-0.9815858	0.6917318	-1.3395407
C	1.5786326	2.9307240	-2.1594305
O	1.7133152	4.1241102	-2.0366086
O	2.5640235	2.0124522	-2.1753524
C	3.9243707	2.5589712	-2.1562505
H	4.0901021	3.0561132	-3.1220041
C	4.8636793	1.4230305	-1.9314338
H	4.7880293	0.9159882	-0.9641909
C	-0.8582416	3.2117298	-2.3140593
H	3.9707759	3.3034302	-1.3479970
N	-1.7540109	3.9523423	-2.3054841
C	0.3242339	1.9305846	-5.0163851
C	0.1566529	1.3243713	-3.6018305
H	-0.8141005	0.8104676	-3.6045805
H	0.9402691	0.5629439	-3.4824522
C	-0.8311359	2.8436703	-5.4533943
O	-0.6947739	3.9080532	-6.0115897
O	-2.0131780	2.2397080	-5.1856451
C	-3.1883799	2.8728953	-5.7780237
H	-3.0270746	3.9611662	-5.7613239
C	-4.3820595	2.4803701	-4.9758569
H	-4.3768172	2.7868193	-3.9244586
C	1.5874938	2.6515147	-5.1502688
H	-3.2452355	2.5285174	-6.8227444
N	2.6274882	3.1677629	-5.2261037
C	5.7697796	1.0311075	-2.8309088

H	5.8435567	1.5103775	-3.8091436
H	6.4610454	0.2129060	-2.6253799
C	-5.4310731	1.8289642	-5.4863853
H	-5.4406433	1.5112346	-6.5309866
H	-6.3101107	1.5972791	-4.8830194
C	0.2630432	0.8618854	-7.4777983
C	0.3360994	0.6376159	-6.0082391
H	1.2551243	0.0945072	-5.7500928
H	-0.5296670	0.0507334	-5.6625189
C	1.4070431	0.8443668	-8.3281654
O	1.4592620	1.0014266	-9.5488072
O	2.5920841	0.5839489	-7.5877465
C	3.8013752	0.6175865	-8.3472891
H	4.0932939	-0.4064701	-8.6441451
C	4.8718273	1.2599266	-7.5272067
H	4.5962052	2.2176092	-7.0743566
C	-1.0108168	1.0134117	-8.0483348
H	3.6079929	1.1843631	-9.2755601
N	-2.1175128	1.1207147	-8.4377197
C	6.0952906	0.7520765	-7.3393177
H	6.3813886	-0.2138007	-7.7641760
H	6.8563918	1.2850601	-6.7672536

2-phenylethyl-CA monomer

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C	-5.3710327	0.2135028	-0.0319917
C	-4.1897117	-0.2092381	0.4540902
C	-2.9169394	0.2587598	-0.2076639
O	-2.8904771	1.0033656	-1.1665521
O	-1.8363306	-0.2584382	0.4072208
C	-4.1122313	-1.0888564	1.5784613
H	-5.3774060	0.8831486	-0.8918848
H	-6.3144890	-0.0973124	0.4125345
N	-4.0587841	-1.8064144	2.4956349
C	-0.5490345	0.1279005	-0.1513890
H	-0.5109194	-0.1916459	-1.2026821
H	-0.4698539	1.2242010	-0.1303394
C	0.5342870	-0.5388979	0.6867612
C	1.9096597	-0.1886682	0.1671693
C	2.5307358	-0.9807800	-0.8088530
C	3.7871448	-0.6410567	-1.3141595
C	4.4430412	0.5013393	-0.8502140
C	3.8358655	1.2985032	0.1226984
C	2.5794812	0.9547647	0.6252229
H	0.3828720	-1.6280397	0.6652776
H	0.4260340	-0.2156312	1.7325362
H	2.1140937	1.5779849	1.3923770
H	4.3439780	2.1888368	0.4957033
H	5.4260659	0.7663020	-1.2412013
H	4.2570248	-1.2732798	-2.0688016
H	2.0269260	-1.8803502	-1.1699548

poly(2-phenylethyl-CA)$_1$
28

C	-4.6538053	0.6102277	0.6631444
C	-3.6756005	-0.4309288	0.1540662
C	-2.3998023	0.0250044	-0.2124576
O	-1.9766270	1.2048695	-0.0954781
O	-1.5479640	-0.9663131	-0.7429149
C	-4.0732734	-1.7697838	0.0631623
H	-5.0426527	1.2221221	-0.1809622
H	-5.5160278	0.1082899	1.1261465
N	-4.4687822	-2.8790493	0.0052976
C	-0.2059623	-0.5570691	-0.9510354
H	0.2069801	-1.2468551	-1.7032423
H	-0.1730216	0.4708945	-1.3438163
C	0.6254958	-0.6317286	0.3475000
C	2.0472207	-0.1952122	0.1269095
C	3.0789142	-1.1256582	-0.0737046
C	4.3903737	-0.7118659	-0.3205029
C	4.6974755	0.6497170	-0.3767262
C	3.6805450	1.5897781	-0.1838035
C	2.3723327	1.1709510	0.0632162
H	0.5899273	-1.6624709	0.7299957
H	0.1325674	0.0204975	1.0823885
H	1.5795753	1.9070885	0.2134527
H	3.9087849	2.6567733	-0.2236506
H	5.7213827	0.9763947	-0.5669579
H	5.1757651	-1.4561903	-0.4672718
H	2.8455418	-2.1921098	-0.0276662
O	-4.0936963	1.4903500	1.6493188
H	-3.2256666	1.7222770	1.2455920

poly(2-phenylethyl-CA)$_2$
54

C	-0.2651904	-1.5037896	1.1702146
C	-0.4148307	-2.9683527	1.6743248
H	0.4705549	-3.5289998	1.3507270
H	-1.3064909	-3.3996984	1.1829724
C	1.0538788	-0.8766872	1.6450554
O	1.1604874	0.1636549	2.2562947
O	2.0907896	-1.6402648	1.2325145
C	3.4005567	-1.0240674	1.3386632
H	3.3352000	-0.0083322	0.9271886
C	4.3652830	-1.8758183	0.5208341
H	3.9221524	-1.9959851	-0.4783641
H	4.4676427	-2.8717544	0.9785576
C	-1.3872130	-0.7617203	1.7455091
H	3.6881997	-0.9640362	2.3991154
C	5.7139783	-1.2081025	0.3981727
N	-2.3267154	-0.3157984	2.2705174
O	-0.4836299	-3.0988446	3.0875450
H	-1.2074138	-2.5230275	3.3931394

C	0.0693801	-0.2734581	-1.1593516
C	-0.3053052	-1.5269117	-0.4245785
H	-1.3240677	-1.8374048	-0.6944514
H	0.3805504	-2.3434257	-0.6989322
C	-0.8874261	0.7063938	-1.5556953
O	-0.7139299	1.7674683	-2.1573871
O	-2.1963341	0.3178357	-1.1701482
C	-3.1942323	1.3099273	-1.3798355
H	-2.9128958	2.2493714	-0.8755815
C	-4.5025994	0.7562288	-0.8071032
H	-4.3332488	0.4967379	0.2483268
H	-4.7508187	-0.1761551	-1.3383194
C	1.4144209	-0.0804301	-1.4978166
H	-3.2969230	1.5433300	-2.4533924
C	-5.6363445	1.7414002	-0.9316008
N	2.5628761	0.0138998	-1.7507190
C	6.8047298	-1.6052478	1.1832956
C	8.0422905	-0.9652932	1.0699909
C	8.2027672	0.0874649	0.1668092
C	7.1197992	0.4924602	-0.6200405
C	5.8843562	-0.1472351	-0.5075935
C	-6.4133945	1.8101692	-2.0983405
C	-7.4441759	2.7435448	-2.2267567
C	-7.7186995	3.6328790	-1.1847954
C	-6.9531063	3.5785646	-0.0173036
C	-5.9235159	2.6430843	0.1047430
H	9.1677668	0.5893317	0.0747543
H	8.8815845	-1.2909135	1.6877555
H	6.6830948	-2.4313723	1.8886328
H	-5.3288697	2.6024620	1.0199439
H	-8.0360612	2.7759046	-3.1435717
H	-8.5246184	4.3623909	-1.2815355
H	-7.1590232	4.2674900	0.8040819
H	-6.2048885	1.1161175	-2.9159870
H	7.2375402	1.3132528	-1.3299366
H	5.0320828	0.1617620	-1.1205419

poly(2-phenylethyl-CA)$_3$

80

C	-1.5351985	-1.1085183	3.0456245
C	-1.9693799	-2.4298197	3.7763628
H	-1.2658411	-3.2195087	3.4842899
H	-2.9780295	-2.6951858	3.4119840
C	-0.1111804	-0.7353467	3.5225191
O	0.1636485	0.2374228	4.1856470
O	0.7629033	-1.6769339	3.1099516
C	2.1671540	-1.3595528	3.3213206
H	2.3178731	-0.2998079	3.0797003
C	2.9803152	-2.2579476	2.3968070
H	2.5747616	-2.1439893	1.3808459
H	2.8573867	-3.3105356	2.6929695
C	-2.4735884	-0.0802082	3.5095707

H	2.4109878	-1.5201449	4.3818621
C	4.4414985	-1.8746783	2.4090890
N	-3.2859610	0.6221306	3.9575327
O	-1.9193963	-2.3438471	5.1854581
H	-2.5123599	-1.6227061	5.4621451
C	-1.2891108	-0.2871335	0.4801855
C	-1.6390573	-1.3848658	1.5197287
H	-2.6743377	-1.6869449	1.3096451
H	-0.9931019	-2.2500873	1.3138187
C	-2.2058636	0.9460720	0.5627372
O	-1.8240592	2.0935237	0.6029583
O	-3.4972811	0.5521262	0.5179121
C	-4.4670465	1.6191648	0.3297489
H	-4.5815793	2.1625588	1.2792023
C	-5.7668571	0.9705322	-0.1324300
H	-6.1795427	0.3415724	0.6710424
H	-5.5220102	0.3246250	-0.9882493
C	0.1021838	0.1426840	0.6122977
H	-4.0770923	2.3017791	-0.4360441
C	-6.7740645	2.0120176	-0.5589843
N	1.2303449	0.4070714	0.7182699
C	-1.4021236	-0.1246721	-2.1853736
C	-1.4979948	-0.9791352	-0.9644564
H	-0.7536468	-1.7855121	-1.0113815
H	-2.4975744	-1.4356630	-0.8873467
C	-0.2382774	-0.0636632	-3.0064169
O	-0.0647234	0.5726172	-4.0481135
O	0.7976610	-0.8912696	-2.4954595
C	2.0344334	-0.8011981	-3.1941435
H	2.5672136	-1.7414675	-2.9847192
C	2.8719197	0.4011073	-2.7185305
H	2.9844800	0.3408525	-1.6264452
H	2.2979642	1.3107092	-2.9448739
C	-2.5517323	0.5690964	-2.5914998
H	1.8522886	-0.7197537	-4.2766513
C	4.2157439	0.4428289	-3.3942192
N	-3.5617542	1.1106018	-2.8660209
C	-6.6383953	2.6405748	-1.8084349
C	-7.5516177	3.6167883	-2.2099204
C	-8.6111981	3.9830453	-1.3738990
C	-8.7518744	3.3657460	-0.1293130
C	-7.8370085	2.3884848	0.2729655
C	5.3838888	-2.6093858	3.1406756
C	6.7306684	-2.2365621	3.1543073
C	7.1534461	-1.1176371	2.4341905
C	6.2218216	-0.3746080	1.7030580
C	4.8773449	-0.7485599	1.6922138
C	4.3541405	0.9882882	-4.6816230
C	5.5892568	0.9962082	-5.3321962
C	6.7170824	0.4544047	-4.7088397
C	6.5956732	-0.0947063	-3.4300445
C	5.3570782	-0.1008027	-2.7837482
H	-7.9499888	1.9065236	1.2472946
H	-9.5751123	3.6444501	0.5313752
H	-9.3241649	4.7459765	-1.6917904

H	-7.4347124	4.0942367	-3.1844586
H	-5.8062855	2.3505621	-2.4568092
H	5.0584856	-3.4898231	3.7001428
H	7.4508474	-2.8242720	3.7263058
H	8.2049380	-0.8263898	2.4396556
H	6.5428742	0.4992247	1.1338960
H	4.1492206	-0.1656900	1.1229218
H	5.2710301	-0.5281764	-1.7816231
H	7.4694410	-0.5182717	-2.9307730
H	7.6840540	0.4637034	-5.2148745
H	5.6726641	1.4308445	-6.3302439
H	3.4754065	1.4148258	-5.1702782

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C	-0.5132970	-0.9016070	4.1861063
C	-0.7650598	-2.2434182	4.9700222
H	0.0855459	-2.9082374	4.7738116
H	-1.6824350	-2.7027934	4.5600011
C	0.7778364	-0.2546388	4.7462100
O	0.8171266	0.7811432	5.3671124
O	1.8311747	-1.0456790	4.4606988
C	3.1389879	-0.4965917	4.7952660
H	3.1678568	0.5477795	4.4588795
C	4.1817816	-1.3432732	4.0762424
H	3.9266924	-1.3592474	3.0064197
H	4.1377870	-2.3783652	4.4468565
C	-1.6612603	-0.0462014	4.5052402
H	3.2621455	-0.5206358	5.8876767
C	5.5697069	-0.7770339	4.2652051
N	-2.6326510	0.5067762	4.8283247
O	-0.8321353	-2.0750347	6.3681136
H	-1.5806693	-1.4855590	6.5680971
C	-0.1965808	-0.1913776	1.5850853
C	-0.4341714	-1.2806406	2.6825413
H	-1.3763620	-1.7797004	2.4175669
H	0.3742566	-2.0184483	2.5898088
C	-1.3067001	0.8948656	1.6363855
O	-1.1100344	2.0636430	1.8686259
O	-2.5042735	0.3222277	1.4101886
C	-3.6285498	1.2480014	1.3322773
H	-3.7453338	1.7368177	2.3096353
C	-4.8547021	0.4306230	0.9456709
H	-5.0465069	-0.3239693	1.7238447
H	-4.6367975	-0.1026054	0.0087770
C	1.1006967	0.4643146	1.7933725
H	-3.3883139	2.0052265	0.5738985
C	-6.0669772	1.3143194	0.7653920
N	2.1549060	0.9212178	1.9687947
C	0.0237712	-0.2832909	-1.1258106
C	-0.2026864	-0.9864192	0.2355032
H	0.5726237	-1.7607843	0.3129384

H	-1.1764229	-1.4937278	0.1827226
C	1.4295127	0.3129502	-1.2985875
O	1.6664761	1.4181857	-1.7286225
O	2.3572519	-0.6159690	-0.9752396
C	3.7233010	-0.2775466	-1.3371262
H	3.7184962	0.1044154	-2.3661690
C	4.5458230	-1.5566284	-1.2385611
H	4.0329638	-2.3217378	-1.8397030
H	4.5808446	-1.9025298	-0.1938364
C	-0.9767251	0.7558339	-1.3578223
H	4.0841435	0.5095766	-0.6585340
C	5.9435211	-1.3467024	-1.7703704
N	-1.8311257	1.5303785	-1.5140555
C	0.2307771	-1.1722261	-3.6480845
C	-0.1487191	-1.4602391	-2.2358267
H	-1.2051225	-1.7552448	-2.1732012
H	0.4659991	-2.2798205	-1.8322260
C	-0.7105785	-0.7464433	-4.6346853
O	-0.5203637	-0.4674200	-5.8179307
O	-2.0159942	-0.6763287	-4.0898593
C	-2.9782962	-0.0381230	-4.9227107
H	-2.5805379	0.9172306	-5.3009727
C	-4.2234923	0.1912724	-4.0598317
H	-3.9066832	0.7479982	-3.1651619
H	-4.6058371	-0.7856765	-3.7240272
C	1.5660135	-1.3804878	-4.0230566
H	-3.2125748	-0.6598740	-5.8039751
C	-5.3027607	0.9473109	-4.7912338
N	2.7031837	-1.5865997	-4.2549039
C	6.4315812	-1.2807377	5.2487120
C	7.7065619	-0.7393242	5.4297291
C	8.1372792	0.3187597	4.6268253
C	7.2859977	0.8309971	3.6439934
C	6.0123141	0.2885741	3.4662764
C	-6.3734087	1.8572747	-0.4908764
C	-7.4796074	2.6921348	-0.6592292
C	-8.2965844	3.0016324	0.4308762
C	-8.0001613	2.4700776	1.6883504
C	-6.8939255	1.6336581	1.8520402
C	7.0371118	-1.1773177	-0.9105654
C	8.3221950	-0.9662571	-1.4183095
C	8.5280381	-0.9181309	-2.7985431
C	7.4423476	-1.0823978	-3.6645578
C	6.1592988	-1.2945316	-3.1577792
C	-6.2809023	0.2776269	-5.5418646
C	-7.2660897	0.9822716	-6.2372592
C	-7.2911795	2.3783590	-6.1953481
C	-6.3227378	3.0603730	-5.4538411
C	-5.3395656	2.3504787	-4.7613876
H	8.3660534	-1.1485994	6.1968052
H	9.1342995	0.7402113	4.7628120
H	7.6152276	1.6542378	3.0084312
H	5.3491076	0.6922560	2.6977540
H	6.1018965	-2.1137799	5.8741514
H	-9.1626090	3.6523939	0.3005362

H	-7.7020574	3.0968993	-1.6477381
H	-5.7396489	1.6199650	-1.3478567
H	-6.6675228	1.2189173	2.8371677
H	-8.6333816	2.7052598	2.5455561
H	-4.5839570	2.8875235	-4.1836081
H	-6.3320944	4.1511549	-5.4138445
H	-6.2690885	-0.8143500	-5.5754075
H	-8.0184012	0.4388731	-6.8121084
H	-8.0611583	2.9313923	-6.7358237
H	6.8810205	-1.2162864	0.1706972
H	9.1625388	-0.8400252	-0.7329873
H	9.5302434	-0.7537420	-3.1984845
H	7.5949167	-1.0464621	-4.7447042
H	5.3055803	-1.4225903	-3.8297778

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C	-0.9520536	0.9655226	5.2757450
C	-1.6307000	-0.0486646	6.2726256
H	-1.1330919	-1.0191204	6.1503844
H	-2.6906043	-0.1481705	5.9774475
C	0.5275402	1.1316685	5.7073696
O	0.9965465	2.1388123	6.1810407
O	1.1822718	-0.0318477	5.5193676
C	2.6098804	0.0023704	5.8129288
H	3.0723813	0.7516778	5.1556342
C	3.1598774	-1.3947820	5.5553394
H	2.9307916	-1.6789765	4.5177468
H	2.6474881	-2.1116459	6.2150621
C	-1.6554265	2.2372618	5.4726463
H	2.7489233	0.3169345	6.8565154
C	4.6525787	-1.4452929	5.7863533
N	-2.3059322	3.1709186	5.7144336
O	-1.4842205	0.3119301	7.6262141
H	-1.9310580	1.1651599	7.7670146
C	-0.6547905	1.1637030	2.5928660
C	-1.1428330	0.3759755	3.8536538
H	-2.2173078	0.2004096	3.7077676
H	-0.6372203	-0.5991070	3.8511518
C	-1.3886890	2.5281423	2.4607745
O	-0.8301718	3.5952899	2.3789101
O	-2.7176299	2.3199049	2.4527319
C	-3.5338415	3.5136376	2.2420689
H	-3.4737668	4.1313688	3.1493419
C	-4.9530110	3.0474045	1.9476219
H	-5.3523502	2.5060277	2.8184099
H	-4.9148713	2.3456895	1.1014616
C	0.7884829	1.4147972	2.6952294
H	-3.1092594	4.0711702	1.3976569
C	-5.8447435	4.2183928	1.6048235
N	1.9384630	1.5372186	2.8109315
C	-0.7411725	0.6228161	-0.0974073

C	-0.9675777	0.2038880	1.3938552
H	-0.3686277	-0.7036372	1.5501846
H	-2.0264002	-0.0727562	1.4888896
C	0.7106310	1.1250171	-0.3302375
O	0.9992778	2.2522831	-0.6529702
O	1.5751413	0.1227398	-0.0849307
C	2.9764014	0.4436450	-0.3258922
H	3.0853659	0.6867725	-1.3918580
C	3.7892857	-0.7829473	0.0668047
H	3.4597352	-1.6399549	-0.5381887
H	3.5796585	-1.0199243	1.1220045
C	-1.6735834	1.6944332	-0.4690927
H	3.2401948	1.3234551	0.2764607
C	5.2693148	-0.5492126	-0.1289808
N	-2.4693193	2.4988190	-0.7348565
C	-0.9885372	-0.7146520	-2.4561959
C	-1.0558098	-0.6801044	-0.9095661
H	-2.0731063	-0.9958923	-0.6401704
H	-0.3592163	-1.4452325	-0.5391368
C	-2.0728655	0.1225428	-3.1544429
O	-1.8749694	0.8828404	-4.0737370
O	-3.2864572	-0.1861735	-2.6424063
C	-4.4222465	0.3157344	-3.3989782
H	-4.5276459	1.3934223	-3.2048429
C	-5.6462629	-0.4796119	-2.9602662
H	-5.8733380	-0.2704287	-1.9034660
H	-5.3939421	-1.5459062	-3.0562124
C	0.3255876	-0.3043417	-2.9460003
H	-4.2172866	0.1587338	-4.4657332
C	-6.8407590	-0.1628086	-3.8288094
N	1.4026880	-0.0225647	-3.2842469
C	-1.4030653	-2.6378857	-4.2762298
C	-1.2455113	-2.2731169	-2.8403620
H	-0.3976623	-2.8151981	-2.3998136
H	-2.1544319	-2.5267184	-2.2726896
C	-0.3202972	-3.1162848	-5.0759844
O	-0.3150054	-3.4356141	-6.2640195
O	0.8663187	-3.2181746	-4.3081216
C	2.0495120	-3.4629095	-5.0605145
H	2.0581310	-4.4920271	-5.4596815
C	3.2288876	-3.2291709	-4.1104236
H	3.1465491	-3.9347070	-3.2681922
H	3.1280456	-2.2121864	-3.7024429
C	-2.6864211	-2.5558191	-4.8349403
H	2.0992445	-2.7824750	-5.9255641
C	4.5636029	-3.3893000	-4.7920653
N	-3.7971676	-2.4649402	-5.2186529
C	5.1863750	-2.2952647	-5.4135531
C	6.4119480	-2.4399088	-6.0671745
C	7.0404892	-3.6871187	-6.1145091
C	6.4323136	-4.7859109	-5.5026513
C	5.2069292	-4.6351073	-4.8496595
C	6.0016017	0.2102509	0.7967199
C	7.3654138	0.4442118	0.6113865
C	8.0204431	-0.0773784	-0.5076527

C	7.3015895	-0.8301183	-1.4385785
C	5.9370034	-1.0615342	-1.2498732
C	-6.9283004	-0.7128702	-5.1188747
C	-8.0168668	-0.4145378	-5.9399698
C	-9.0322719	0.4354086	-5.4902584
C	-8.9520868	0.9880843	-4.2104860
C	-7.8614775	0.6903150	-3.3885052
C	-5.8432612	4.7506521	0.3063488
C	-6.6463014	5.8460592	-0.0149304
C	-7.4621871	6.4291286	0.9583321
C	-7.4688788	5.9100735	2.2546285
C	-6.6642901	4.8135188	2.5733323
C	5.1747777	-1.6664702	7.0688969
C	6.5537367	-1.6848187	7.2869671
C	7.4342985	-1.4818104	6.2216383
C	6.9270080	-1.2620461	4.9390273
C	5.5473436	-1.2428450	4.7262749
H	-8.0722000	-0.8508198	-6.9389050
H	-6.1301751	-1.3763905	-5.4650736
H	-7.8026385	1.1237870	-2.3868673
H	-9.7392968	1.6525563	-3.8492383
H	-9.8826666	0.6651798	-6.1347550
H	-6.6358969	6.2433235	-1.0308985
H	-5.2053893	4.2982800	-0.4564137
H	-8.0919023	7.2835509	0.7061020
H	-8.1034380	6.3582116	3.0209857
H	-6.6743385	4.4093023	3.5882745
H	4.4917403	-1.8335910	7.9051803
H	6.9414583	-1.8625272	8.2912826
H	8.5119336	-1.4996964	6.3897873
H	7.6038258	-1.1092963	4.0970829
H	5.1596217	-1.0752943	3.7191448
H	4.7380841	-5.4975983	-4.3700204
H	6.9147094	-5.7647278	-5.5321845
H	7.9986924	-3.8016140	-6.6239560
H	6.8777233	-1.5741202	-6.5413353
H	4.6989220	-1.3184691	-5.3783713
H	5.3829625	-1.6496458	-1.9845780
H	7.7994601	-1.2404035	-2.3184456
H	9.0862786	0.1044121	-0.6537695
H	7.9169816	1.0390847	1.3415791
H	5.4936597	0.6282963	1.6693706

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C	-0.5972784	0.7648323	6.3665017
C	-1.1128811	-0.5002907	7.1528255
H	-0.4130991	-1.3224104	6.9560154
H	-2.1045764	-0.7663123	6.7452857
C	0.7755436	1.1644079	6.9663216
O	0.9810592	2.1729067	7.5980935
O	1.6732542	0.1904226	6.7172088

C	3.0269842	0.4534964	7.1926696
H	3.4025092	1.3444595	6.6705128
C	3.8655419	-0.7812367	6.8884262
H	3.8355626	-0.9758424	5.8062095
H	3.4179975	-1.6514343	7.3925089
C	-1.5714655	1.8242826	6.6476124
H	2.9856829	0.6705051	8.2688619
C	5.2957246	-0.5944154	7.3408793
N	-2.4254311	2.5606073	6.9334727
O	-1.1387218	-0.3186840	8.5485923
H	-1.7752180	0.3876491	8.7567049
C	-0.1530962	1.4087568	3.7762510
C	-0.5505750	0.3615559	4.8696536
H	-1.5480405	-0.0069335	4.5938551
H	0.1531925	-0.4787398	4.7954330
C	-1.1396089	2.6122058	3.7651488
O	-0.8070049	3.7644956	3.9000240
O	-2.3916743	2.1556984	3.5835935
C	-3.4248972	3.1836878	3.4667427
H	-3.5724105	3.6312812	4.4596822
C	-4.6807606	2.5013136	2.9415614
H	-5.0281169	1.7547292	3.6712417
H	-4.4189193	1.9683792	2.0152147
C	1.2007540	1.9111685	4.0424716
H	-3.0618407	3.9535027	2.7742147
C	-5.7735862	3.5071609	2.6619449
N	2.2934664	2.2312401	4.2750849
C	0.0740166	1.2736383	1.0463741
C	-0.1950347	0.6005120	2.4353973
H	0.5385254	-0.2116537	2.5284273
H	-1.1945260	0.1478975	2.3833277
C	1.4642652	1.9693329	1.0108021
O	1.6280233	3.1495943	0.8195901
O	2.4242038	1.0576713	1.2512252
C	3.7887521	1.5766269	1.2426505
H	4.0378678	1.8450701	0.2066392
C	4.6909374	0.4790313	1.7898088
H	4.6396809	-0.4002293	1.1313785
H	4.3075935	0.1783225	2.7776430
C	-0.9599404	2.2768963	0.7630218
H	3.8173930	2.4792808	1.8666051
C	6.1205529	0.9532117	1.9148939
N	-1.8310541	3.0179665	0.5578152
C	0.1746947	0.2804703	-1.5041285
C	-0.0206943	0.0812698	0.0336556
H	-1.0149786	-0.3685212	0.1567666
H	0.7265229	-0.6549585	0.3590273
C	-0.8739262	1.2594864	-2.0979774
O	-0.5991477	2.2634368	-2.7097472
O	-2.1137443	0.8085511	-1.8254017
C	-3.1951376	1.5723545	-2.4368273
H	-3.2958697	2.5208848	-1.8898996
C	-4.4549726	0.7199803	-2.3653680
H	-4.7326396	0.5473247	-1.3145717
H	-4.2289551	-0.2561057	-2.8198418

C	1.5162425	0.8086067	-1.7815136
H	-2.9148947	1.7837547	-3.4762174
C	-5.5943466	1.3807347	-3.1057532
N	2.6043085	1.1825480	-1.9473768
C	0.0659683	-1.4520845	-3.6153981
C	0.0186687	-1.1669365	-2.0931801
H	0.8106293	-1.7813156	-1.6428071
H	-0.9459553	-1.5454815	-1.7259596
C	1.4021496	-1.0828551	-4.2809082
O	1.5159595	-0.4319456	-5.2939023
C	-1.0294319	-0.7880611	-4.3191082
N	-1.9557483	-0.2969683	-4.8239824
C	-0.1265083	-3.0608032	-3.7393126
C	0.0346174	-3.6944435	-5.0782178
C	-1.0690693	-4.0243590	-5.9227530
O	-1.0574800	-4.5518361	-7.0343795
C	1.3290155	-4.0550563	-5.4809155
N	2.4451191	-4.3339161	-5.7362179
H	-1.1314794	-3.2601524	-3.3428418
H	0.6145960	-3.4597559	-3.0289176
O	-2.3015474	-3.6865289	-5.3083507
C	-3.4423006	-3.8200528	-6.1496983
C	-4.6792487	-3.6477434	-5.2650458
H	-3.4228491	-3.0512179	-6.9415266
H	-3.4392128	-4.8006813	-6.6512304
H	-4.6233546	-2.6689764	-4.7657142
H	-4.6468607	-4.4171581	-4.4766348
C	-5.9668912	-3.7573363	-6.0431413
O	2.4172629	-1.6574763	-3.5996654
C	3.7144052	-1.6007339	-4.2537116
C	4.6113932	-2.6214336	-3.5631314
H	4.7954645	-2.3157708	-2.5215205
H	4.0693354	-3.5783914	-3.5534545
C	5.9170675	-2.7884352	-4.3032870
H	3.5732991	-1.8578940	-5.3114059
H	4.1039846	-0.5752502	-4.1753466
C	5.6658929	-0.8483234	8.6696432
C	6.9802067	-0.6504454	9.0967042
C	7.9475482	-0.1938993	8.1980447
C	7.5917331	0.0618201	6.8720502
C	6.2757527	-0.1364284	6.4495105
C	-5.7707564	4.2394882	1.4649106
C	-6.7668399	5.1813902	1.2030495
C	-7.7808697	5.4087772	2.1372633
C	-7.7912700	4.6891777	3.3338092
C	-6.7934816	3.7464614	3.5924642
C	-5.6349505	1.3446085	-4.5088363
C	-6.6706435	1.9679945	-5.2063146
C	-7.6820228	2.6396479	-4.5133791
C	-7.6491979	2.6850569	-3.1183502
C	-6.6108301	2.0608393	-2.4220608
C	6.4894895	1.8335385	2.9442958
C	7.8047213	2.2866079	3.0601203
C	8.7743553	1.8674586	2.1449801
C	8.4183016	0.9955654	1.1142866

C	7.1009531	0.5447738	1.0010589
C	7.0959609	-2.1748664	-3.8594386
C	8.2928459	-2.3236535	-4.5656378
C	8.3232006	-3.0901897	-5.7323165
C	7.1511982	-3.7037313	-6.1857055
C	5.9562226	-3.5552353	-5.4800145
C	-6.4228886	-5.0017966	-6.5071797
C	-7.6023701	-5.1079266	-7.2456889
C	-8.3543770	-3.9661763	-7.5364737
C	-7.9146167	-2.7214634	-7.0815563
C	-6.7320259	-2.6212835	-6.3442437
H	4.9161614	-1.2127958	9.3760067
H	7.2504777	-0.8580039	10.1331705
H	8.9758060	-0.0428196	8.5292346
H	8.3385573	0.4129324	6.1584304
H	6.0100770	0.0621490	5.4090110
H	-6.8080447	3.1832713	4.5284293
H	-8.5799315	4.8593525	4.0683907
H	-8.5611496	6.1429034	1.9318004
H	-6.7510750	5.7369751	0.2643572
H	-4.9780237	4.0675076	0.7331515
H	5.7346131	2.1700136	3.6591373
H	8.0718524	2.9715660	3.8665115
H	9.8023770	2.2214694	2.2337607
H	9.1669807	0.6646859	0.3931011
H	6.8279924	-0.1360697	0.1918603
H	5.0350340	-4.0298845	-5.8306058
H	7.1664720	-4.3039282	-7.0971839
H	9.2559718	-3.2091266	-6.2864542
H	9.2018720	-1.8394294	-4.2037462
H	7.0747635	-1.5728830	-2.9471985
H	-6.5925042	2.0976670	-1.3300519
H	-8.4344442	3.2055757	-2.5674459
H	-8.4927468	3.1243241	-5.0594924
H	-6.6875751	1.9277810	-6.2965946
H	-4.8421935	0.8243089	-5.0520371
H	-6.3955478	-1.6443826	-5.9894526
H	-5.8414416	-5.8990131	-6.2832920
H	-8.4940972	-1.8224629	-7.2992706
H	-7.9367206	-6.0864057	-7.5954844
H	-9.2775410	-4.0474466	-8.1126168

poly(2-phenylethyl-CA)$_7$
184

C	-1.0175398	1.2288559	7.3083835
C	-1.5640760	-0.0568536	8.0392420
H	-0.9087972	-0.8954125	7.7710308
H	-2.5796198	-0.2557186	7.6526569
C	0.3883762	1.5362348	7.8860821
O	0.6548014	2.4971696	8.5670695
O	1.2362548	0.5432505	7.5523018
C	2.6141255	0.7238345	7.9971306

H	3.0049566	1.6372822	7.5279181
C	3.3959283	-0.5130356	7.5742185
H	3.3146507	-0.6299859	6.4833614
H	2.9401187	-1.4019346	8.0361772
C	-1.9358399	2.3112633	7.6761781
H	2.6163084	0.8621951	9.0870002
C	4.8492115	-0.4029739	7.9753030
N	-2.7480164	3.0681686	8.0235170
O	-1.5348430	0.0437694	9.4425858
H	-2.1383531	0.7568624	9.7154689
C	-0.6210451	2.0017933	4.7468555
C	-1.0316140	0.9099044	5.7906990
H	-2.0515248	0.5993910	5.5258101
H	-0.3666714	0.0472442	5.6478504
C	-1.5565002	3.2431341	4.8294052
O	-1.1697735	4.3724438	5.0072520
O	-2.8318408	2.8484987	4.6686057
C	-3.8237959	3.9235819	4.6535251
H	-3.9144112	4.3142027	5.6768236
C	-5.1273353	3.3290415	4.1387755
H	-5.4780874	2.5506592	4.8326424
H	-4.9260033	2.8483116	3.1695715
C	0.7588618	2.4348234	5.0010774
H	-3.4528563	4.7197290	3.9958092
C	-6.1850072	4.3961016	3.9725182
N	1.8700875	2.6983029	5.2163438
C	-0.4774311	2.0226781	2.0092323
C	-0.7286325	1.2748595	3.3639390
H	-0.0192755	0.4363496	3.3879594
H	-1.7432937	0.8568720	3.3155724
C	0.9200875	2.7068164	1.9883484
O	1.0900564	3.8971827	1.8888114
O	1.8759961	1.7697970	2.1233090
C	3.2468560	2.2757603	2.1173316
H	3.4605610	2.6493600	1.1063427
C	4.1564682	1.1209433	2.5120891
H	4.0452042	0.3022075	1.7861992
H	3.8302192	0.7418421	3.4933511
C	-1.5070262	3.0484478	1.8007761
H	3.3087114	3.1086408	2.8294832
C	5.6014762	1.5598009	2.5796332
N	-2.3760427	3.8044387	1.6470641
C	-0.4576326	1.1898823	-0.5970056
C	-0.6006911	0.8920753	0.9325802
H	-1.5874919	0.4273837	1.0597504
H	0.1624656	0.1452470	1.1892426
C	-1.5599460	2.1640931	-1.1024826
O	-1.3375117	3.2039980	-1.6725446
O	-2.7714674	1.6586757	-0.8059669
C	-3.9043664	2.4430888	-1.2916058
H	-3.9216518	3.3932032	-0.7393763
C	-5.1619877	1.6162155	-1.0633258
H	-5.2729809	1.4046844	0.0110954
H	-5.0450512	0.6544671	-1.5846145
C	0.8571289	1.7798898	-0.8770805

H	-3.7431238	2.6489431	-2.3575391
C	-6.3833989	2.3415972	-1.5790307
N	1.9291047	2.1938602	-1.0501497
C	-0.5621606	-0.4338454	-2.8096548
C	-0.5816984	-0.2270365	-1.2592070
H	0.2415038	-0.8367738	-0.8627466
H	-1.5248529	-0.6547655	-0.8929931
C	0.7251056	0.1629549	-3.4438858
O	0.7371088	1.0592266	-4.2523353
C	-1.7325171	0.2048427	-3.4239605
N	-2.7037421	0.6746012	-3.8563598
C	-0.6365355	-1.9908787	-2.9806056
C	-0.6583841	-2.6609393	-4.3761591
C	-1.9327175	-2.3820577	-5.1894542
O	-1.9538651	-2.0604103	-6.3548831
C	0.5124314	-2.2888079	-5.1669412
N	1.4891330	-2.0058331	-5.7326643
H	-1.5439255	-2.3322747	-2.4636941
H	0.2297484	-2.3985628	-2.4404974
O	-3.0213879	-2.6343910	-4.4273844
C	-4.2835155	-2.6806710	-5.1475690
C	-5.2937520	-3.3781327	-4.2443117
H	-4.5832471	-1.6532033	-5.4016310
H	-4.1275368	-3.2516260	-6.0718753
H	-5.4792833	-2.7693633	-3.3458557
H	-4.8461504	-4.3325344	-3.9302389
C	-6.5876069	-3.6431713	-4.9769901
O	1.8024422	-0.4584781	-2.9277364
C	3.0850593	-0.0411688	-3.4808599
C	4.1617459	-0.8296201	-2.7461897
H	4.0779879	-0.6200363	-1.6680631
H	3.9776191	-1.9040281	-2.8917745
C	5.5441337	-0.4696288	-3.2384852
H	3.0741376	-0.2619651	-4.5570442
H	3.1920247	1.0420134	-3.3323317
C	-0.6135901	-4.2566624	-4.0627834
C	-0.7994150	-5.2113336	-5.1909932
C	0.2958760	-5.7981035	-5.8964173
O	1.5317467	-5.3742683	-5.3488232
O	0.2775420	-6.5799945	-6.8458511
C	2.6776914	-5.7035135	-6.1268291
C	3.8530938	-4.9265587	-5.5244474
H	2.5176116	-5.4207519	-7.1796366
H	2.8676023	-6.7905544	-6.1105634
H	3.5709447	-3.8631969	-5.5063354
C	5.1319323	-5.1135740	-6.2999801
H	3.9915387	-5.2515171	-4.4808631
H	0.3585583	-4.4210094	-3.5782178
H	-1.4058986	-4.3882585	-3.3092809
C	-2.1102994	-5.5784817	-5.5271582
N	-3.2414504	-5.8357817	-5.7356344
C	5.2716493	-0.7920369	9.2546170
C	6.6087252	-0.6654082	9.6358842
C	7.5463898	-0.1456315	8.7403097
C	7.1384705	0.2446134	7.4629074

C	5.8001019	0.1172400	7.0863470
C	-6.1806832	5.2257498	2.8406756
C	-7.1434508	6.2242392	2.6850430
C	-8.1248922	6.4113280	3.6620480
C	-8.1364067	5.5944218	4.7943484
C	-7.1719561	4.5955376	4.9468401
C	6.0589781	2.3386290	3.6540288
C	7.3882578	2.7605404	3.7149531
C	8.2825983	2.4115502	2.6992250
C	7.8380322	1.6403645	1.6235581
C	6.5070561	1.2201851	1.5657204
C	-6.7138306	2.2935400	-2.9417603
C	-7.8246205	2.9834495	-3.4301864
C	-8.6221274	3.7350634	-2.5631643
C	-8.3016377	3.7920683	-1.2051826
C	-7.1894666	3.1005484	-0.7195252
C	-6.6599566	-4.6987988	-5.9015182
C	-7.8432596	-4.9445155	-6.5997437
C	-8.9701038	-4.1436275	-6.3889301
C	-8.9063257	-3.0911970	-5.4735128
C	-7.7209809	-2.8442473	-4.7752306
C	6.1963678	0.6785108	-2.7638498
C	7.4654462	1.0257396	-3.2310087
C	8.1032065	0.2282890	-4.1850235
C	7.4626008	-0.9148168	-4.6682112
C	6.1928963	-1.2585137	-4.1987772
C	5.4585372	-4.2527318	-7.3599470
C	6.6308075	-4.4312149	-8.0977029
C	7.5017628	-5.4800002	-7.7905584
C	7.1891826	-6.3467500	-6.7404408
C	6.0159012	-6.1628282	-6.0053752
H	5.4928718	0.4196998	6.0828743
H	7.8621729	0.6452483	6.7515727
H	8.5921770	-0.0505134	9.0352700
H	6.9197924	-0.9782628	10.6337089
H	4.5450465	-1.2066516	9.9574013
H	-7.1873010	3.9568447	5.8329189
H	-8.8998291	5.7324637	5.5615005
H	-8.8787745	7.1901827	3.5398379
H	-7.1270381	6.8562685	1.7960295
H	-5.4136390	5.0855777	2.0754675
H	5.3635225	2.6202505	4.4484234
H	7.7254691	3.3661105	4.5577315
H	9.3215649	2.7405839	2.7461699
H	8.5264407	1.3623817	0.8241832
H	6.1683438	0.6154935	0.7215048
H	-6.0923842	1.7087863	-3.6237304
H	-8.0685608	2.9308861	-4.4921639
H	-9.4917664	4.2718765	-2.9448829
H	-8.9187913	4.3736819	-0.5184191
H	-6.9477798	3.1469698	0.3451033
H	5.7001615	1.3099048	-2.0226155
H	7.9558454	1.9232284	-2.8500140
H	9.0951966	0.4977321	-4.5506992
H	7.9485991	-1.5455730	-5.4140960

H	5.6997158	-2.1539691	-4.5829781
H	5.7787576	-6.8420407	-5.1830826
H	7.8626781	-7.1688370	-6.4910515
H	8.4187691	-5.6200995	-8.3652180
H	6.8643807	-3.7478552	-8.9161282
H	4.7803371	-3.4318793	-7.6034836
H	-5.7747034	-5.3212644	-6.0623278
H	-7.8850776	-5.7691427	-7.3135006
H	-9.8942214	-4.3399714	-6.9355097
H	-9.7802019	-2.4601280	-5.3009605
H	-7.6752928	-2.0205841	-4.0580747

β-methoxy-CA monomer

20

C	-3.9721206	0.2794397	-1.5284511
C	-2.8678723	-0.2195138	-0.9434443
C	-1.6439101	0.6536957	-0.8289057
O	-1.5868398	1.7957287	-1.2351906
O	-0.6380256	-0.0059251	-0.2203611
C	-2.8268050	-1.5532423	-0.4301095
H	-3.9521849	1.3022503	-1.9043264
H	-4.8787140	-0.3131721	-1.6335402
N	-2.8017383	-2.6419432	-0.0141607
C	0.5917028	0.7427194	-0.0589441
C	1.5736444	-0.1850638	0.6335929
H	0.9621726	1.0574954	-1.0441549
H	0.3974503	1.6432782	0.5395132
H	1.1695090	-0.5065375	1.6132770
H	1.7333517	-1.0952971	0.0233722
O	2.7784997	0.5411315	0.7919269
C	3.7837575	-0.2281587	1.4328796
H	4.6741630	0.4062764	1.5122747
H	4.0342717	-1.1328436	0.8488946
H	3.4696880	-0.5403180	2.4458574

poly(β-methoxy-CA)$_1$

22

C	-3.6727953	0.2046388	-1.4460505
C	-2.4238964	-0.3456074	-0.8423140
C	-1.2981653	0.5130718	-0.7069195
O	-1.1979992	1.7046081	-1.0359143
O	-0.1862207	-0.1386013	-0.1232051
C	-2.3918962	-1.6884565	-0.4292989
H	-3.3998853	1.0517842	-2.0979265
H	-4.1980134	-0.5558487	-2.0445828
N	-2.4116036	-2.8218427	-0.1085055
C	0.9606719	0.6829731	0.0351604
C	2.0240018	-0.2099044	0.6502328
H	1.3029099	1.0876025	-0.9317705
H	0.7509772	1.5455272	0.6899666

H	1.6669595	-0.6155370	1.6166869
H	2.2279940	-1.0706522	-0.0156614
O	3.2138104	0.5574894	0.8454386
C	4.2435864	-0.2176001	1.4139195
H	5.1208341	0.4324837	1.5355745
H	4.5196962	-1.0744005	0.7671438
H	3.9565568	-0.6210134	2.4056466
O	-4.6704969	0.6677902	-0.4757948
H	-4.1370258	0.9114951	0.2981741

poly(β-methoxy-CA)$_2$

42

C	-0.1391504	-0.8417730	1.0524365
C	-0.1875859	-2.2714016	1.6701630
H	0.7078682	-2.8114497	1.3390789
H	-1.0798349	-2.7789754	1.2589767
C	1.1678388	-0.1260180	1.4250753
O	1.2520327	0.9321194	2.0078806
O	2.2214602	-0.8519086	0.9881657
C	3.5162366	-0.2226520	1.1227491
H	3.4387677	0.8325313	0.8328992
C	4.4559250	-0.9749208	0.1986085
H	4.1529963	-0.7916631	-0.8475602
H	4.4057892	-2.0640262	0.4019918
C	-1.2654824	-0.1180142	1.6429429
H	3.8456471	-0.2832712	2.1711832
N	-2.1962839	0.3082705	2.1991167
O	-0.1778269	-2.3003553	3.0901778
H	-0.9082180	-1.7308989	3.3926344
C	0.0727372	0.1879558	-1.3913451
C	-0.2666876	-0.9927669	-0.5295291
H	-1.2997519	-1.3206410	-0.7139271
H	0.4010235	-1.8330188	-0.7760906
C	-0.8936928	1.1493159	-1.8060856
O	-0.7543693	2.1319826	-2.5364358
O	-2.1705178	0.8494400	-1.2634947
C	-3.1806257	1.8034947	-1.5722208
H	-2.8451133	2.8225824	-1.3257629
C	-4.3911324	1.4158813	-0.7408471
H	-4.1394466	1.4528314	0.3352191
H	-4.6996011	0.3773838	-0.9764282
C	1.3826132	0.2908124	-1.8798171
H	-3.4246521	1.7914476	-2.6479010
N	2.4995922	0.3073412	-2.2571384
O	5.7727820	-0.4866031	0.4496232
C	6.6913298	-0.9545081	-0.5171917
H	7.6717678	-0.5247544	-0.2722759
H	6.4013886	-0.6422513	-1.5370221
H	6.7727903	-2.0598514	-0.5032263
O	-5.4544677	2.3216401	-1.0408065
C	-6.6001555	2.0510016	-0.2654519
H	-7.3690794	2.7849300	-0.5426597
H	-6.3929897	2.1388361	0.8189742

H	-6.9939212	1.0319249	-0.4546794

poly(β-methoxy-CA)$_3$

62

C	-0.9180312	-0.3549352	2.6611624
C	-1.3173942	-1.6433473	3.4700043
H	-0.6391537	-2.4512084	3.1671355
H	-2.3478863	-1.9110741	3.1755018
C	0.5241961	0.0291646	3.0672791
O	0.8230962	0.9871522	3.7401903
O	1.3869701	-0.9021335	2.6057802
C	2.7880080	-0.6150536	2.8341461
H	2.9823382	0.4374823	2.5940717
C	3.5669138	-1.5441060	1.9211563
H	3.3754977	-1.2748802	0.8660120
H	3.2434905	-2.5937474	2.0730344
C	-1.8332947	0.6943659	3.1239361
H	3.0304657	-0.7972450	3.8910858
N	-2.6231989	1.4194820	3.5758436
O	-1.1832759	-1.5054144	4.8689047
H	-1.7483179	-0.7647274	5.1522829
C	-0.8517654	0.3665003	0.0575203
C	-1.0961712	-0.7002131	1.1576608
H	-2.1277535	-1.0519451	1.0200890
H	-0.4267769	-1.5466413	0.9486782
C	-1.8474684	1.5369973	0.1171745
O	-1.5461840	2.7077693	0.0860612
O	-3.1106919	1.0544210	0.1611575
C	-4.1675925	2.0414149	0.0788569
H	-4.3450661	2.4541025	1.0831193
C	-5.3903136	1.3181758	-0.4554719
H	-5.5984648	0.4121558	0.1497675
H	-5.2004252	1.0152280	-1.5005049
C	0.5097690	0.8922570	0.1427255
H	-3.8581260	2.8464723	-0.5981376
N	1.6201469	1.2277528	0.2357373
C	-1.1255104	0.3678528	-2.6107897
C	-1.0518036	-0.4169185	-1.3444385
H	-0.2215686	-1.1358851	-1.3874779
H	-1.9863472	-0.9792888	-1.1905173
C	-0.0076606	0.5696255	-3.4736290
O	0.0396197	1.1566731	-4.5546711
O	1.1627534	-0.0345102	-2.9458808
C	2.3417237	0.1938658	-3.7096335
H	2.3420252	-0.4109672	-4.6328719
C	3.5047724	-0.1971714	-2.8139446
H	3.3962006	-1.2508690	-2.4844080
H	3.5120805	0.4389463	-1.9090755
C	-2.3868172	0.8294770	-3.0175155
H	2.4129503	1.2495728	-4.0102693
N	-3.4815386	1.1703232	-3.2891696
O	4.9421669	-1.3945395	2.2434045

C	5.7714444	-2.1328103	1.3655961
H	6.8092248	-1.9622135	1.6781544
H	5.6503863	-1.8019455	0.3174787
H	5.5539054	-3.2172587	1.4158564
O	-6.4852890	2.2269570	-0.3741646
C	-7.6204647	1.7347060	-1.0569405
H	-8.4106442	2.4915648	-0.9655806
H	-7.4061552	1.5599888	-2.1272013
H	-7.9834689	0.7848666	-0.6158869
O	4.7179580	-0.0399764	-3.5501917
C	5.8473864	-0.3361080	-2.7615799
H	6.7381544	-0.1833751	-3.3857289
H	5.8371398	-1.3874733	-2.4073128
H	5.9138362	0.3226690	-1.8735717

poly(β-methoxy-CA)$_4$

82

C	-0.1942018	-0.2793410	4.0640649
C	-0.4632466	-1.5926322	4.8927533
H	0.3090053	-2.3229105	4.6190453
H	-1.4506649	-1.9818213	4.5854632
C	1.1897533	0.2687230	4.4934834
O	1.3609250	1.2594757	5.1619685
O	2.1535356	-0.5642632	4.0487633
C	3.5223573	-0.1359715	4.2747948
H	3.5874575	0.9498253	4.1360606
C	4.3745053	-0.8753943	3.2579175
H	4.0882564	-0.5575849	2.2386694
H	4.2075617	-1.9692056	3.3367905
C	-1.2422591	0.6599649	4.4753807
H	3.8118671	-0.3884038	5.3047993
N	-2.1412470	1.2844563	4.8696947
O	-0.3716841	-1.4112879	6.2869060
H	-1.0407210	-0.7563803	6.5539812
C	-0.1235521	0.3803751	1.4321421
C	-0.2908742	-0.6811548	2.5692438
H	-1.2739718	-1.1453743	2.4102026
H	0.4737777	-1.4523558	2.4072829
C	-1.2383411	1.4599279	1.5170230
O	-1.0403302	2.6316219	1.7282422
O	-2.4439127	0.8782578	1.3468876
C	-3.5773869	1.7853962	1.3203181
H	-3.8581400	2.0301561	2.3546236
C	-4.6913054	1.0539818	0.5934762
H	-4.8751777	0.0654448	1.0613804
H	-4.3987274	0.8876835	-0.4597831
C	1.1709901	1.0613291	1.5564439
H	-3.2901660	2.7022240	0.7920829
N	2.2181458	1.5514621	1.6751224
C	0.0041984	0.1913979	-1.2811408
C	-0.1941289	-0.4573998	0.1112603
H	0.5687886	-1.2432464	0.1899732
H	-1.1778546	-0.9478595	0.1087637

C	1.4153873	0.7563268	-1.5019802
O	1.6673189	1.8378462	-1.9782604
O	2.3307989	-0.1714536	-1.1340805
C	3.7129432	0.1659853	-1.3962237
H	3.7842945	0.6711962	-2.3667245
C	4.4772640	-1.1458795	-1.3979868
H	4.2327752	-1.7065363	-2.3172469
H	4.1870218	-1.7596148	-0.5203910
C	-0.9878406	1.2383886	-1.5112585
H	4.0695906	0.8412880	-0.6038112
N	-1.8456676	2.0135857	-1.6454341
C	0.1954205	-0.8411977	-3.7565160
C	-0.2240745	-1.0248378	-2.3391847
H	-1.2978116	-1.2506758	-2.2795556
H	0.3320358	-1.8602669	-1.8853097
C	-0.7024940	-0.4467740	-4.7940064
O	-0.4796937	-0.3027904	-5.9955617
O	-2.0060909	-0.2292187	-4.2838876
C	-2.9460651	0.2503403	-5.2399435
H	-2.5115415	1.0642306	-5.8389730
C	-4.1419336	0.7398868	-4.4411009
H	-3.8332959	1.5610373	-3.7676409
H	-4.5409490	-0.0806100	-3.8099862
C	1.5190503	-1.1693401	-4.0883963
H	-3.2452653	-0.5489302	-5.9393394
N	2.6414304	-1.4746936	-4.2766739
O	5.7271881	-0.5525307	3.5296711
C	6.6004574	-1.0601642	2.5310122
H	7.6160869	-0.7491416	2.8045582
H	6.3538906	-0.6607163	1.5309331
H	6.5627539	-2.1656295	2.4873934
O	-5.8512297	1.8681790	0.6765729
C	-6.9186777	1.3438926	-0.0909455
H	-7.7674509	2.0297793	0.0220123
H	-6.6517574	1.2714729	-1.1616713
H	-7.2189179	0.3384756	0.2623117
O	5.8675819	-0.8311692	-1.3387729
C	6.6705400	-1.9639851	-1.6080274
H	7.7183609	-1.6388429	-1.5676232
H	6.4577037	-2.3820800	-2.6085153
H	6.5146086	-2.7645495	-0.8576048
O	-5.1458039	1.1854368	-5.3527070
C	-6.2665211	1.7085718	-4.6765620
H	-6.9880396	2.0390154	-5.4357444
H	-5.9956745	2.5718085	-4.0379026
H	-6.7509386	0.9457684	-4.0329965

poly(β-methoxy-CA)$_5$

102

C	-0.7318225	0.9631771	5.1404892
C	-1.2188786	-0.2081145	6.0774256
H	-0.5418074	-1.0586205	5.9261952
H	-2.2345165	-0.4943396	5.7501206

C	0.6867330	1.3754250	5.6070169
O	0.9517015	2.4085374	6.1717721
O	1.5537251	0.3787837	5.3284422
C	2.9491642	0.6489049	5.6264413
H	3.1734940	1.6951271	5.3868196
C	3.7634556	-0.3019353	4.7665184
H	3.5943735	-0.0672004	3.6991188
H	3.4476774	-1.3504508	4.9428884
C	-1.6658111	2.0677716	5.3796880
H	3.1263952	0.4769678	6.6974682
N	-2.4931593	2.8427641	5.6408006
O	-1.1679282	0.1090819	7.4478665
H	-1.7694481	0.8563222	7.6134553
C	-0.4316567	1.3257469	2.4704474
C	-0.7996823	0.4170109	3.6910924
H	-1.8264224	0.0682632	3.5135622
H	-0.1367659	-0.4580832	3.6590091
C	-1.3918023	2.5482814	2.3826477
O	-1.0402684	3.6969849	2.4912145
O	-2.6507551	2.1090823	2.1879628
C	-3.6647775	3.1343612	1.9891208
H	-4.0238194	3.4635377	2.9742160
C	-4.7678184	2.4906146	1.1666404
H	-5.1408959	1.5738954	1.6679546
H	-4.3665089	2.2021358	0.1776629
C	0.9425625	1.8221815	2.6058256
H	-3.2168888	3.9835338	1.4601820
N	2.0516684	2.1463523	2.7300882
C	-0.2411677	0.8446318	-0.2172226
C	-0.5641414	0.3730245	1.2375103
H	0.0866522	-0.4916341	1.4237344
H	-1.6032477	0.0183743	1.2389556
C	1.2485631	1.2617080	-0.3609325
O	1.6260052	2.3534807	-0.7067755
O	2.0382541	0.2194370	-0.0229715
C	3.4638446	0.4499573	-0.1630139
H	3.6518677	0.9583514	-1.1162922
C	4.1173530	-0.9196671	-0.1185571
H	3.8741208	-1.4810420	-1.0395584
H	3.7351122	-1.4994974	0.7464864
C	-1.0776238	1.9938427	-0.5818408
H	3.8030078	1.0870246	0.6664618
N	-1.7900938	2.8771076	-0.8327962
C	-0.4480738	-0.3923067	-2.6392604
C	-0.5913217	-0.4053319	-1.0974131
H	-1.6406871	-0.6560423	-0.8923880
H	0.0286340	-1.2308937	-0.7196154
C	-1.3872350	0.6055957	-3.3340607
O	-1.0618709	1.3853127	-4.1978984
O	-2.6445737	0.4346254	-2.8618652
C	-3.6762229	1.2229624	-3.5005739
H	-3.6675130	2.2345536	-3.0675765
C	-4.9879405	0.5099166	-3.2231267
H	-5.0476434	0.2228835	-2.1529346
H	-5.0407598	-0.4064905	-3.8369879

C	0.9345010	-0.1285402	-3.0299390
H	-3.4719467	1.2826055	-4.5761452
N	2.0650363	0.0221773	-3.2616415
C	-1.0922027	-2.1695299	-4.5471529
C	-0.8682360	-1.8944528	-3.1009941
H	-0.0744784	-2.5428799	-2.7048303
H	-1.7906759	-2.0842289	-2.5292955
C	-0.1004076	-2.7502153	-5.3940435
O	-0.1822738	-3.0578585	-6.5824066
O	1.1022886	-2.9854175	-4.6811740
C	2.1776486	-3.4842608	-5.4695216
H	2.0413351	-4.5559778	-5.6955348
C	3.4351745	-3.2672234	-4.6447030
H	3.3354550	-3.7663391	-3.6588521
H	3.5801654	-2.1865531	-4.4596432
C	-2.3780258	-1.9337268	-5.0582439
H	2.2359631	-2.9511793	-6.4297069
N	-3.4857069	-1.7131432	-5.3936371
O	5.1242319	-0.1207364	5.1155932
C	5.9912240	-0.8408328	4.2531357
H	7.0167927	-0.6360905	4.5830496
H	5.8053355	-1.9303110	4.3109620
H	5.8772681	-0.5188779	3.2019079
O	-5.8037724	3.4473076	1.0336401
C	-6.8068129	3.0155403	0.1259840
H	-7.5546127	3.8158301	0.0694723
H	-6.3932648	2.8327226	-0.8822145
H	-7.2984231	2.0887436	0.4791126
O	5.5188693	-0.7191512	-0.0025965
C	6.2386504	-1.9302220	-0.1468266
H	7.3044847	-1.6874085	-0.0548909
H	6.0566996	-2.3943279	-1.1337200
H	5.9663419	-2.6625065	0.6378513
O	-6.0429666	1.4125269	-3.5488612
C	-7.2980943	0.7611341	-3.5719091
H	-8.0502081	1.5109110	-3.8499283
H	-7.3140317	-0.0611649	-4.3100407
H	-7.5600424	0.3415444	-2.5800738
O	4.5469402	-3.8114231	-5.3550891
C	5.7597336	-3.5865638	-4.6730171
H	6.5665416	-4.0224532	-5.2772922
H	5.7639313	-4.0673329	-3.6731580
H	5.9587554	-2.5060979	-4.5332663

poly(β-methoxy-CA)$_6$

122

C	-0.3435669	1.1804709	6.3417215
C	-0.7549987	-0.0618371	7.2208824
H	-0.0876598	-0.8920806	6.9536919
H	-1.7911843	-0.3325048	6.9476024
C	1.0999129	1.5718554	6.7454797
O	1.3912173	2.5152966	7.4378657

O	1.9552401	0.6572980	6.2393660
C	3.3715272	0.9314874	6.4019515
H	3.5397739	2.0137994	6.3463167
C	4.0744626	0.2007764	5.2701732
H	3.7558445	0.6329375	4.3022683
H	3.7924336	-0.8724507	5.2731182
C	-1.2737419	2.2541435	6.6986930
H	3.6986306	0.5624291	7.3840464
N	-2.0977154	3.0059082	7.0282568
O	-0.6005451	0.1492652	8.6030086
H	-1.1787827	0.8845097	8.8719997
C	-0.2208379	1.7712065	3.7170355
C	-0.4817483	0.7422632	4.8652971
H	-1.5002885	0.3608285	4.7105807
H	0.2174132	-0.0921240	4.7264329
C	-1.3563960	2.8348429	3.6565094
O	-1.1949783	4.0191130	3.8070735
O	-2.5232880	2.2044337	3.4044734
C	-3.6817092	3.0452463	3.1467287
H	-4.2070438	3.2150991	4.0966546
C	-4.5403982	2.2853563	2.1490546
H	-4.7792525	1.2732312	2.5366279
H	-3.9770729	2.1669968	1.2048314
C	1.0589212	2.4608873	3.9081773
H	-3.3485969	4.0055163	2.7359896
N	2.1042449	2.9463572	4.0551530
C	0.0963832	1.5247178	1.0266999
C	-0.1850782	0.8968089	2.4269041
H	0.5896498	0.1328147	2.5727048
H	-1.1577621	0.3903352	2.3739604
C	1.5263858	2.1324805	0.9576833
O	1.7743354	3.2803291	0.6912531
O	2.4150229	1.1562560	1.2375916
C	3.8206801	1.4915635	1.0970064
H	3.9400514	2.2276744	0.2934518
C	4.5217169	0.1852032	0.7678746
H	4.2005784	-0.1595971	-0.2320933
H	4.2410144	-0.5956222	1.5059540
C	-0.8825951	2.5688821	0.7115081
H	4.1728584	1.9239061	2.0448342
N	-1.7135928	3.3457951	0.4753538
C	0.1521548	0.4613345	-1.4834293
C	-0.0544306	0.3119750	0.0535946
H	-1.0691529	-0.0866965	0.1839286
H	0.6567717	-0.4479190	0.4029727
C	-0.8805374	1.4470204	-2.0915251
O	-0.6059931	2.4604916	-2.6830099
O	-2.1225508	0.9883681	-1.8272615
C	-3.2125175	1.7641082	-2.3838721
H	-3.3511793	2.6697045	-1.7754457
C	-4.4277907	0.8572035	-2.3265206
H	-4.5260306	0.4173015	-1.3122639
H	-4.3088518	0.0272941	-3.0480918
C	1.5016979	0.9538601	-1.7785382
H	-2.9638596	2.0469044	-3.4140421

N	2.5942086	1.3055672	-1.9594149
C	0.1207751	-1.3264903	-3.5205705
C	-0.0427762	-0.9948328	-2.0207509
H	0.6732860	-1.6339085	-1.4871260
H	-1.0550286	-1.3019859	-1.7230918
C	1.5432373	-1.0714517	-4.0397333
O	1.8291974	-0.4825255	-5.0541522
C	-0.8476344	-0.5796414	-4.3186507
N	-1.6837463	0.0137034	-4.8687026
C	-0.1712268	-2.9146410	-3.6290311
C	0.1274030	-3.5932595	-4.9203466
C	-0.8645323	-3.7955832	-5.9253307
O	-0.7639333	-4.3295008	-7.0284058
C	1.4359376	-4.0634587	-5.1041695
N	2.5585368	-4.4192758	-5.1478411
H	-1.2306767	-3.0320476	-3.3625246
H	0.4416027	-3.3429360	-2.8203463
O	-2.1150664	-3.2852673	-5.4914077
C	-3.1443229	-3.2759594	-6.4735742
C	-4.2180944	-2.3540926	-5.9200886
H	-2.7628230	-2.9056115	-7.4369137
H	-3.5459923	-4.2895779	-6.6438762
H	-3.8042466	-1.3361200	-5.7963138
H	-4.5414639	-2.7107202	-4.9198652
O	2.4222815	-1.6590217	-3.1939694
C	3.8121447	-1.6128986	-3.5846638
C	4.5004605	-2.6933689	-2.7708878
H	4.1634067	-2.6440366	-1.7142086
H	4.2295413	-3.6834601	-3.1789141
H	3.8935684	-1.8071683	-4.6610641
H	4.2144240	-0.6146489	-3.3541445
O	5.4655066	0.3591336	5.4700808
C	6.2245758	-0.1810880	4.3957320
H	7.2820078	-0.0304280	4.6435807
H	6.0352837	-1.2649162	4.2744544
H	6.0052851	0.3246589	3.4385031
O	-5.7201413	3.0404836	1.9464019
C	-6.4916686	2.5376666	0.8641428
H	-7.3815483	3.1731802	0.7816696
H	-5.9338609	2.5735940	-0.0890111
H	-6.8125302	1.4938600	1.0471234
O	5.9167933	0.4289344	0.8003581
C	6.6557640	-0.6747338	0.2900179
H	6.4922024	-1.5841602	0.9003837
H	7.7163625	-0.3997661	0.3379205
H	6.3834285	-0.8985844	-0.7567841
O	-5.5653667	1.6474302	-2.6389749
C	-6.7382062	0.8601709	-2.7547751
H	-7.5627223	1.5407249	-3.0003176
H	-6.9719235	0.3371449	-1.8069217
H	-6.6411920	0.1040300	-3.5553006
O	5.9058747	-2.4667575	-2.8491586
C	6.6410643	-3.5552618	-2.3236235
H	7.7061593	-3.3111093	-2.4286452
H	6.4269534	-4.4911781	-2.8711516

H	6.4155143	-3.7219851	-1.2510378
O	-5.3273824	-2.3433158	-6.8178690
C	-6.3296033	-1.4494564	-6.3895849
H	-7.1392561	-1.4759689	-7.1311207
H	-6.7434905	-1.7393015	-5.4010746
H	-5.9495264	-0.4118377	-6.3091817

poly(β-methoxy-CA)$_7$

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C	-0.9142312	1.0773053	7.2233994
C	-1.0610879	-0.3449822	7.8902643
H	-0.1504088	-0.9137898	7.6628903
H	-1.9257518	-0.8464688	7.4194877
C	0.2821342	1.7916044	7.9006179
O	0.1865874	2.7430531	8.6365167
O	1.4251808	1.1531237	7.5738085
C	2.6479814	1.7518874	8.0812274
H	2.5814653	2.8425165	7.9879789
C	3.7819183	1.1936189	7.2398407
H	3.6540015	1.5160057	6.1891180
H	3.7728286	0.0848600	7.2632939
C	-2.1542801	1.7905890	7.5442331
H	2.7634626	1.4869197	9.1414248
N	-3.1927682	2.2249977	7.8372685
O	-1.1664978	-0.2972967	9.2919023
H	-1.9861915	0.1721832	9.5264332
C	-0.5904922	2.0315479	4.7076413
C	-0.7405652	0.8305655	5.7025096
H	-1.6104676	0.2535721	5.3588745
H	0.1502470	0.1980004	5.5888611
C	-1.8269653	2.9750106	4.7904051
O	-1.7782610	4.1207432	5.1636808
O	-2.9276795	2.3020941	4.4042554
C	-4.1648244	3.0710106	4.3807596
H	-4.5711140	3.1044031	5.4010298
C	-5.0974965	2.3550488	3.4197314
H	-5.2394513	1.2992408	3.7286945
H	-4.6553943	2.3587032	2.4050985
C	0.6090004	2.8107854	5.0362634
H	-3.9465835	4.0899350	4.0402721
N	1.5966736	3.3658585	5.2949052
C	-0.2004857	2.1886339	2.0086151
C	-0.4465413	1.3514432	3.3080444
H	0.3894882	0.6424869	3.3742559
H	-1.3685064	0.7751036	3.1550505
C	1.1480565	2.9628490	2.0719183
O	1.2557284	4.1562095	1.9428627
O	2.1522804	2.0908332	2.2965127
C	3.4781233	2.6835717	2.3751779
H	3.6348168	3.3261373	1.5001613
C	4.4584790	1.5249444	2.4062466
H	4.4580952	1.0017869	1.4309067
H	4.1619706	0.7928489	3.1852959

C	-1.2872353	3.1557571	1.8160468
H	3.5388640	3.2884637	3.2905197
N	-2.1981579	3.8654185	1.6866840
C	0.0095221	1.4870778	-0.6309776
C	-0.2054208	1.1099834	0.8726332
H	-1.1769309	0.6002887	0.9206422
H	0.5727771	0.3816394	1.1382519
C	-1.0682913	2.4998245	-1.1156896
O	-0.8294944	3.6030412	-1.5378811
O	-2.2843735	1.9374864	-0.9687216
C	-3.4184034	2.7196399	-1.4365027
H	-3.6742371	3.4579579	-0.6636011
C	-4.5439364	1.7260576	-1.6679588
H	-4.6898929	1.0947187	-0.7666720
H	-4.2823940	1.0607109	-2.5112443
C	1.3464300	2.0628390	-0.8161313
H	-3.1394860	3.2369098	-2.3619352
N	2.4423972	2.4383873	-0.9097871
C	0.0215369	-0.0163537	-2.9262427
C	-0.1026651	0.1115471	-1.3725575
H	0.6682535	-0.5491766	-0.9530016
H	-1.0837334	-0.2986813	-1.0994394
C	1.4216679	0.4410257	-3.4225465
O	1.6116342	1.3728869	-4.1644868
C	-0.9912967	0.8075576	-3.5966006
N	-1.8336830	1.4406019	-4.0867535
C	-0.2386782	-1.5404419	-3.1886595
C	-0.2992477	-2.1288710	-4.6191674
C	-1.4798056	-1.6056147	-5.4507353
O	-1.4137669	-1.2338068	-6.5983342
C	0.9534138	-1.8922888	-5.3313757
N	2.0011621	-1.7214295	-5.8086391
H	-1.2025965	-1.7849884	-2.7228458
H	0.5441434	-2.0855497	-2.6423579
O	-2.6131388	-1.6823748	-4.7135641
C	-3.8384212	-1.3323826	-5.3989748
C	-4.9672285	-1.9493329	-4.5921847
H	-3.9219692	-0.2358011	-5.4380895
H	-3.8096311	-1.7337931	-6.4188776
H	-4.8202838	-1.7456963	-3.5111771
H	-4.9692102	-3.0425538	-4.7475654
O	2.3710782	-0.3500136	-2.8801787
C	3.7297205	-0.0884829	-3.3209411
C	4.5119172	-1.3653167	-3.0710253
H	4.3810003	-1.7002870	-2.0214564
H	4.1370201	-2.1649551	-3.7360972
H	3.7170258	0.1712852	-4.3859379
H	4.1313769	0.7555013	-2.7422449
C	-0.5103907	-3.7291988	-4.3922222
C	-0.9344101	-4.5754186	-5.5409286
C	-0.0192718	-5.3295648	-6.3366205
O	1.3152744	-5.1253433	-5.9080567
O	-0.2561047	-6.0914177	-7.2728757
C	2.3006826	-5.7838392	-6.6976967
C	3.6332357	-5.1740449	-6.2971494

H	2.1041861	-5.6347272	-7.7696143
H	2.2982529	-6.8712793	-6.5110158
H	3.6341895	-4.0911410	-6.5219496
H	3.7931784	-5.2906526	-5.2054351
H	0.4466253	-4.0821645	-3.9834253
H	-1.2669122	-3.7708659	-3.5924322
C	-2.3121935	-4.7042712	-5.7760405
N	-3.4832908	-4.7590105	-5.8928311
O	4.9884510	1.6994784	7.7806576
C	6.1087364	1.3743403	6.9730631
H	6.9921755	1.8060577	7.4581380
H	6.2429908	0.2791280	6.8894055
H	6.0099395	1.7977317	5.9565707
O	-6.3271512	3.0549302	3.4373468
C	-7.2270404	2.5725200	2.4519235
H	-8.1432395	3.1692208	2.5328923
H	-6.8105615	2.6855813	1.4340860
H	-7.4748800	1.5069919	2.6168636
O	5.7376983	2.0657537	2.6881731
C	6.7626333	1.0929160	2.5763427
H	7.7113307	1.5959759	2.7982856
H	6.8078807	0.6692455	1.5564962
H	6.6161916	0.2635855	3.2945807
O	-5.7155958	2.4693565	-1.9537433
C	-6.7748793	1.6335106	-2.3982813
H	-7.6268012	2.2868084	-2.6222201
H	-6.4962095	1.0722220	-3.3080672
H	-7.0726828	0.9093874	-1.6155088
O	5.8769096	-1.0803238	-3.3363046
C	6.6769107	-2.2476654	-3.2967924
H	7.7074248	-1.9426062	-3.5168893
H	6.3502371	-2.9894270	-4.0488109
H	6.6486943	-2.7273994	-2.2991945
O	-6.1861394	-1.3603228	-5.0411669
C	-7.3147621	-2.0576886	-4.5508468
H	-8.2064895	-1.5615575	-4.9555680
H	-7.3088252	-3.1146493	-4.8730057
H	-7.3624173	-2.0331691	-3.4437382
O	4.6711985	-5.8393585	-7.0153743
C	5.9360628	-5.2836311	-6.7361768
H	6.6789821	-5.8349608	-7.3278641
H	5.9834054	-4.2112558	-7.0085104
H	6.1969647	-5.3756970	-5.6618219