

Thermodynamic and Kinetic Considerations in the Copolymerization of Ethylene and Carbon Dioxide

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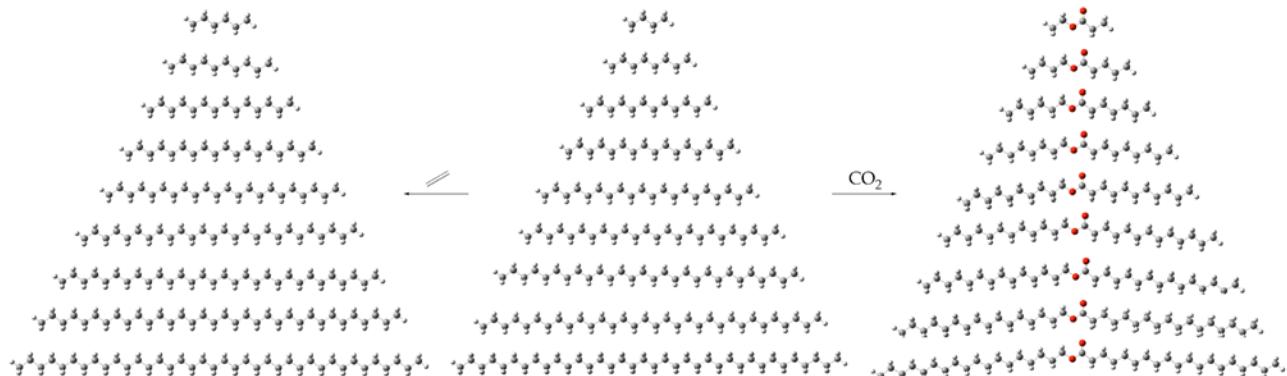
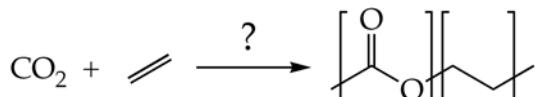
College Station, Texas 77843-3255

Supporting Information

Supporting Information Available: Theoretical and synthetic details, DFT optimized structures, as well as additional characterization data (^{13}C NMR, GC-MS) for the formed oligomers and polymers.

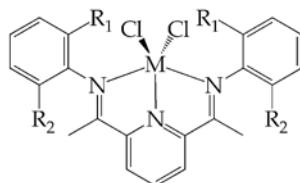
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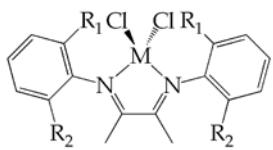


General Considerations and Instrumentation. All air-sensitive procedures were performed under a purified nitrogen atmosphere in a glove box or by using standard Schlenk line and vacuum line techniques. 2,6-Diisopropyl aniline (Acros, 92%) was distilled at 145°C under dynamic vacuum before use. Methylaluminoxane (MAO) (Albemarle, 30% in toluene) was concentrated to dryness and used as a solid. Ethanol was distilled from magnesium sulfate into an oven-dried Straus flask and stored until use. Tetrahydrofuran was distilled from sodium/benzophenone under a nitrogen atmosphere and stored in an oven-dried Straus flask until use. All other chemicals and solvents were used as received.

Precatalyst Synthesis. Precatalysts **1 - 5** and the ligand for precatalyst **6** were prepared according to the following modified literature procedures.



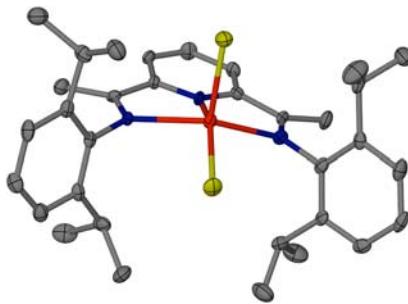
- 1: M = Fe, R₁ = R₂ = iPr
- 2: M = Fe, R₁ = R₂ = Me
- 3: M = Co, R₁ = iPr, R₂ = H
- 4: M = Fe, R₁ = Me, R₂ = H



- 5: M = Ni, R₁ = R₂ = iPr
- 6: M = Cu, R₁ = iPr, R₂ = H

Synthesis of N,N'-bis-(2,6-diisopropylaniline) diacetylpyridine [204203-14-5] (CJP-I-48). In a 50 mL round bottom flask, 2.00 g (12.25 mmol) of 2,6-diacetylpyridine and 5.43 g (30.46 mmol, 2.5 eq.) of 2,6-diisopropylaniline were dissolved in 25 mL of dry ethanol. Five drops of glacial acetic acid were added. The mixture refluxed for 18 hours in an oil bath. The heat was turned off and the mixture was allowed to slowly cool to room temperature in the oil bath. The mixture was cooled in an ice bath for 30 minutes and then filtered to yield 3.103 g (52.6 %) of a yellow powder, which was triturated in ethyl acetate. MS (ESI) *m/z* 482.3 (M+H)⁺

Synthesis of 1 [204203-10-1] or [308359-85-5] (CJP-I-49).¹ Inside the glove box, 2.00 g (4.15 mmol) of *N,N'*-bis-(2,6-diisopropylaniline) diacetylpyridine and 0.52 g (4.15 mmol) of FeCl₂·4H₂O were combined in a 200 mL round bottom flask and a swivel frit apparatus was attached. The frit was evacuated and 75 mL of dry ethanol were condensed in. The frit was back-filled with nitrogen and the blue solution was refluxed for 30 minutes. The frit was flipped and all soluble material was washed to the lower collection flask. The solution was condensed to approximately half of its original volume and placed in an ice-water bath for 30 minutes. The frit was again flipped to collect 0.658 g (26.0 %) of a dark blue crystalline solid. The filtrate was concentrated to dryness and redissolved in dichloromethane. The second crop was purified by the same recrystallization method to yield 0.744 g (29.5 %). The total yield of first and second crops is 1.402 g (55.5 %). Blue needle-like crystals suitable for X-ray diffraction can be grown by vapor diffusion of hexanes into a saturated dichloromethane solution. The molecule cocrystallizes with 0.5 molecules of H₂O. The X-ray data, shown below, are identical to that previously reported.²



Crystal data: triclinic, *P*-1, *a* = 8.6390(10) Å, *b* = 9.8363(10) Å, *c* = 20.714(2) Å, α = 83.513(6)°, β = 88.300(7)°, γ = 65.758(6)°, *V* = 1594.5(3) Å³, *Z* = 2, *T* = 110(2) K, *R*₁ (on F₀) = 0.0500, *wR*₂ (on F₀²) = 0.1195, GOF = 1.012 for 366 parameters and 4244 unique data.

Synthesis of N,N'-bis-(2,6-dimethylaniline) diacetylpyridine [204203-16-7] (BJR-II-14). A 50 mL round bottom flask was charged with 2,6-diacetylpyridine (3.00 g, 18.39 mmol), 2,6-dimethylaniline, and 30 mL of ethanol. When the mixture was perceived to be homogeneous, 4 drops of glacial acetic acid were added. The mixture was stirred overnight. The solution was concentrated to 15 mL and the product was isolated by filtration and washed with 15 mL of cold ethanol. The product was recrystallized in ethanol and dried *in vacuo* to yield 4.34 g (64.0 %) of yellow crystals.

Synthesis of 2 [207129-93-9] (BJR-II-18).¹ In the glove box a 100 mL pear shaped flask was charged with *N,N'*-bis-(2,6-dimethylaniline) diacetylpyridine (3.70 g, 10 mmol) and FeCl₂ (1.90 g, 15 mmol). The flask was attached to a swivel frit and connected to a high vacuum line and evacuated. 20 mL of dry ethanol were vacuum transferred into the vessel. The frit was opened to N₂ and the solution was heated at reflux for 15 minutes. The frit was allowed to cool to room temperature and the frit was flipped. The frit was evacuated and refluxing ethanol was used to extract excess FeCl₂ from the reaction solids. After 10-15 mL of ethanol had washed the material, solvent was removed by high vacuum and the purple powder was dried *in vacuo* to yield 4.74 g (96.0 %).

Synthesis of N,N'-bis-(2-isopropylaniline) diacetylpyridine [210537-34-1] (BJR-II-75). 2,6-diacetyl pyridine (3.00 g, 18.4 mmol) and 2-isopropylaniline (6.85 g, 45.9 mmol) were dissolved in 200 mL of toluene. *Para*-toluenesulfonic acid monohydrate (0.10 g) was added. A Dean-Stark trap was attached to the flask and the reaction was heated to reflux. After 16 hours 0.8 mL of water had come over and the heat source was removed. The solution was poured into a separatory funnel and the organic layer was rinsed with 100 mL of a dilute aqueous sodium bicarbonate solution (3 g/100 mL). The aqueous layer was rinsed with diethyl ether (2 x 100 mL) and all organics were combined and dried *in vacuo*. The yellow powder was triturated in refluxing ethanol, cooled to RT, and filtered to yield 6.44 g (88.0 %) of the desired product.

Synthesis of 3 [590367-46-7] (BJR-II-83).³ Inside the glove box *N,N'*-bis-(2-isopropylaniline) diacetylpyridine (3.10 g, 7.8 mmol) and CoCl₂ (1.00 g, 7.7 mmol) were combined in a flask and this was attached to a swivel frit.

The frit was brought into air and evacuated on a Schlenk line. THF (40mL) was vacuum transferred into the flask at liquid nitrogen temperatures and warmed to room temperature. The solution stirred for 16 hours at which time the THF was removed *in vacuo* and diethyl ether (40 mL) was vacuum transferred into the flask. The frit was flipped and gentle reflux of ether allowed for the extraction of the product. The solution was concentrated and the frit flipped again. The powder was collected on the frit and a positive pressure of nitrogen isolated the powder on the frit. The powder was dried *in vacuo* to yield 3.66 g (90.2 %) of the cobalt complex.

Synthesis of *N,N'*-bis-(2-methylaniline) diacetylpyridine [210537-32-9] (BJR-II-74). 2,6-diacetyl pyridine (3.00 g, 18.4 mmol) and *o*-toluidine (4.93 g, 45.9 mmol) were dissolved in 200 mL of toluene. *Para*-toluenesulfonic acid monohydrate (0.10 g) was added. A Dean-Stark trap was attached to the flask and the reaction was heated to reflux. After 16 hours 0.8 mL of water had come over and the heat source was removed. The solution was poured into a separatory funnel and the organic layer was rinsed with 100 mL of a dilute aqueous sodium bicarbonate solution (3 g/100 mL). The aqueous layer was rinsed with diethyl ether (2 x 100 mL) and all organics were combined and dried *in vacuo*. The yellow powder was recrystallized from hot ethanol and isolated by filtration to yield 3.41 g (54.3 %) of crystalline product.

Synthesis of 4 [210537-35-2] (BJR-II-76).⁴ Inside the glove box *N,N'*-bis-(2-methylaniline) diacetylpyridine (2.83 g, 8.29 mmol) and FeCl₂ (1.00 g, 7.89 mmol) were combined in a flask and this was attached to a swivel frit. The frit was brought into air and evacuated on a Schlenk line. THF (40 mL) was vacuum transferred into the flask at liquid nitrogen temperatures and warmed to room temperature. The solution stirred for 16 hours at which time the THF was removed *in vacuo* and hexanes (40 mL) were vacuum transferred into the flask. The frit was flipped and then gently refluxed to extract the product. Hexanes were removed *in vacuo* and diethyl ether (40 mL) was vacuum transferred into the flask. Gentle reflux of ether allowed for the full extraction of the product. Ether was removed and hexanes were again added and the solution concentrated. The frit was flipped again and the powder was collected on the frit. The powder was dried *in vacuo* to yield 2.94 g (79.6 %) of the iron complex.

Synthesis of *N,N'*-(butane-2,3-diylidene)-bis-(2,6-diisopropylaniline) [74663-77-7] (AKJ-I-97). 2,3-

butanedione (12.93 g, 0.16 mol) and 2,6-diisopropylaniline (53.19 g, 0.30 mol) were combined in methanol and allowed to shake for 36 hours. The solution was heated until all the material was in solution and then cooled to precipitate a crystalline solid, which was collected by filtration.

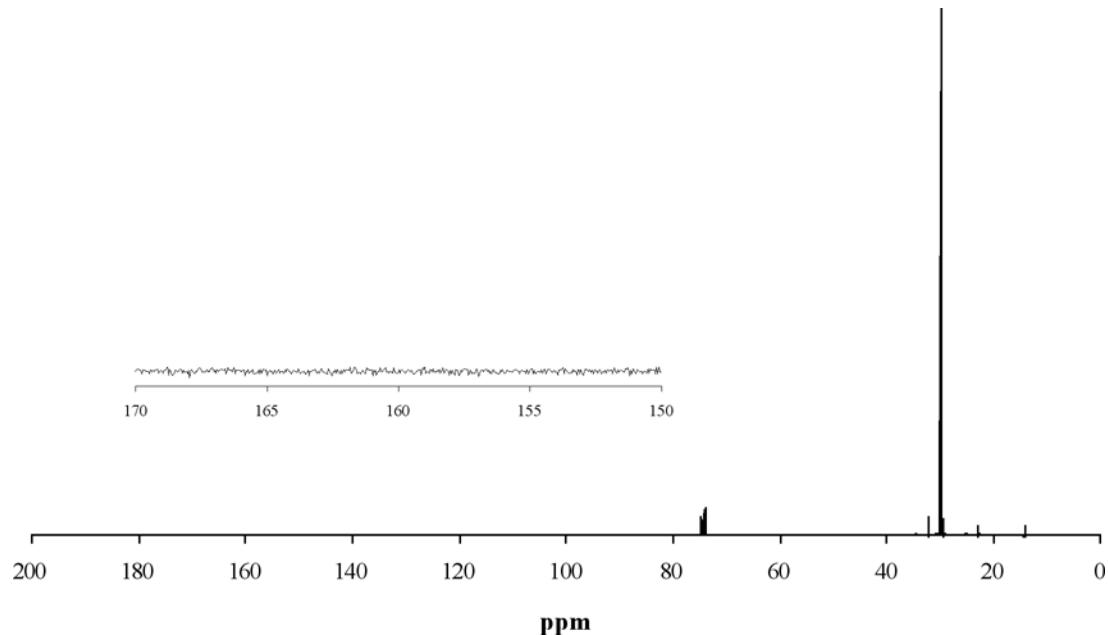
Synthesis of 5 [200879-37-4] (BJR-II-51).⁵ In the glove box a 100 mL pear shaped flask was charged with NiCl₂ (1.94 g, 15 mmol) and *N,N'*-(butane-2,3-diylidene)-bis-(2,6-diisopropylaniline) (4.05 g, 10 mmol). The flask was attached to a swivel frit and the frit was evacuated on the line. 40-50 mL of dry ethanol were vacuum transferred into the flask. The flask was exposed to the nitrogen line and the reaction was heated to reflux for 25 minutes. Heat was removed and after one hour, the frit was flipped. By refluxing the solvent, all of the material was extracted through the frit. The volume was concentrated under high vacuum and the frit was flipped. The solid was isolated on the frit and washed with ethanol. Solvent was removed under high vacuum and the product was dried to yield 1.60 g (29.9 %).

Synthesis of *N,N'*-(butane-2,3-diylidene)-bis-(2-isopropylaniline) [49673-33-8] (BJR-II-73).⁶ 2,3-butanedione (4.30 g, 50 mmol) and 2-isopropylaniline (13.52 g, 100 mmol) were combined in methanol and allowed to shake for 36 hours. The solution was heated until all the material was in solution and then precipitated out to yield 4.77 g in the first crop, 1.62 g in the second, 3.18 g in the third, and 1.47 g in the fourth for an overall yield of 11.04 g (68.9 %).

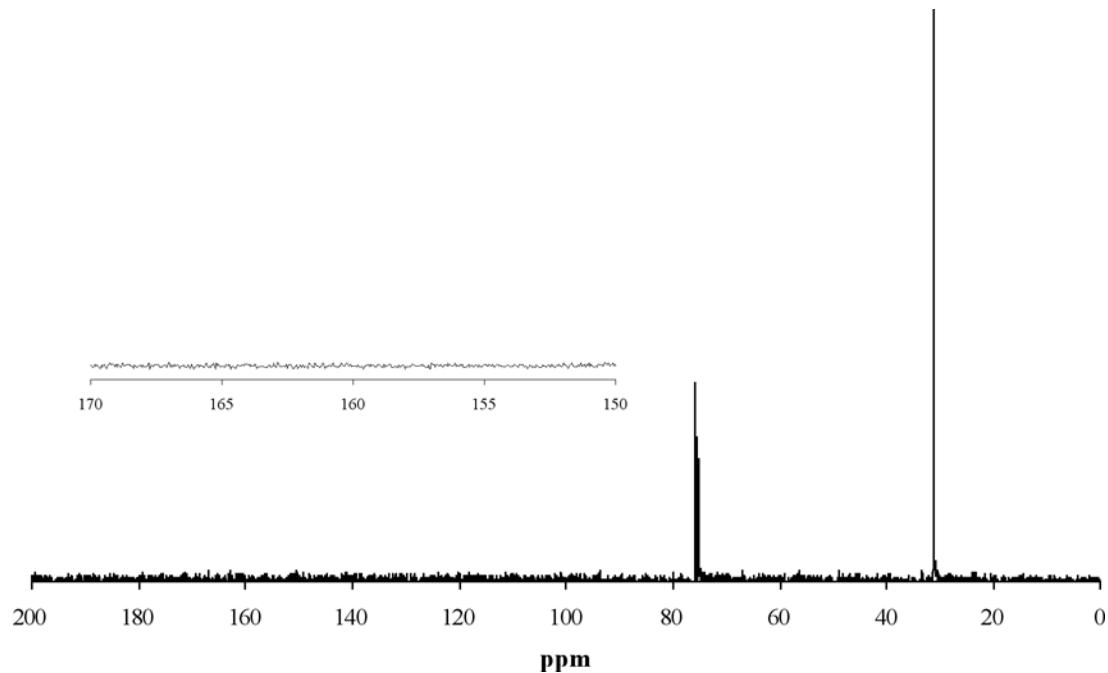
Synthesis of 6 (BJR-II-79). In air *N,N'*-(butane-2,3-diylidene)-bis-(2-isopropylaniline) (2.63 g, 8.2 mmol) was placed in a pear shaped flask and this was attached to a swivel frit. The frit was evacuated and taken into the glove box where CuCl₂ (1.00 g, 7.4 mmol) was added. The frit was brought onto the line and evacuated. 50 mL of THF were vacuum transferred into the flask and the reaction was allowed to stir at room temperature for 24 hours. THF was removed *in vacuo* and diethyl ether was vacuum transferred into the flask. The frit was flipped and gentle reflux allowed for extraction of the product. Solvent was removed *in vacuo* and hexanes (50 mL) were vacuum transferred into the flask and gentle reflux further extracted the product. The hexane solution was concentrated and the solid was collected and washed on the frit. *In vacuo* drying provided 2.79 g (82.9 %) of the product.

¹³C NMR Spectra

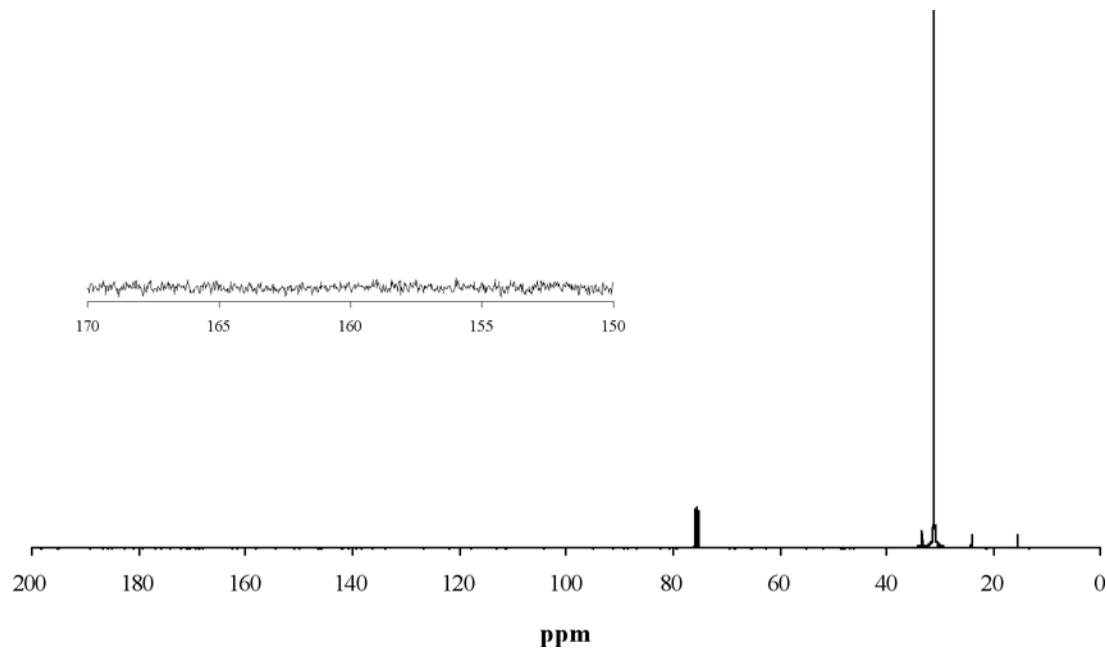
Polymer produced with **1**/MAO (Table 5, entry 1), showing the absence of carbonyl peaks:



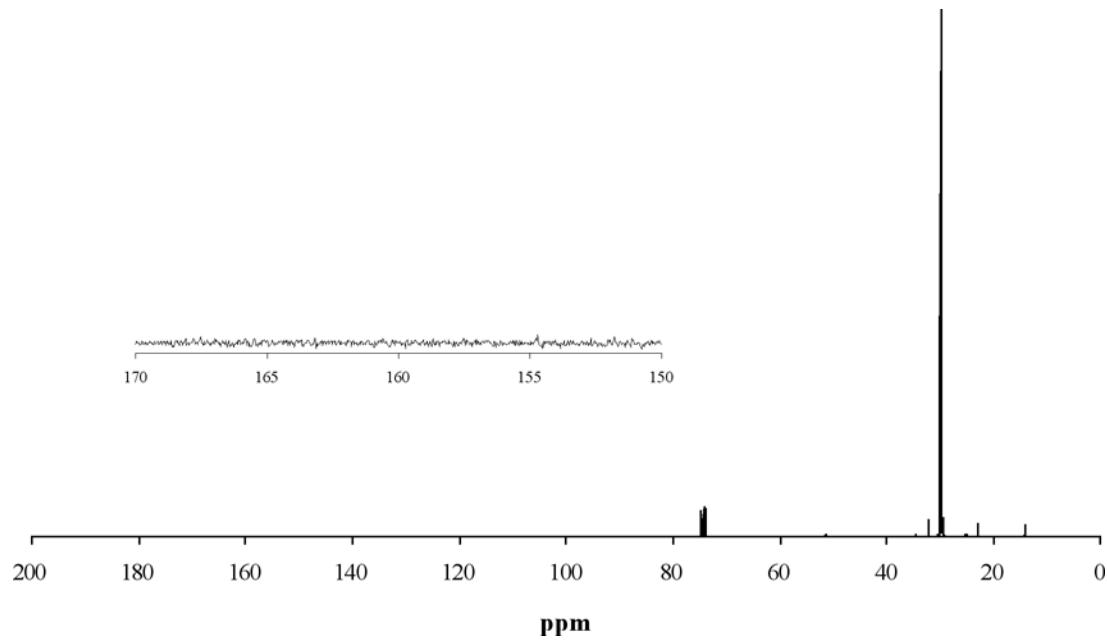
Polymer produced with **1**/MAO (Table 5, entry 2), showing the absence of carbonyl peaks:



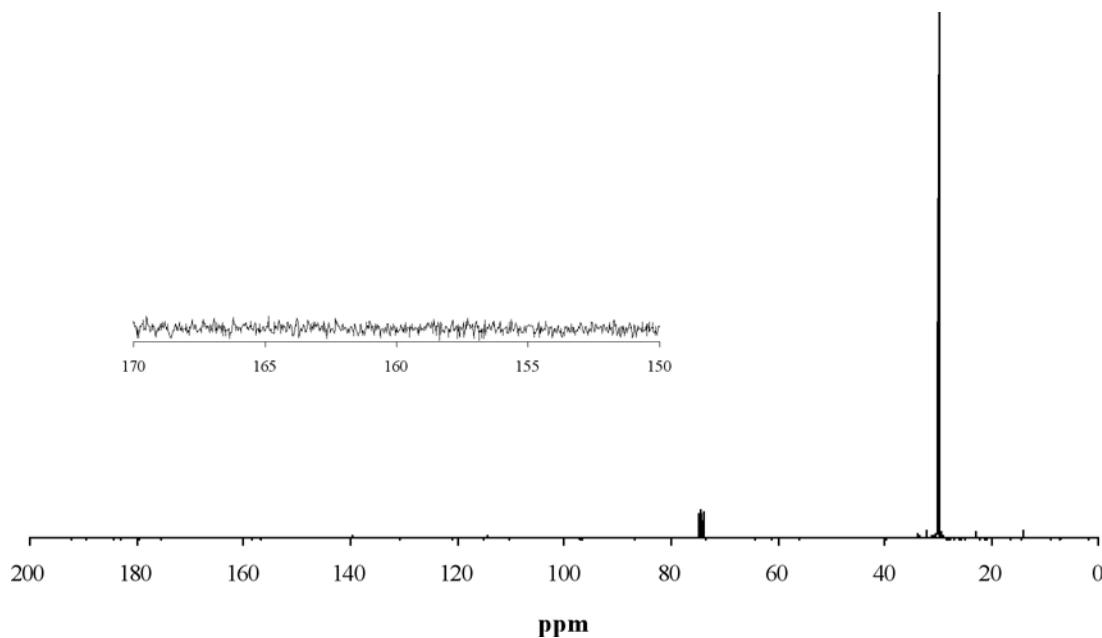
Polymer produced by the homopolymerization of ethylene with **1**/MAO (Table 5, entry 3) showing the necessary absence of carbonyl peaks:



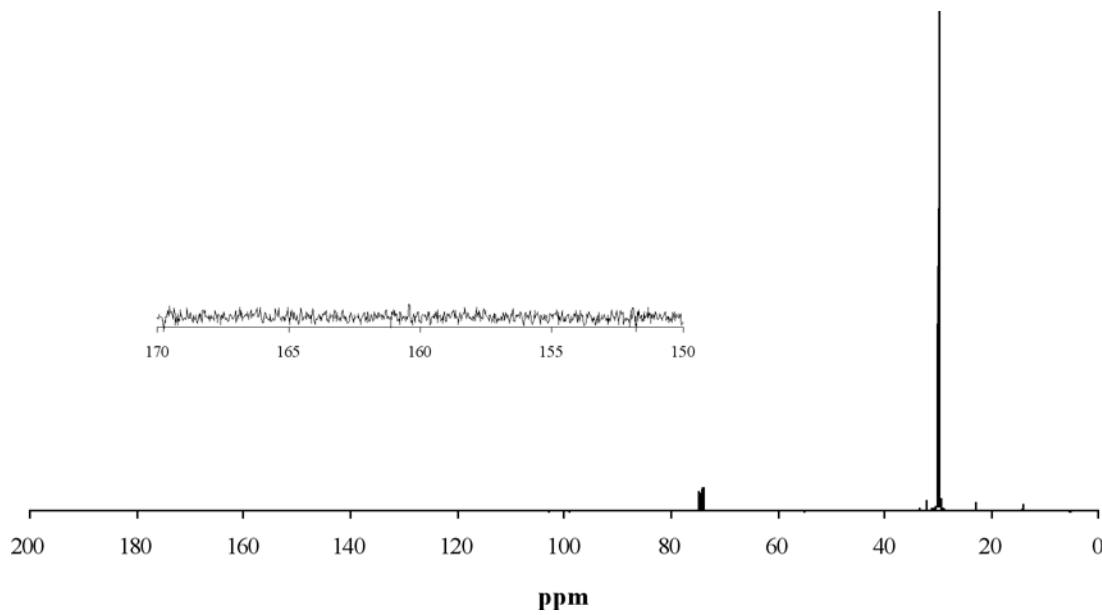
Polymer produced with **2**/MAO (Table 5, entry 4), showing the absence of carbonyl peaks:



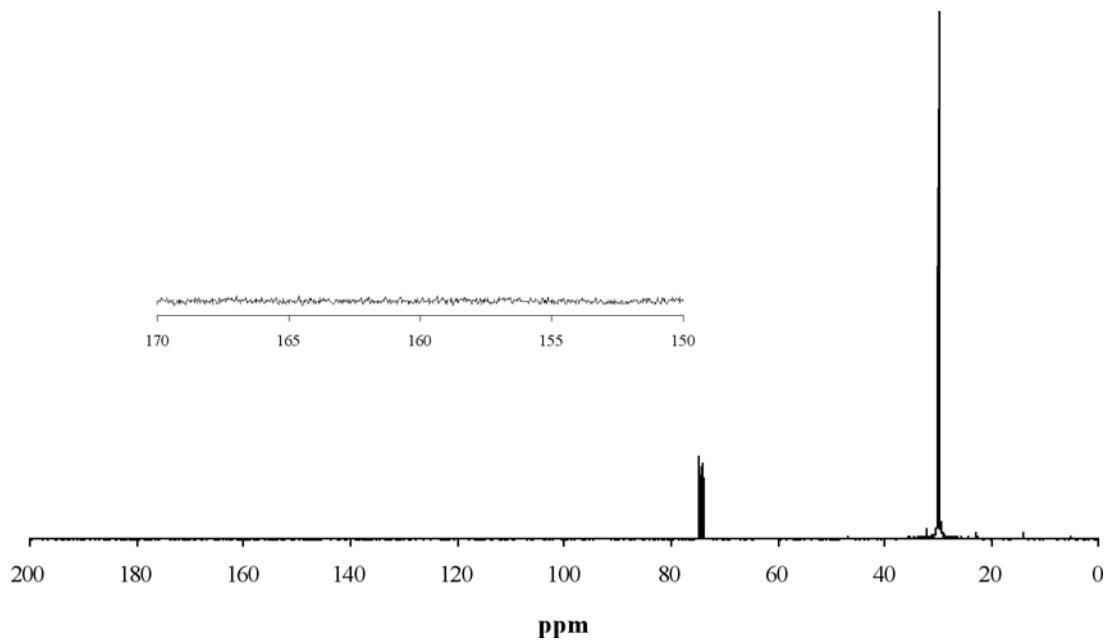
Polymer produced with **2**/MAO (Table 5, entry 5), showing the absence of carbonyl peaks:



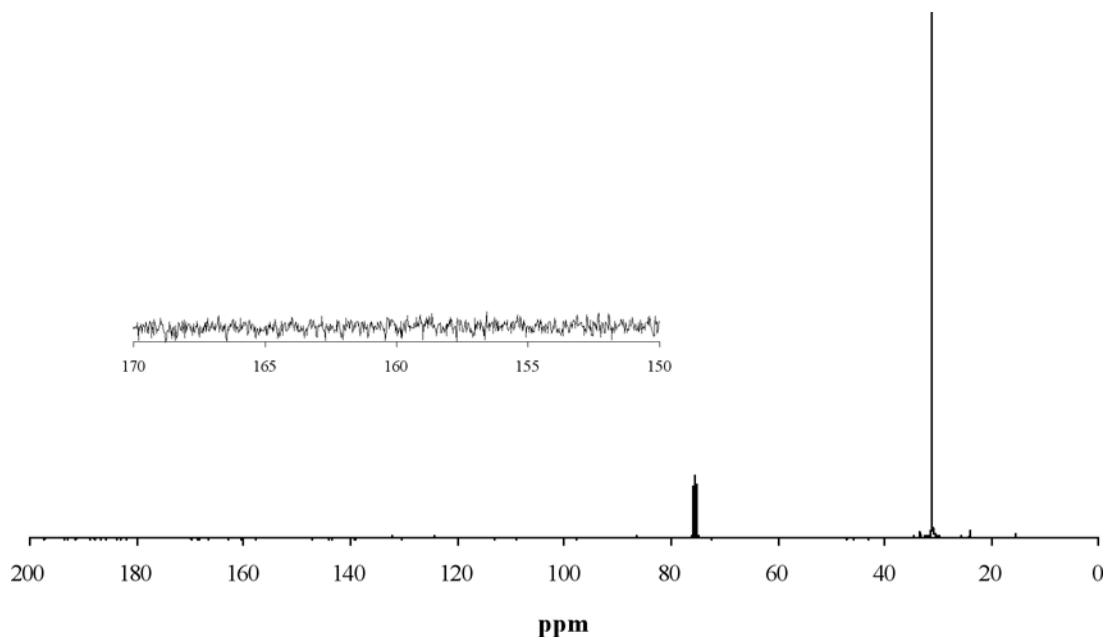
Polymer produced with **2**/MAO (Table 5, entry 6), showing the absence of carbonyl peaks:



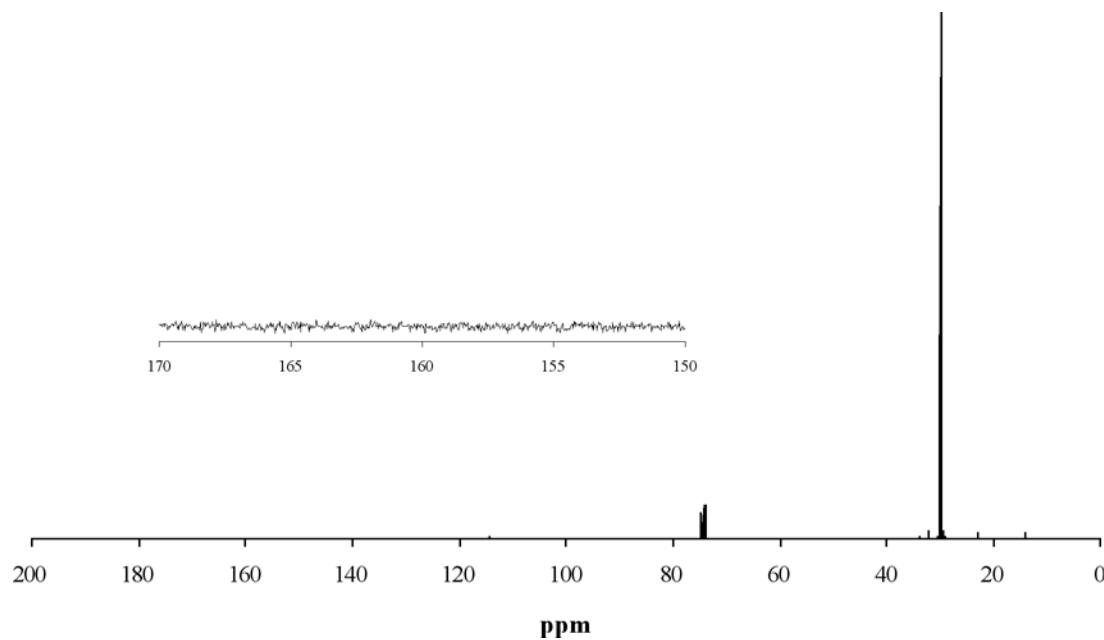
Polymer produced with **2**/MAO (Table 5, entry 7), showing the absence of carbonyl peaks:



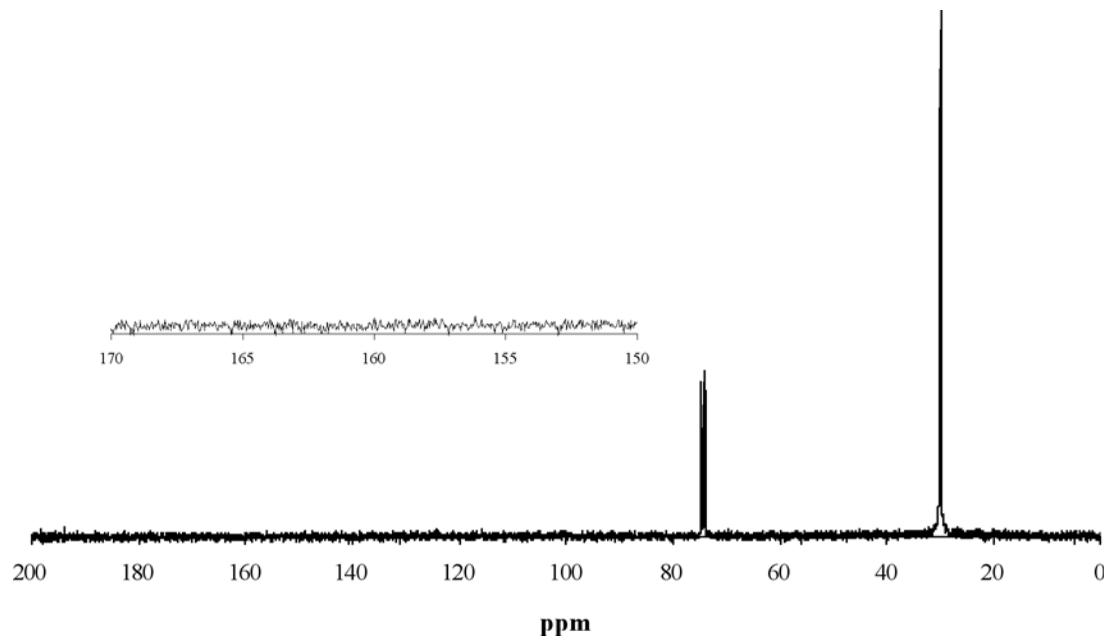
Polymer produced with **2**/MAO (Table 5, entry 8), showing the absence of carbonyl peaks:



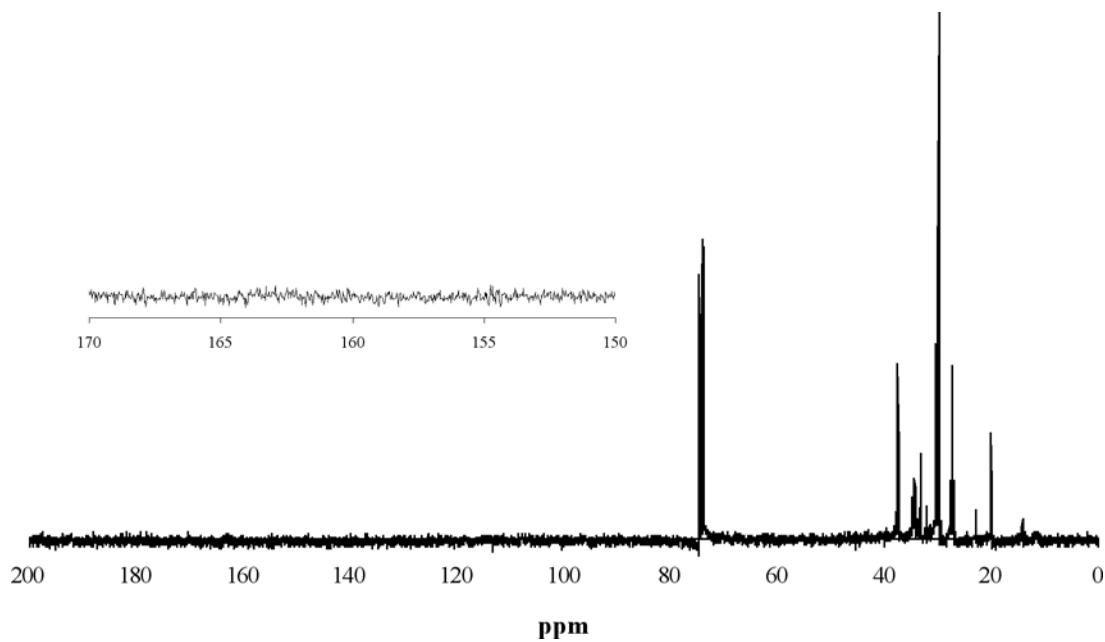
Polymer produced by the homopolymerization of ethylene with **2**/MAO (Table 5, entry 9), showing the necessary absence of carbonyl peaks:



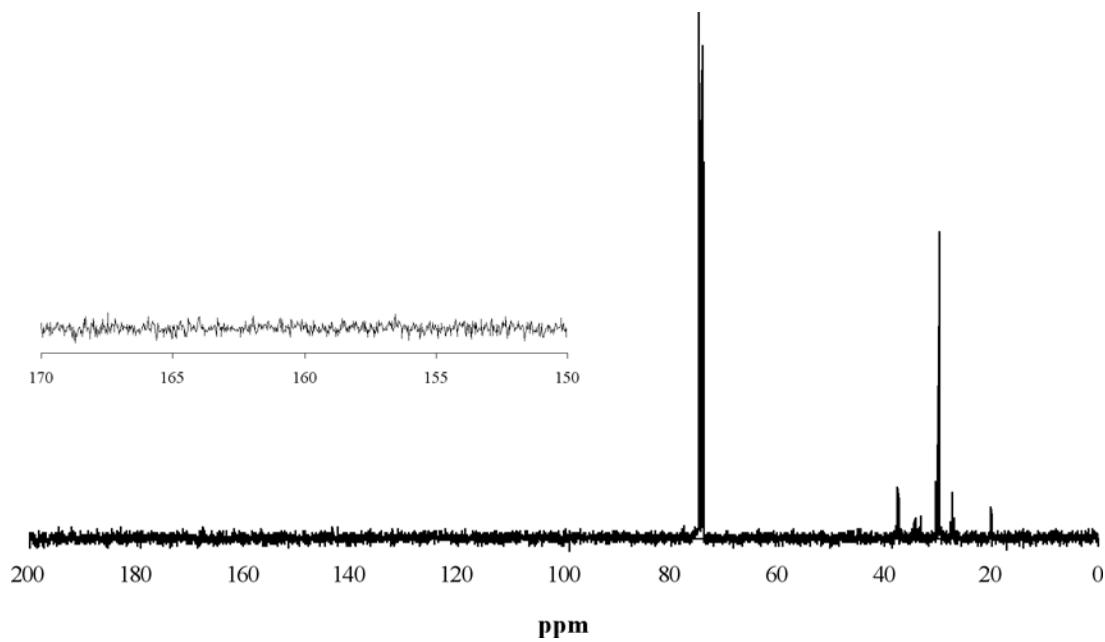
Polymer produced with **3**/MAO (Table 5, entry 10), showing the absence of carbonyl peaks:



Polymer produced with **5**/MAO (Table 5, entry 14), showing the absence of carbonyl peaks:

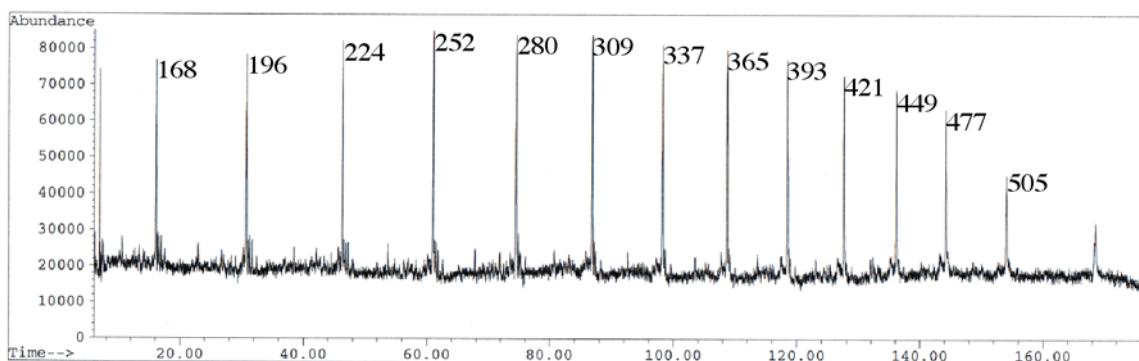


Polymer produced with **5**/MAO, (Table 5, entry 15), showing the absence of carbonyl peaks:

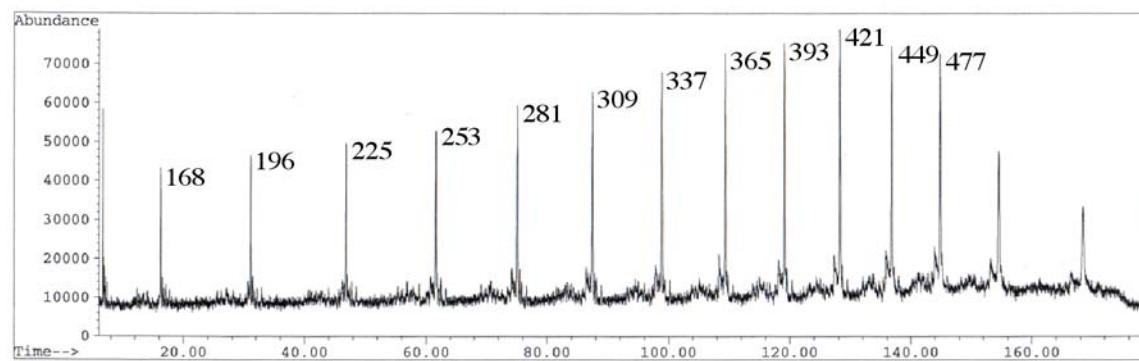


GC-MS Spectra

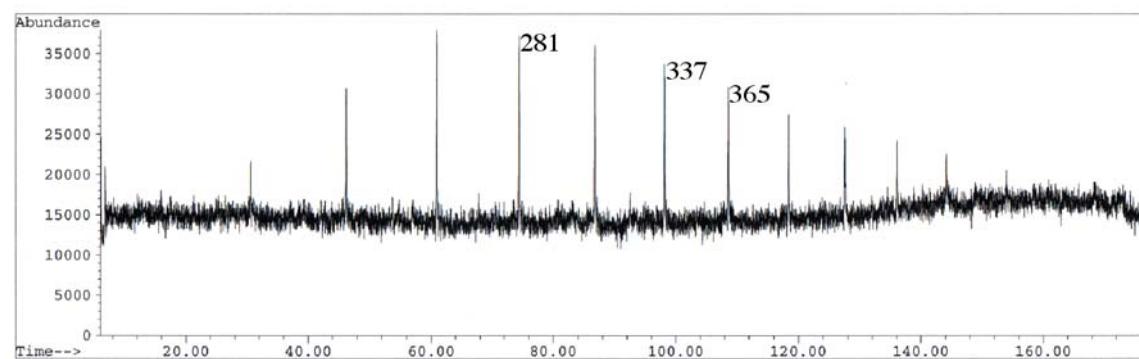
GC traces of oligomers produced with **4**/MAO, (Table 5, entry 12), with the representative masses for each peak:



GC traces of oligomers produced with **4**/MAO, (Table 5, entry 13), with the representative masses for each peak:



GC traces of oligomers produced with **6**/MAO, (Table 5, entry 16), with the representative masses for each peak:

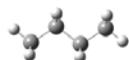


Computational Methods

All calculations were performed using the Gaussian 03 suite of programs.⁷ Optimized structure calculations and frequency calculations were performed using Density Function Theory (DFT) employing the Becke's 3-parameter hybrid functional (B3)⁸ with the correlation functional of Lee, Yang and Parr (LYP).^{9,10} The Pople style basis set, 6-31G(d') (= 6-31G \dagger) was used. The compounds are named in the following manner: XchainY where X is the total number of monomer units in the chain and Y is the number of CO₂ units in the chain.

DFT Structures and Coordinates

2chain0



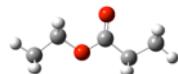
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H	-1.7255	-2.2399	0.0000
H	-0.1899	-2.2337	0.8854
H	-0.1899	-2.2337	-0.8854
H	-1.2565	0.0640	0.8788
H	-1.2565	0.0640	-0.8788
H	1.2565	-0.0640	-0.8788
H	1.2565	-0.0640	0.8788
H	1.7255	2.2399	0.0000
H	0.1899	2.2337	0.8854
H	0.1899	2.2337	-0.8854

3chain0



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C	0.0000	-0.7672	0.0000
C	0.0000	0.7672	0.0000
C	1.4059	1.3827	0.0000
C	1.3953	2.9156	0.0000
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H	-0.8779	-3.3094	0.8854
H	-0.8779	-3.3094	-0.8854
H	-1.9608	-1.0195	0.8785
H	-1.9608	-1.0195	-0.8785
H	0.5556	-1.1316	-0.8789
H	0.5556	-1.1316	0.8789
H	-0.5556	1.1316	0.8789
H	-0.5556	1.1316	-0.8789
H	1.9608	1.0195	-0.8785
H	1.9608	1.0195	0.8785
H	2.4136	3.3253	0.0000
H	0.8779	3.3094	0.8854
H	0.8779	3.3094	-0.8854

3chain1



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C	-1.8571	0.4317	0.0002
C	-3.0882	-0.4567	0.0002
O	0.6320	1.3935	-0.0004
H	3.8039	-0.9248	0.0003
H	3.1489	0.4719	0.8840
H	3.1498	0.4738	-0.8810
H	1.5011	-1.4735	0.8722
H	1.5021	-1.4715	-0.8752
H	-1.8158	1.0798	-0.8835
H	-1.8158	1.0797	0.8840
H	-3.9945	0.1613	0.0003
H	-3.1084	-1.0987	0.8886
H	-3.1085	-1.0985	-0.8883

4chain0



C	2.8131	-3.5239	0.0000
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C	1.4056	-1.3825	0.0000
C	-0.0001	-0.7673	0.0000
C	0.0001	0.7673	0.0000
C	-1.4056	1.3825	0.0000
C	-1.4056	2.9171	0.0000
C	-2.8131	3.5239	0.0000
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H	3.3822	-3.2092	-0.8854
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H	0.8498	-3.2795	-0.8784
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H	1.9625	-1.0196	0.8787
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H	-0.5563	-1.1310	-0.8787
H	0.5563	1.1310	-0.8787
H	0.5563	1.1310	0.8787
H	-1.9625	1.0196	0.8787
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H	-3.3822	3.2092	-0.8854

5chain0



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C	1.4064	1.3817	0.0000
C	0.0000	0.7673	0.0000
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C	-1.4062	-1.3818	0.0000
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H	3.8188	5.4753	0.0000
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H	2.2831	5.4587	-0.8854
H	3.3669	3.1692	0.8785
H	3.3669	3.1692	-0.8785
H	0.8504	3.2807	-0.8788
H	0.8504	3.2807	0.8788
H	1.9623	1.0181	0.8788
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H	-0.5559	1.1310	-0.8788
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H	0.5561	-1.1312	0.8788
H	0.5561	-1.1312	-0.8788
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H	-1.9621	-1.0182	0.8788
H	-0.8503	-3.2808	0.8788
H	-0.8503	-3.2808	-0.8788
H	-3.3668	-3.1689	-0.8785
H	-3.3668	-3.1689	0.8785
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H	-2.2836	-5.4587	0.8854
H	-2.2836	-5.4587	-0.8854

5chain1



C	-3.0480	0.1723	0.0001
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C	-0.5135	0.3986	-0.0001
O	0.6520	-0.2881	0.0001
C	1.8565	0.5104	0.0001
C	3.0449	-0.4396	0.0001
O	-0.5761	1.6062	-0.0002
C	-4.2398	-0.7930	-0.0002
C	-5.5926	-0.0723	0.0004
C	4.3865	0.3062	-0.0001
C	5.5927	-0.6396	0.0001

H	-3.1026	0.8347	-0.8748
H	-3.1025	0.8340	0.8754
H	-1.6004	-1.2103	-0.8743
H	-1.6003	-1.2110	0.8732
H	1.8517	1.1609	0.8840
H	1.8518	1.1609	-0.8837
H	2.9794	-1.0945	-0.8805
H	2.9796	-1.0943	0.8810
H	-4.1764	-1.4540	0.8780
H	-4.1767	-1.4531	-0.8792
H	-6.4264	-0.7858	-0.0001
H	-5.7015	0.5689	-0.8845
H	-5.7013	0.5677	0.8862
H	4.4383	0.9666	0.8786
H	4.4382	0.9662	-0.8791
H	6.5371	-0.0812	-0.0002
H	5.5885	-1.2891	-0.8854
H	5.5887	-1.2886	0.8859

6chain0



C	-4.2201	5.6727	0.0000
C	-2.8123	5.0664	0.0000
C	-2.8117	3.5318	0.0000
C	-1.4059	2.9170	0.0000
C	-1.4059	1.3823	0.0000
C	0.0002	0.7674	0.0000
C	-0.0002	-0.7674	0.0000
C	1.4059	-1.3823	0.0000
C	1.4059	-2.9170	0.0000
C	2.8117	-3.5318	0.0000
C	2.8123	-5.0664	0.0000
C	4.2201	-5.6727	0.0000
H	-4.1853	6.7698	0.0000
H	-4.7891	5.3580	0.8854
H	-4.7891	5.3580	-0.8854
H	-2.2570	5.4292	0.8785
H	-2.2570	5.4292	-0.8785
H	-3.3683	3.1688	-0.8788
H	-3.3683	3.1688	0.8788
H	-0.8500	3.2808	0.8788
H	-0.8500	3.2808	-0.8788
H	-1.9618	1.0186	-0.8788
H	-1.9618	1.0186	0.8788
H	0.5561	1.1310	0.8788
H	0.5561	1.1310	-0.8788
H	-0.5561	-1.1310	-0.8788
H	-0.5561	-1.1310	0.8788
H	1.9618	-1.0186	0.8788
H	1.9618	-1.0186	-0.8788
H	0.8500	-3.2808	-0.8788
H	0.8500	-3.2808	0.8788

H	3.3683	-3.1688	0.8788
H	3.3683	-3.1688	-0.8788
H	2.2570	-5.4292	-0.8785
H	2.2570	-5.4292	0.8785
H	4.1853	-6.7698	0.0000
H	4.7891	-5.3580	0.8854
H	4.7891	-5.3580	-0.8854

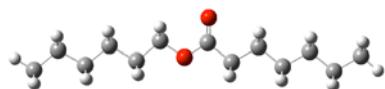
7chain0



C	-8.3458	-0.3237	-0.0005
C	-7.0580	0.5077	-0.0005
C	-5.7838	-0.3476	-0.0003
C	-4.4893	0.4765	-0.0003
C	-3.2155	-0.3796	-0.0001
C	-1.9209	0.4446	-0.0001
C	-0.6474	-0.4117	0.0000
C	0.6474	0.4123	0.0000
C	1.9208	-0.4442	0.0002
C	3.2156	0.3799	0.0001
C	4.4892	-0.4764	0.0003
C	5.7839	0.3474	0.0003
C	7.0579	-0.5082	0.0004
C	8.3459	0.3230	0.0004
H	-9.2378	0.3159	-0.0006
H	-8.4008	-0.9715	0.8850
H	-8.4007	-0.9717	-0.8858
H	-7.0494	1.1710	0.8780
H	-7.0493	1.1709	-0.8790
H	-5.7928	-1.0121	-0.8790
H	-5.7929	-1.0120	0.8785
H	-4.4812	1.1409	0.8784
H	-4.4811	1.1407	-0.8791
H	-3.2237	-1.0439	-0.8788
H	-3.2238	-1.0438	0.8787
H	-1.9127	1.1090	0.8786
H	-1.9126	1.1088	-0.8789
H	-0.6556	-1.0761	-0.8786
H	-0.6557	-1.0760	0.8788
H	0.6557	1.0766	0.8787
H	0.6558	1.0765	-0.8788
H	1.9125	-1.1085	-0.8785
H	1.9125	-1.1083	0.8790
H	3.2239	1.0443	0.8788
H	3.2240	1.0441	-0.8786
H	4.4810	-1.1408	-0.8784
H	4.4809	-1.1406	0.8791
H	5.7931	1.0120	0.8790
H	5.7931	1.0118	-0.8786
H	7.0492	-1.1715	-0.8780
H	7.0491	-1.1713	0.8789
H	9.2377	-0.3168	0.0005

H	8.4010	0.9710	0.8857
H	8.4010	0.9708	-0.8851

7chain1



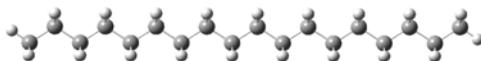
C	3.0550	0.3428	0.0000
C	1.7134	-0.3939	-0.0002
C	0.5186	0.5427	-0.0001
O	-0.6402	-0.1554	-0.0001
C	-1.8523	0.6316	0.0000
C	-3.0321	-0.3292	-0.0001
O	0.5692	1.7509	0.0000
C	4.2571	-0.6099	-0.0002
C	5.6073	0.1191	0.0001
C	-4.3795	0.4061	0.0000
C	-5.5857	-0.5425	0.0001
C	6.8158	-0.8264	0.0000
C	8.1604	-0.0903	0.0003
C	-6.9362	0.1859	0.0000
C	-8.1368	-0.7670	0.0002
H	3.1015	1.0052	0.8752
H	3.1016	1.0055	-0.8749
H	1.6218	-1.0557	0.8734
H	1.6219	-1.0554	-0.8740
H	-1.8536	1.2823	-0.8838
H	-1.8535	1.2822	0.8838
H	-2.9600	-0.9832	0.8806
H	-2.9601	-0.9831	-0.8808
H	4.2016	-1.2719	-0.8792
H	4.2015	-1.2724	0.8785
H	5.6632	0.7808	0.8790
H	5.6633	0.7813	-0.8783
H	-4.4370	1.0670	-0.8791
H	-4.4369	1.0670	0.8790
H	-5.5290	-1.2038	0.8791
H	-5.5290	-1.2040	-0.8788
H	6.7597	-1.4870	-0.8788
H	6.7596	-1.4875	0.8783
H	9.0031	-0.7934	0.0001
H	8.2624	0.5515	0.8859
H	8.2625	0.5520	-0.8849
H	-6.9919	0.8466	-0.8786
H	-6.9918	0.8468	0.8785
H	-9.0860	-0.2164	0.0001
H	-8.1289	-1.4168	0.8858
H	-8.1289	-1.4171	-0.8852

8chain0



C	5.6318	-7.8173	0.0000
C	4.2227	-7.2136	0.0000
C	4.2209	-5.6788	0.0000
C	2.8142	-5.0653	0.0000
C	2.8136	-3.5304	0.0000
C	1.4068	-2.9165	0.0000
C	1.4067	-1.3816	0.0000
C	0.0000	-0.7675	0.0000
C	0.0000	0.7675	0.0000
C	-1.4067	1.3816	0.0000
C	-1.4068	2.9165	0.0000
C	-2.8136	3.5304	0.0000
C	-2.8142	5.0653	0.0000
C	-4.2209	5.6788	0.0000
C	-4.2227	7.2136	0.0000
C	-5.6318	7.8173	0.0000
H	5.5995	-8.9145	0.0000
H	6.1998	-7.5009	0.8854
H	6.1998	-7.5009	-0.8854
H	3.6678	-7.5768	0.8785
H	3.6678	-7.5768	-0.8785
H	4.7771	-5.3154	-0.8788
H	4.7771	-5.3154	0.8788
H	2.2586	-5.4293	0.8788
H	2.2586	-5.4293	-0.8788
H	3.3692	-3.1665	-0.8788
H	3.3692	-3.1665	0.8788
H	0.8511	-3.2803	0.8788
H	0.8511	-3.2803	-0.8788
H	1.9624	-1.0178	-0.8788
H	1.9624	-1.0178	0.8788
H	-0.5557	-1.1312	0.8788
H	-0.5557	-1.1312	-0.8788
H	0.5557	1.1312	-0.8788
H	0.5557	1.1312	0.8788
H	-1.9624	1.0178	0.8788
H	-1.9624	1.0178	-0.8788
H	-0.8511	3.2803	-0.8788
H	-0.8511	3.2803	0.8788
H	-3.3692	3.1665	0.8788
H	-3.3692	3.1665	-0.8788
H	-2.2586	5.4293	-0.8788
H	-2.2586	5.4293	0.8788
H	-4.7771	5.3154	0.8788
H	-4.7771	5.3154	-0.8788
H	-3.6678	7.5768	-0.8785
H	-3.6678	7.5768	0.8785
H	-5.5995	8.9145	0.0000
H	-6.1998	7.5009	0.8854
H	-6.1998	7.5009	-0.8854

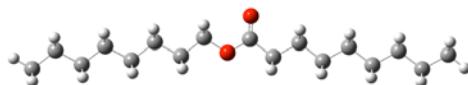
9chain0



C	10.9125	-0.3458	-0.0001
C	9.6289	0.4922	0.0002
C	8.3504	-0.3565	0.0003
C	7.0601	0.4741	0.0006
C	5.7821	-0.3755	0.0006
C	4.4916	0.4552	0.0008
C	3.2138	-0.3948	0.0008
C	1.9231	0.4355	0.0009
C	0.6454	-0.4147	0.0007
C	-0.6454	0.4155	0.0007
C	-1.9230	-0.4349	0.0004
C	-3.2138	0.3954	0.0003
C	-4.4915	-0.4548	-0.0002
C	-5.7821	0.3756	-0.0003
C	-7.0600	-0.4743	-0.0008
C	-8.3505	0.3561	-0.0011
C	-9.6288	-0.4929	-0.0016
C	-10.9126	0.3448	-0.0018
H	11.8077	0.2892	-0.0001
H	10.9639	-0.9939	-0.8856
H	10.9642	-0.9941	0.8853
H	9.6236	1.1556	-0.8782
H	9.6239	1.1554	0.8788
H	8.3562	-1.0211	0.8790
H	8.3560	-1.0209	-0.8785
H	7.0552	1.1386	-0.8781
H	7.0554	1.1384	0.8794
H	5.7870	-1.0399	0.8793
H	5.7869	-1.0397	-0.8782
H	4.4865	1.1196	-0.8779
H	4.4866	1.1194	0.8796
H	3.2189	-1.0592	0.8794
H	3.2188	-1.0591	-0.8780
H	1.9180	1.1000	-0.8778
H	1.9179	1.0997	0.8797
H	0.6505	-1.0792	0.8793
H	0.6506	-1.0790	-0.8781
H	-0.6505	1.0799	-0.8780
H	-0.6507	1.0796	0.8795
H	-1.9180	-1.0993	0.8790
H	-1.9177	-1.0991	-0.8784
H	-3.2188	1.0598	-0.8784
H	-3.2191	1.0595	0.8791
H	-4.4866	-1.1193	0.8785
H	-4.4862	-1.1190	-0.8790
H	-5.7869	1.0401	-0.8789
H	-5.7874	1.0398	0.8785
H	-7.0553	-1.1387	0.8778
H	-7.0548	-1.1384	-0.8797
H	-8.3561	1.0208	-0.8797

H	-8.3566	1.0205	0.8778
H	-9.6237	-1.1564	0.8768
H	-9.6232	-1.1560	-0.8802
H	-11.8076	-0.2905	-0.0022
H	-10.9641	0.9931	-0.8871
H	-10.9646	0.9928	0.8837

9chain1



C	3.0587	0.4736	0.0001
C	1.7197	-0.2677	-0.0002
C	0.5219	0.6651	-0.0002
O	-0.6348	-0.0363	0.0000
C	-1.8490	0.7476	0.0001
C	-3.0268	-0.2157	0.0001
O	0.5689	1.8735	-0.0003
C	4.2644	-0.4746	-0.0001
C	5.6115	0.2607	0.0001
C	-4.3753	0.5176	0.0002
C	-5.5805	-0.4327	-0.0001
C	6.8243	-0.6794	0.0000
C	8.1708	0.0565	0.0000
C	-6.9312	0.2955	0.0002
C	-8.1389	-0.6510	-0.0001
C	9.3847	-0.8822	0.0001
C	10.7256	-0.1393	0.0001
C	-9.4897	0.0774	0.0002
C	-10.6911	-0.8745	-0.0001
H	3.1028	1.1361	0.8752
H	3.1029	1.1365	-0.8748
H	1.6301	-0.9299	0.8733
H	1.6304	-0.9294	-0.8741
H	-1.8518	1.3983	-0.8837
H	-1.8518	1.3982	0.8839
H	-2.9535	-0.8695	0.8808
H	-2.9536	-0.8694	-0.8808
H	4.2116	-1.1368	-0.8790
H	4.2116	-1.1371	0.8787
H	5.6633	0.9228	0.8787
H	5.6633	0.9229	-0.8785
H	-4.4336	1.1785	-0.8787
H	-4.4337	1.1782	0.8793
H	-5.5222	-1.0940	0.8787
H	-5.5223	-1.0935	-0.8792
H	6.7719	-1.3416	-0.8788
H	6.7719	-1.3416	0.8789
H	8.2241	0.7189	0.8787
H	8.2241	0.7188	-0.8788
H	-6.9875	0.9576	-0.8784
H	-6.9875	0.9570	0.8793
H	-8.0836	-1.3134	0.8785
H	-8.0837	-1.3127	-0.8792

H	9.3320	-1.5435	-0.8784
H	9.3320	-1.5434	0.8786
H	11.5721	-0.8379	0.0002
H	10.8244	0.5033	0.8854
H	10.8245	0.5032	-0.8854
H	-9.5451	0.7387	-0.8780
H	-9.5450	0.7379	0.8790
H	-11.6403	-0.3236	0.0002
H	-10.6835	-1.5250	0.8850
H	-10.6836	-1.5242	-0.8859

10chain0



C	5.6279	-7.8280	0.0000
C	4.2214	-7.2146	0.0000
C	4.2198	-5.6799	0.0000
C	2.8133	-5.0661	0.0000
C	2.8125	-3.5314	0.0000
C	1.4063	-2.9169	0.0000
C	1.4061	-1.3822	0.0000
C	0.0000	-0.7673	0.0000
C	0.0000	0.7673	0.0000
C	-1.4061	1.3822	0.0000
C	-1.4063	2.9169	0.0000
C	-2.8125	3.5314	0.0000
C	-2.8133	5.0661	0.0000
C	-4.2198	5.6799	0.0000
C	-4.2214	7.2146	0.0000
C	-5.6279	7.8280	0.0000
C	5.6306	-9.3626	0.0000
C	7.0395	-9.9663	0.0000
C	-5.6305	9.3626	0.0000
C	-7.0395	9.9663	0.0000
H	6.1844	-7.4642	0.8786
H	6.1844	-7.4642	-0.8786
H	3.6656	-7.5790	0.8786
H	3.6656	-7.5790	-0.8786
H	4.7757	-5.3156	-0.8785
H	4.7757	-5.3156	0.8785
H	2.2573	-5.4302	0.8785
H	2.2573	-5.4302	-0.8785
H	3.3686	-3.1674	-0.8785
H	3.3686	-3.1674	0.8785
H	0.8501	-3.2808	0.8785
H	0.8501	-3.2808	-0.8785
H	1.9623	-1.0184	-0.8785
H	1.9623	-1.0184	0.8785
H	-0.5563	-1.1311	0.8785
H	-0.5563	-1.1311	-0.8785
H	0.5563	1.1311	-0.8785
H	0.5563	1.1311	0.8785
H	-1.9623	1.0184	0.8785

H	-1.9623	1.0184	-0.8785
H	-0.8501	3.2808	-0.8785
H	-0.8501	3.2808	0.8785
H	-3.3686	3.1674	0.8785
H	-3.3686	3.1674	-0.8785
H	-2.2573	5.4302	-0.8785
H	-2.2573	5.4302	0.8785
H	-4.7757	5.3156	0.8785
H	-4.7757	5.3156	-0.8785
H	-3.6656	7.5790	-0.8786
H	-3.6656	7.5790	0.8786
H	-6.1843	7.4642	0.8786
H	-6.1843	7.4642	-0.8786
H	5.0755	-9.7261	-0.8783
H	5.0755	-9.7261	0.8783
H	7.0073	-11.0634	0.0000
H	7.6076	-9.6498	0.8854
H	7.6076	-9.6498	-0.8854
H	-5.0755	9.7261	-0.8783
H	-5.0755	9.7261	0.8783
H	-7.0073	11.0634	0.0000
H	-7.6076	9.6498	0.8854
H	-7.6076	9.6498	-0.8854

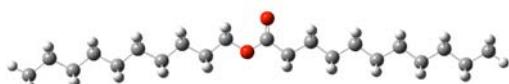
11chain0



C	-13.4799	-0.3607	-0.0004
C	-12.1987	0.4808	-0.0002
C	-10.9179	-0.3645	-0.0003
C	-9.6298	0.4697	0.0000
C	-8.3495	-0.3765	-0.0001
C	-7.0612	0.4575	0.0001
C	-5.7812	-0.3892	0.0001
C	-4.4927	0.4445	0.0002
C	-3.2128	-0.4025	0.0002
C	-1.9241	0.4309	0.0003
C	-0.6444	-0.4163	0.0002
C	0.6444	0.4169	0.0002
C	1.9241	-0.4303	0.0003
C	3.2129	0.4030	0.0002
C	4.4926	-0.4441	0.0002
C	5.7813	0.3894	0.0001
C	7.0612	-0.4574	0.0001
C	8.3496	0.3765	-0.0001
C	9.6298	-0.4699	0.0000
C	10.9179	0.3640	-0.0003
C	12.1986	-0.4815	-0.0002
C	13.4800	0.3598	-0.0005
H	-14.3769	0.2718	-0.0004
H	-13.5298	-1.0092	0.8848
H	-13.5297	-1.0089	-0.8860
H	-12.1954	1.1439	0.8784
H	-12.1953	1.1443	-0.8786

H	-10.9217	-1.0288	-0.8792
H	-10.9218	-1.0292	0.8784
H	-9.6269	1.1338	0.8789
H	-9.6268	1.1341	-0.8787
H	-8.3526	-1.0407	-0.8789
H	-8.3527	-1.0410	0.8785
H	-7.0580	1.1217	0.8790
H	-7.0579	1.1220	-0.8785
H	-5.7845	-1.0534	-0.8788
H	-5.7846	-1.0536	0.8787
H	-4.4892	1.1087	0.8790
H	-4.4892	1.1089	-0.8785
H	-3.2163	-1.0668	-0.8786
H	-3.2164	-1.0669	0.8789
H	-1.9206	1.0951	0.8790
H	-1.9205	1.0952	-0.8785
H	-0.6480	-1.0807	-0.8785
H	-0.6480	-1.0807	0.8790
H	0.6480	1.0813	0.8790
H	0.6480	1.0813	-0.8785
H	1.9205	-1.0947	-0.8784
H	1.9205	-1.0946	0.8790
H	3.2164	1.0674	0.8789
H	3.2164	1.0673	-0.8786
H	4.4891	-1.1085	-0.8784
H	4.4892	-1.1083	0.8790
H	5.7847	1.0539	0.8787
H	5.7847	1.0537	-0.8787
H	7.0578	-1.1219	-0.8785
H	7.0579	-1.1216	0.8790
H	8.3529	1.0410	0.8786
H	8.3528	1.0407	-0.8789
H	9.6266	-1.1344	-0.8787
H	9.6267	-1.1341	0.8789
H	10.9220	1.0287	0.8784
H	10.9219	1.0284	-0.8792
H	12.1951	-1.1449	-0.8786
H	12.1952	-1.1446	0.8784
H	14.3768	-0.2729	-0.0004
H	13.5300	1.0083	0.8848
H	13.5299	1.0079	-0.8860

11chain1

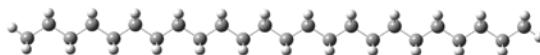


C	-3.0611	0.5872	0.0000
C	-1.7231	-0.1558	-0.0006
C	-0.5243	0.7756	-0.0002
O	0.6318	0.0731	-0.0013
C	1.8465	0.8562	-0.0009
C	3.0239	-0.1076	-0.0007
O	-0.5701	1.9841	0.0011

C	-4.2685	-0.3588	-0.0003
C	-5.6140	0.3792	0.0001
C	4.3725	0.6256	-0.0004
C	5.5780	-0.3242	-0.0003
C	-6.8291	-0.5579	-0.0001
C	-8.1735	0.1824	0.0002
C	6.9282	0.4050	0.0000
C	8.1369	-0.5405	0.0001
C	-9.3903	-0.7527	0.0001
C	-10.7343	-0.0120	0.0004
C	9.4864	0.1903	0.0003
C	10.6968	-0.7527	0.0004
C	-11.9516	-0.9463	0.0003
C	-13.2899	-0.1987	0.0005
C	12.0458	-0.0212	0.0006
C	13.2497	-0.9700	0.0006
H	-3.1044	1.2505	-0.8747
H	-3.1041	1.2497	0.8753
H	-1.6346	-0.8173	-0.8747
H	-1.6344	-0.8184	0.8727
H	1.8495	1.5068	0.8829
H	1.8500	1.5068	-0.8847
H	2.9507	-0.7613	-0.8814
H	2.9504	-0.7613	0.8801
H	-4.2168	-1.0217	0.8783
H	-4.2170	-1.0209	-0.8794
H	-5.6644	1.0418	-0.8782
H	-5.6642	1.0412	0.8789
H	4.4306	1.2864	0.8786
H	4.4309	1.2865	-0.8794
H	5.5202	-0.9852	-0.8792
H	5.5200	-0.9853	0.8786
H	-6.7784	-1.2204	0.8786
H	-6.7786	-1.2199	-0.8791
H	-8.2237	0.8450	-0.8783
H	-8.2235	0.8446	0.8791
H	6.9838	1.0668	0.8788
H	6.9840	1.0669	-0.8788
H	8.0816	-1.2023	-0.8788
H	8.0813	-1.2024	0.8788
H	-9.3403	-1.4153	0.8788
H	-9.3404	-1.4149	-0.8788
H	-10.7854	0.6507	-0.8783
H	-10.7852	0.6504	0.8792
H	9.5410	0.8523	0.8791
H	9.5412	0.8525	-0.8784
H	10.6434	-1.4150	-0.8785
H	10.6431	-1.4151	0.8791
H	-11.9012	-1.6078	0.8787
H	-11.9013	-1.6075	-0.8783
H	-14.1389	-0.8942	0.0005
H	-13.3865	0.4444	-0.8848
H	-13.3863	0.4442	0.8860
H	12.0995	0.6399	0.8791
H	12.0997	0.6400	-0.8778

H	14.1977	-0.4169	0.0008
H	13.2438	-1.6201	-0.8848
H	13.2436	-1.6203	0.8860

12chain0



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C	5.6264	-9.3644	0.0000
C	5.6254	-7.8296	0.0000
C	4.2188	-7.2157	0.0000
C	4.2183	-5.6810	0.0000
C	2.8119	-5.0666	0.0000
C	2.8119	-3.5318	0.0000
C	1.4057	-2.9171	0.0000
C	1.4060	-1.3823	0.0000
C	-0.0002	-0.7674	0.0000
C	0.0002	0.7674	0.0000
C	-1.4060	1.3823	0.0000
C	-1.4057	2.9171	0.0000
C	-2.8119	3.5318	0.0000
C	-2.8119	5.0666	0.0000
C	-4.2183	5.6810	0.0000
C	7.0349	-11.5126	0.0000
C	8.4439	-12.1166	0.0000
C	-4.2188	7.2157	0.0000
C	-5.6254	7.8296	0.0000
C	-5.6264	9.3644	0.0000
C	-7.0329	9.9780	0.0000
C	-7.0349	11.5126	0.0000
C	-8.4439	12.1166	0.0000
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H	7.5892	-9.6145	-0.8788
H	5.0708	-9.7285	0.8788
H	5.0708	-9.7285	-0.8788
H	6.1811	-7.4656	-0.8787
H	6.1811	-7.4656	0.8787
H	3.6630	-7.5797	0.8787
H	3.6630	-7.5797	-0.8787
H	4.7742	-5.3171	-0.8787
H	4.7742	-5.3171	0.8787
H	2.2561	-5.4303	0.8787
H	2.2561	-5.4303	-0.8787
H	3.3679	-3.1681	-0.8787
H	3.3679	-3.1681	0.8787
H	0.8497	-3.2807	0.8787
H	0.8497	-3.2807	-0.8787
H	1.9620	-1.0187	-0.8787
H	1.9620	-1.0187	0.8787
H	-0.5562	-1.1310	0.8787
H	-0.5562	-1.1310	-0.8787
H	0.5562	1.1310	-0.8787
H	0.5562	1.1310	0.8787

H	-1.9620	1.0187	0.8787
H	-1.9620	1.0187	-0.8787
H	-0.8497	3.2807	-0.8787
H	-0.8497	3.2807	0.8787
H	-3.3679	3.1681	0.8787
H	-3.3679	3.1681	-0.8787
H	-2.2561	5.4303	-0.8787
H	-2.2561	5.4303	0.8787
H	-4.7742	5.3171	0.8787
H	-4.7742	5.3171	-0.8787
H	6.4800	-11.8759	-0.8785
H	6.4800	-11.8759	0.8785
H	8.4114	-13.2137	0.0000
H	9.0120	-11.8004	0.8854
H	9.0120	-11.8004	-0.8854
H	-3.6630	7.5797	-0.8787
H	-3.6630	7.5797	0.8787
H	-6.1811	7.4656	0.8787
H	-6.1811	7.4656	-0.8787
H	-5.0708	9.7285	-0.8788
H	-5.0708	9.7285	0.8788
H	-7.5892	9.6145	0.8788
H	-7.5892	9.6145	-0.8788
H	-6.4800	11.8759	-0.8785
H	-6.4800	11.8759	0.8785
H	-8.4114	13.2137	0.0000
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H	-9.0120	11.8004	-0.8854

13chain0

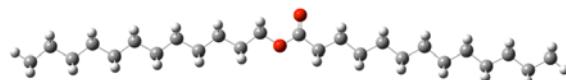


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C	-13.4857	-0.3711	0.0001
C	-12.1991	0.4651	-0.0002
C	-10.9174	-0.3790	0.0001
C	-9.6304	0.4572	-0.0002
C	-8.3491	-0.3875	0.0001
C	-7.0618	0.4482	-0.0001
C	-5.7807	-0.3969	0.0001
C	-4.4932	0.4384	0.0000
C	-3.2123	-0.4070	0.0001
C	-1.9247	0.4281	0.0000
C	-0.6439	-0.4174	0.0000
C	0.6438	0.4176	0.0001
C	1.9246	-0.4279	0.0000
C	3.2123	0.4071	0.0001
C	4.4932	-0.4382	-0.0001
C	5.7807	0.3970	0.0001
C	7.0618	-0.4481	-0.0001
C	8.3491	0.3875	0.0001
C	9.6304	-0.4572	-0.0002

C	10.9174	0.3789	0.0001
C	12.1991	-0.4653	-0.0002
C	13.4857	0.3710	0.0001
C	14.7679	-0.4723	-0.0002
C	16.0478	0.3713	0.0002
H	-16.9458	0.2594	-0.0002
H	-16.0965	-1.0196	0.8858
H	-16.0965	-1.0204	-0.8850
H	-14.7657	1.1357	0.8779
H	-14.7657	1.1349	-0.8790
H	-13.4885	-1.0360	-0.8784
H	-13.4886	-1.0353	0.8792
H	-12.1972	1.1298	0.8783
H	-12.1971	1.1291	-0.8793
H	-10.9194	-1.0437	-0.8783
H	-10.9195	-1.0430	0.8791
H	-9.6282	1.1218	0.8784
H	-9.6282	1.1212	-0.8791
H	-8.3514	-1.0521	-0.8784
H	-8.3514	-1.0516	0.8791
H	-7.0594	1.1127	0.8785
H	-7.0594	1.1123	-0.8790
H	-5.7832	-1.0614	-0.8784
H	-5.7833	-1.0610	0.8790
H	-4.4906	1.1029	0.8786
H	-4.4906	1.1026	-0.8789
H	-3.2150	-1.0714	-0.8785
H	-3.2150	-1.0712	0.8789
H	-1.9220	1.0925	0.8787
H	-1.9220	1.0924	-0.8788
H	-0.6466	-1.0817	-0.8787
H	-0.6466	-1.0817	0.8788
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H	0.6465	1.0820	-0.8786
H	1.9220	-1.0922	-0.8788
H	1.9219	-1.0923	0.8787
H	3.2150	1.0713	0.8789
H	3.2149	1.0716	-0.8785
H	4.4906	-1.1024	-0.8789
H	4.4906	-1.1027	0.8786
H	5.7833	1.0612	0.8790
H	5.7832	1.0616	-0.8785
H	7.0593	-1.1122	-0.8790
H	7.0594	-1.1126	0.8785
H	8.3514	1.0516	0.8790
H	8.3514	1.0521	-0.8784
H	9.6282	-1.1212	-0.8791
H	9.6282	-1.1218	0.8784
H	10.9195	1.0430	0.8790
H	10.9195	1.0435	-0.8784
H	12.1971	-1.1293	-0.8792
H	12.1971	-1.1299	0.8783
H	13.4886	1.0351	0.8792
H	13.4886	1.0358	-0.8784
H	14.7657	-1.1352	-0.8790

H	14.7657	-1.1359	0.8780
H	16.9458	-0.2598	-0.0001
H	16.0966	1.0193	0.8858
H	16.0966	1.0201	-0.8850

13chain1



C	-3.0628	0.6915	0.0000
C	-1.7252	-0.0524	-0.0005
C	-0.5260	0.8785	-0.0003
O	0.6299	0.1757	-0.0004
C	1.8447	0.9587	-0.0002
C	3.0221	-0.0050	0.0000
O	-0.5715	2.0870	0.0000
C	-4.2710	-0.2536	-0.0004
C	-5.6157	0.4859	0.0000
C	4.3705	0.7286	0.0001
C	5.5765	-0.2205	0.0002
C	-6.8321	-0.4495	-0.0003
C	-8.1753	0.2930	0.0000
C	6.9261	0.5099	0.0003
C	8.1359	-0.4343	0.0003
C	-9.3940	-0.6397	-0.0002
C	-10.7362	0.1046	0.0001
C	9.4843	0.2985	0.0003
C	10.6963	-0.6428	0.0002
C	-11.9558	-0.8268	0.0000
C	-13.2977	-0.0824	0.0002
C	12.0437	0.0919	0.0001
C	13.2569	-0.8475	0.0000
C	-14.5176	-1.0133	0.0002
C	-15.8538	-0.2621	0.0004
C	14.6039	-0.1122	0.0000
C	15.8105	-1.0575	-0.0002
H	-3.1056	1.3548	-0.8747
H	-3.1055	1.3540	0.8753
H	-1.6371	-0.7141	-0.8746
H	-1.6368	-0.7149	0.8729
H	1.8478	1.6094	0.8835
H	1.8481	1.6093	-0.8840
H	2.9491	-0.6588	-0.8807
H	2.9489	-0.6587	0.8808
H	-4.2200	-0.9165	0.8782
H	-4.2201	-0.9158	-0.8795
H	-5.6652	1.1486	-0.8783
H	-5.6651	1.1480	0.8788
H	4.4283	1.3895	0.8791
H	4.4285	1.3895	-0.8789
H	5.5192	-0.8816	-0.8787
H	5.5191	-0.8816	0.8791
H	-6.7825	-1.1122	0.8784
H	-6.7825	-1.1116	-0.8793

H	-8.2242	0.9558	-0.8785
H	-8.2241	0.9553	0.8789
H	6.9812	1.1717	0.8790
H	6.9812	1.1718	-0.8785
H	8.0813	-1.0962	-0.8786
H	8.0813	-1.0962	0.8791
H	-9.3454	-1.3024	0.8785
H	-9.3454	-1.3020	-0.8791
H	-10.7844	0.7674	-0.8785
H	-10.7843	0.7670	0.8789
H	9.5381	0.9607	0.8790
H	9.5380	0.9607	-0.8784
H	10.6429	-1.3049	-0.8786
H	10.6430	-1.3050	0.8789
H	-11.9076	-1.4896	0.8786
H	-11.9077	-1.4892	-0.8790
H	-13.3470	0.5805	-0.8784
H	-13.3468	0.5801	0.8791
H	12.0966	0.7542	0.8789
H	12.0965	0.7543	-0.8786
H	13.2053	-1.5099	-0.8788
H	13.2054	-1.5100	0.8788
H	-14.4689	-1.6751	0.8785
H	-14.4691	-1.6747	-0.8785
H	-16.7048	-0.9553	0.0004
H	-15.9487	0.3813	-0.8848
H	-15.9485	0.3810	0.8860
H	14.6559	0.5491	0.8785
H	14.6558	0.5492	-0.8784
H	16.7570	-0.5018	-0.0002
H	15.8063	-1.7077	-0.8856
H	15.8064	-1.7078	0.8852

14chain0

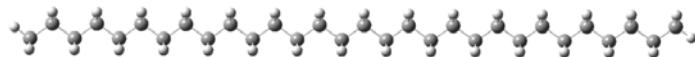


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C	0.4197	-9.6317	0.0000
C	-0.4211	-8.3478	0.0000
C	0.4189	-7.0634	0.0000
C	-0.4214	-5.7791	0.0000
C	0.4190	-4.4950	0.0000
C	-0.4211	-3.2105	0.0000
C	0.4195	-1.9265	0.0000
C	-0.4203	-0.6420	0.0000
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C	-0.4195	1.9265	0.0000
C	0.4211	3.2105	0.0000
C	-0.4190	4.4950	0.0000

C	-0.4132	-16.0541	0.0000
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C	0.4214	5.7791	0.0000
C	-0.4189	7.0634	0.0000
C	0.4211	8.3478	0.0000
C	-0.4197	9.6317	0.0000
C	0.4197	10.9165	0.0000
C	-0.4217	12.2000	0.0000
C	0.4171	13.4852	0.0000
C	-0.4245	14.7683	0.0000
C	0.4132	16.0541	0.0000
C	-0.4359	17.3304	0.0000
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H	1.0891	-14.7684	-0.8788
H	-1.0815	-13.4860	0.8788
H	-1.0815	-13.4860	-0.8788
H	1.0860	-12.1993	-0.8787
H	1.0860	-12.1993	0.8787
H	-1.0840	-10.9170	0.8787
H	-1.0840	-10.9170	-0.8787
H	1.0841	-9.6314	-0.8787
H	1.0841	-9.6314	0.8787
H	-1.0854	-8.3480	0.8787
H	-1.0854	-8.3480	-0.8787
H	1.0833	-7.0633	-0.8787
H	1.0833	-7.0633	0.8787
H	-1.0857	-5.7791	0.8787
H	-1.0857	-5.7791	-0.8787
H	1.0833	-4.4951	-0.8787
H	1.0833	-4.4951	0.8787
H	-1.0854	-3.2104	0.8787
H	-1.0854	-3.2104	-0.8787
H	1.0839	-1.9267	-0.8787
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H	-1.0847	-0.6418	0.8787
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H	1.0847	0.6418	-0.8787
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H	-1.0839	1.9267	0.8787
H	-1.0839	1.9267	-0.8787
H	1.0854	3.2104	-0.8787
H	1.0854	3.2104	0.8787
H	-1.0833	4.4951	0.8787
H	-1.0833	4.4951	-0.8787
H	-1.0765	-16.0546	-0.8785
H	-1.0765	-16.0546	0.8785
H	-0.1913	-18.2311	0.0000
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H	1.0845	-17.3763	-0.8854
H	1.0857	5.7791	-0.8787
H	1.0857	5.7791	0.8787
H	-1.0833	7.0633	0.8787
H	-1.0833	7.0633	-0.8787
H	1.0854	8.3480	-0.8787
H	1.0854	8.3480	0.8787

H	-1.0841	9.6314	0.8787
H	-1.0841	9.6314	-0.8787
H	1.0840	10.9170	-0.8787
H	1.0840	10.9170	0.8787
H	-1.0860	12.1993	0.8787
H	-1.0860	12.1993	-0.8787
H	1.0815	13.4860	-0.8788
H	1.0815	13.4860	0.8788
H	-1.0891	14.7684	0.8788
H	-1.0891	14.7684	-0.8788
H	1.0765	16.0546	-0.8785
H	1.0765	16.0546	0.8785
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H	-1.0845	17.3763	-0.8854

15chain0

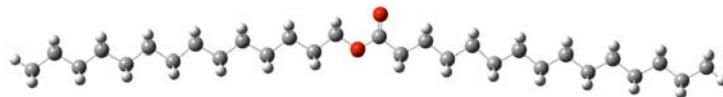


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C	14.7682	0.4602	-0.0003
C	13.4854	-0.3822	-0.0001
C	12.1995	0.4556	-0.0001
C	10.9171	-0.3874	0.0000
C	9.6309	0.4498	0.0000
C	8.3488	-0.3937	0.0002
C	7.0622	0.4430	0.0002
C	5.7804	-0.4010	0.0003
C	4.4936	0.4354	0.0003
C	3.2120	-0.4089	0.0003
C	1.9250	0.4273	0.0003
C	0.6435	-0.4172	0.0003
C	-0.6435	0.4188	0.0003
C	-1.9250	-0.4257	0.0003
C	-3.2120	0.4104	0.0003
C	-4.4935	-0.4341	0.0003
C	-5.7805	0.4021	0.0002
C	-7.0621	-0.4421	0.0002
C	-8.3489	0.3944	0.0001
C	-9.6307	-0.4495	0.0000
C	-10.9172	0.3874	0.0000
C	-12.1994	-0.4560	-0.0001
C	-13.4855	0.3814	-0.0001
C	-14.7681	-0.4614	-0.0003
C	-16.0539	0.3761	-0.0003
C	-17.3369	-0.4658	-0.0005
C	-18.6160	0.3792	-0.0005
H	19.5147	0.2480	-0.0006
H	18.6636	-1.0303	-0.8859
H	18.6637	-1.0302	0.8849
H	17.3357	1.1268	-0.8790

H	17.3358	1.1269	0.8780
H	16.0557	-1.0423	0.8785
H	16.0556	-1.0424	-0.8791
H	14.7671	1.1245	-0.8791
H	14.7672	1.1246	0.8785
H	13.4866	-1.0465	0.8786
H	13.4865	-1.0466	-0.8788
H	12.1981	1.1199	-0.8789
H	12.1983	1.1200	0.8786
H	10.9187	-1.0517	0.8788
H	10.9185	-1.0518	-0.8787
H	9.6292	1.1141	-0.8787
H	9.6293	1.1142	0.8788
H	8.3506	-1.0580	0.8789
H	8.3505	-1.0581	-0.8785
H	7.0603	1.1073	-0.8786
H	7.0604	1.1074	0.8789
H	5.7824	-1.0652	0.8790
H	5.7823	-1.0653	-0.8784
H	4.4915	1.0997	-0.8785
H	4.4916	1.0998	0.8790
H	3.2141	-1.0732	0.8791
H	3.2141	-1.0732	-0.8784
H	1.9229	1.0916	-0.8784
H	1.9229	1.0916	0.8790
H	0.6457	-1.0815	0.8791
H	0.6457	-1.0815	-0.8784
H	-0.6457	1.0832	-0.8784
H	-0.6457	1.0832	0.8791
H	-1.9228	-1.0900	0.8791
H	-1.9228	-1.0900	-0.8784
H	-3.2141	1.0747	-0.8784
H	-3.2142	1.0747	0.8790
H	-4.4914	-1.0984	0.8790
H	-4.4914	-1.0984	-0.8785
H	-5.7825	1.0665	-0.8785
H	-5.7826	1.0665	0.8790
H	-7.0602	-1.1064	0.8789
H	-7.0601	-1.1064	-0.8786
H	-8.3507	1.0588	-0.8786
H	-8.3508	1.0587	0.8789
H	-9.6290	-1.1138	0.8787
H	-9.6289	-1.1138	-0.8787
H	-10.9188	1.0518	-0.8787
H	-10.9190	1.0517	0.8788
H	-12.1979	-1.1204	0.8786
H	-12.1978	-1.1203	-0.8789
H	-13.4869	1.0458	-0.8788
H	-13.4870	1.0457	0.8786
H	-14.7668	-1.1258	0.8784
H	-14.7667	-1.1257	-0.8791
H	-16.0560	1.0407	-0.8790
H	-16.0561	1.0406	0.8785
H	-17.3354	-1.1291	0.8780
H	-17.3353	-1.1290	-0.8790

H	-19.5146	-0.2510	-0.0006
H	-18.6640	1.0277	-0.8858
H	-18.6641	1.0275	0.8850

15chain1



C	-3.0641	0.7901	0.0002
C	-1.7267	0.0460	-0.0001
C	-0.5274	0.9769	-0.0001
O	0.6285	0.2741	0.0000
C	1.8433	1.0572	-0.0001
C	3.0209	0.0937	0.0001
O	-0.5728	2.1854	-0.0004
C	-4.2726	-0.1546	-0.0002
C	-5.6169	0.5856	0.0002
C	4.3690	0.8278	0.0000
C	5.5755	-0.1206	0.0001
C	-6.8340	-0.3490	-0.0002
C	-8.1765	0.3947	0.0002
C	6.9246	0.6106	0.0001
C	8.1352	-0.3325	0.0001
C	-9.3963	-0.5365	-0.0001
C	-10.7374	0.2096	0.0002
C	9.4829	0.4017	0.0001
C	10.6960	-0.5382	0.0001
C	-11.9586	-0.7198	-0.0001
C	-13.2990	0.0276	0.0002
C	12.0423	0.1985	0.0000
C	13.2570	-0.7393	0.0001
C	-14.5208	-0.9010	-0.0002
C	-15.8611	-0.1538	0.0001
C	14.6025	-0.0009	-0.0001
C	15.8182	-0.9371	0.0000
C	-17.0830	-1.0821	-0.0002
C	-18.4176	-0.3280	0.0002
C	17.1633	-0.1985	-0.0002
C	18.3723	-1.1408	-0.0001
H	-3.1067	1.4533	-0.8745
H	-3.1067	1.4526	0.8754
H	-1.6386	-0.6159	-0.8740
H	-1.6383	-0.6162	0.8735
H	1.8464	1.7080	0.8834
H	1.8464	1.7076	-0.8840
H	2.9480	-0.5603	-0.8805
H	2.9478	-0.5598	0.8810
H	-4.2219	-0.8175	0.8784
H	-4.2219	-0.8168	-0.8793
H	-5.6660	1.2483	-0.8781
H	-5.6660	1.2476	0.8790
H	4.4266	1.4888	0.8790
H	4.4266	1.4887	-0.8790

H	5.5185	-0.7818	-0.8788
H	5.5185	-0.7817	0.8791
H	-6.7849	-1.0118	0.8784
H	-6.7850	-1.0110	-0.8793
H	-8.2247	1.0577	-0.8782
H	-8.2246	1.0570	0.8791
H	6.9792	1.2726	0.8788
H	6.9792	1.2725	-0.8787
H	8.0812	-0.9945	-0.8786
H	8.0812	-0.9944	0.8790
H	-9.3485	-1.1994	0.8784
H	-9.3486	-1.1987	-0.8792
H	-10.7847	0.8726	-0.8782
H	-10.7846	0.8720	0.8791
H	9.5359	1.0640	0.8787
H	9.5359	1.0638	-0.8787
H	10.6435	-1.2005	-0.8785
H	10.6436	-1.2003	0.8790
H	-11.9116	-1.3828	0.8784
H	-11.9117	-1.3822	-0.8792
H	-13.3458	0.6907	-0.8783
H	-13.3458	0.6900	0.8791
H	12.0942	0.8610	0.8786
H	12.0941	0.8607	-0.8788
H	13.2056	-1.4018	-0.8785
H	13.2056	-1.4014	0.8790
H	-14.4741	-1.5641	0.8783
H	-14.4742	-1.5634	-0.8792
H	-15.9089	0.5094	-0.8784
H	-15.9089	0.5087	0.8792
H	14.6536	0.6617	0.8785
H	14.6535	0.6613	-0.8790
H	15.7683	-1.6000	-0.8786
H	15.7684	-1.5996	0.8790
H	-17.0357	-1.7441	0.8780
H	-17.0358	-1.7433	-0.8790
H	-19.2701	-1.0194	-0.0001
H	-18.5111	0.3158	-0.8850
H	-18.5110	0.3151	0.8859
H	17.2137	0.4631	0.8782
H	17.2136	0.4628	-0.8788
H	19.3174	-0.5828	-0.0002
H	18.3696	-1.7912	-0.8853
H	18.3698	-1.7909	0.8854

16chain0



C	0.4303	-17.3367	0.0000
C	-0.4118	-16.0539	0.0000
C	0.4265	-14.7683	0.0000
C	-0.4155	-13.4852	0.0000

C	0.4234	-12.2000	0.0000
C	-0.4180	-10.9165	0.0000
C	0.4214	-9.6317	0.0000
C	-0.4195	-8.3479	0.0000
C	0.4204	-7.0633	0.0000
C	-0.4202	-5.7792	0.0000
C	0.4199	-4.4949	0.0000
C	-0.4204	-3.2106	0.0000
C	0.4200	-1.9264	0.0000
C	-0.4202	-0.6421	0.0000
C	0.4202	0.6421	0.0000
C	-0.4200	1.9264	0.0000
C	-0.4070	-18.6228	0.0000
C	0.4426	-19.8987	0.0000
C	0.4204	3.2106	0.0000
C	-0.4199	4.4949	0.0000
C	0.4202	5.7792	0.0000
C	-0.4204	7.0633	0.0000
C	0.4195	8.3479	0.0000
C	-0.4214	9.6317	0.0000
C	0.4180	10.9165	0.0000
C	-0.4234	12.2000	0.0000
C	0.4155	13.4852	0.0000
C	-0.4265	14.7683	0.0000
C	0.4118	16.0539	0.0000
C	-0.4303	17.3367	0.0000
C	0.4070	18.6228	0.0000
C	-0.4426	19.8987	0.0000
H	1.0949	-17.3365	0.8788
H	1.0949	-17.3365	-0.8788
H	-1.0761	-16.0550	0.8788
H	-1.0761	-16.0550	-0.8788
H	1.0908	-14.7674	-0.8787
H	1.0908	-14.7674	0.8787
H	-1.0798	-13.4860	0.8787
H	-1.0798	-13.4860	-0.8787
H	1.0878	-12.1994	-0.8787
H	1.0878	-12.1994	0.8787
H	-1.0823	-10.9170	0.8787
H	-1.0823	-10.9170	-0.8787
H	1.0858	-9.6313	-0.8787
H	1.0858	-9.6313	0.8787
H	-1.0838	-8.3481	0.8787
H	-1.0838	-8.3481	-0.8787
H	1.0847	-7.0631	-0.8787
H	1.0847	-7.0631	0.8787
H	-1.0845	-5.7793	0.8787
H	-1.0845	-5.7793	-0.8787
H	1.0843	-4.4948	-0.8787
H	1.0843	-4.4948	0.8787
H	-1.0847	-3.2106	0.8787
H	-1.0847	-3.2106	-0.8787
H	1.0843	-1.9265	-0.8787
H	1.0843	-1.9265	0.8787
H	-1.0845	-0.6420	0.8787

H	-1.0845	-0.6420	-0.8787
H	1.0845	0.6420	-0.8787
H	1.0845	0.6420	0.8787
H	-1.0843	1.9265	0.8787
H	-1.0843	1.9265	-0.8787
H	-1.0702	-18.6235	-0.8785
H	-1.0702	-18.6235	0.8785
H	-0.1844	-20.7996	0.0000
H	1.0912	-19.9445	0.8854
H	1.0912	-19.9445	-0.8854
H	1.0847	3.2106	-0.8787
H	1.0847	3.2106	0.8787
H	-1.0843	4.4948	0.8787
H	-1.0843	4.4948	-0.8787
H	1.0845	5.7793	-0.8787
H	1.0845	5.7793	0.8787
H	-1.0847	7.0631	0.8787
H	-1.0847	7.0631	-0.8787
H	1.0838	8.3481	-0.8787
H	1.0838	8.3481	0.8787
H	-1.0858	9.6313	0.8787
H	-1.0858	9.6313	-0.8787
H	1.0823	10.9170	-0.8787
H	1.0823	10.9170	0.8787
H	-1.0878	12.1994	0.8787
H	-1.0878	12.1994	-0.8787
H	1.0798	13.4860	-0.8787
H	1.0798	13.4860	0.8787
H	-1.0908	14.7674	0.8787
H	-1.0908	14.7674	-0.8787
H	1.0761	16.0550	-0.8788
H	1.0761	16.0550	0.8788
H	-1.0949	17.3365	0.8788
H	-1.0949	17.3365	-0.8788
H	1.0702	18.6235	-0.8785
H	1.0702	18.6235	0.8785
H	0.1844	20.7996	0.0000
H	-1.0912	19.9445	0.8854
H	-1.0912	19.9445	-0.8854

17chain0

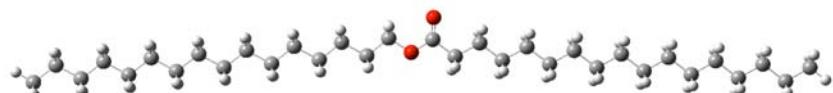


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C	19.9060	0.4564	0.0000
C	18.6218	-0.3838	0.0000
C	17.3371	0.4555	0.0000
C	16.0535	-0.3856	0.0000
C	14.7684	0.4535	0.0000
C	13.4852	-0.3884	-0.0001
C	12.1998	0.4501	-0.0001
C	10.9169	-0.3924	-0.0001
C	9.6311	0.4455	0.0000

C	8.3486	-0.3974	0.0000
C	7.0624	0.4400	0.0000
C	5.7802	-0.4034	0.0000
C	4.4938	0.4337	0.0000
C	3.2118	-0.4100	0.0000
C	1.9252	0.4268	0.0000
C	0.6433	-0.4170	0.0001
C	-0.6433	0.4196	0.0001
C	-1.9252	-0.4242	0.0001
C	-3.2118	0.4124	0.0001
C	-4.4937	-0.4314	0.0001
C	-5.7803	0.4054	0.0001
C	-7.0623	-0.4382	0.0001
C	-8.3487	0.3988	0.0001
C	-9.6309	-0.4445	0.0001
C	-10.9170	0.3929	0.0001
C	-12.1996	-0.4500	0.0000
C	-13.4854	0.3879	0.0000
C	-14.7683	-0.4545	0.0000
C	-16.0537	0.3840	0.0000
C	-17.3369	-0.4578	-0.0001
C	-18.6220	0.3809	-0.0001
C	-19.9058	-0.4599	-0.0001
C	-21.1841	0.3861	-0.0001
H	22.0834	0.2385	0.0000
H	21.2311	-1.0389	-0.8854
H	21.2310	-1.0389	0.8854
H	19.9054	1.1197	-0.8785
H	19.9054	1.1196	0.8785
H	18.6231	-1.0483	0.8788
H	18.6231	-1.0483	-0.8788
H	17.3368	1.1199	-0.8788
H	17.3367	1.1199	0.8788
H	16.0540	-1.0500	0.8787
H	16.0540	-1.0499	-0.8788
H	14.7677	1.1178	-0.8788
H	14.7677	1.1178	0.8787
H	13.4861	-1.0527	0.8787
H	13.4861	-1.0527	-0.8788
H	12.1987	1.1144	-0.8788
H	12.1987	1.1144	0.8787
H	10.9181	-1.0567	0.8787
H	10.9181	-1.0567	-0.8788
H	9.6298	1.1098	-0.8788
H	9.6298	1.1098	0.8787
H	8.3500	-1.0618	0.8787
H	8.3500	-1.0618	-0.8788
H	7.0609	1.1043	-0.8788
H	7.0609	1.1043	0.8787
H	5.7818	-1.0677	0.8787
H	5.7818	-1.0677	-0.8787
H	4.4921	1.0980	-0.8787
H	4.4921	1.0980	0.8787
H	3.2135	-1.0743	0.8788
H	3.2135	-1.0743	-0.8787

H	1.9234	1.0911	-0.8787
H	1.9234	1.0912	0.8788
H	0.6452	-1.0813	0.8788
H	0.6452	-1.0814	-0.8787
H	-0.6452	1.0840	-0.8787
H	-0.6452	1.0840	0.8788
H	-1.9233	-1.0886	0.8788
H	-1.9233	-1.0886	-0.8787
H	-3.2136	1.0768	-0.8787
H	-3.2136	1.0768	0.8788
H	-4.4919	-1.0957	0.8788
H	-4.4919	-1.0957	-0.8786
H	-5.7820	1.0697	-0.8786
H	-5.7820	1.0697	0.8788
H	-7.0606	-1.1026	0.8788
H	-7.0606	-1.1026	-0.8787
H	-8.3503	1.0632	-0.8786
H	-8.3503	1.0631	0.8788
H	-9.6294	-1.1088	0.8788
H	-9.6294	-1.1088	-0.8787
H	-10.9185	1.0573	-0.8787
H	-10.9185	1.0572	0.8788
H	-12.1983	-1.1143	0.8788
H	-12.1983	-1.1143	-0.8787
H	-13.4865	1.0523	-0.8787
H	-13.4866	1.0522	0.8788
H	-14.7673	-1.1188	0.8787
H	-14.7672	-1.1188	-0.8788
H	-16.0545	1.0483	-0.8787
H	-16.0546	1.0483	0.8787
H	-17.3362	-1.1221	0.8787
H	-17.3362	-1.1221	-0.8789
H	-18.6236	1.0454	-0.8788
H	-18.6236	1.0454	0.8787
H	-19.9048	-1.1232	0.8784
H	-19.9048	-1.1232	-0.8786
H	-22.0833	-0.2432	-0.0001
H	-21.2316	1.0346	-0.8855
H	-21.2316	1.0346	0.8853

17chain1

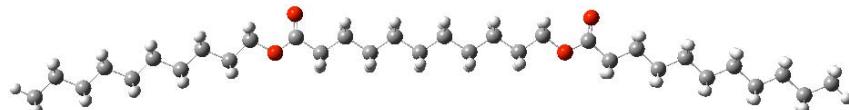


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C	19.6537	-0.6920	0.5674
C	18.3183	-1.2405	0.0468
C	17.1055	-0.3908	0.4488
C	15.7697	-0.9406	-0.0694
C	14.5576	-0.0899	0.3335
C	13.2205	-0.6415	-0.1794
C	12.0098	0.2103	0.2250
C	10.6704	-0.3444	-0.2786

C	9.4617	0.5090	0.1288
C	8.1191	-0.0512	-0.3599
C	6.9131	0.8039	0.0521
C	5.5668	0.2338	-0.4139
C	4.3647	1.0910	0.0051
C	3.0172	0.4995	-0.4313
C	1.8428	1.3639	0.0032
O	0.6271	0.7026	-0.4137
C	-0.5284	1.3051	-0.0507
C	-1.7281	0.5089	-0.5322
C	-3.0620	1.0806	-0.0460
C	-4.2696	0.2586	-0.5138
C	-5.6093	0.8172	-0.0156
C	-6.8241	-0.0094	-0.4578
C	-8.1606	0.5469	0.0518
C	-9.3775	-0.2851	-0.3749
C	-10.7114	0.2703	0.1425
C	-11.9297	-0.5647	-0.2742
C	-13.2617	-0.0095	0.2483
C	-14.4810	-0.8459	-0.1624
C	-15.8117	-0.2905	0.3629
C	-17.0318	-1.1275	-0.0447
C	-18.3619	-0.5720	0.4815
C	-19.5825	-1.4087	0.0754
C	-20.9064	-0.8457	0.6046
O	-0.5734	2.3394	0.5744
H	21.7975	-1.1289	0.5499
H	20.9516	-1.6123	-0.9308
H	20.7681	-2.5719	0.5461
H	19.7922	0.3358	0.1985
H	19.6110	-0.6153	1.6647
H	18.1807	-2.2696	0.4152
H	18.3614	-1.3179	-1.0514
H	17.2436	0.6377	0.0791
H	17.0647	-0.3123	1.5469
H	15.6315	-1.9689	0.3009
H	15.8101	-1.0196	-1.1674
H	14.6944	0.9376	-0.0394
H	14.5197	-0.0084	1.4314
H	13.0836	-1.6687	0.1943
H	13.2575	-0.7236	-1.2773
H	12.1442	1.2362	-0.1531
H	11.9769	0.2968	1.3228
H	10.5359	-1.3698	0.1008
H	10.7015	-0.4316	-1.3763
H	9.5919	1.5322	-0.2578
H	9.4371	0.6034	1.2261
H	7.9891	-1.0739	0.0284
H	8.1408	-0.1465	-1.4571
H	7.0358	1.8230	-0.3475
H	6.9012	0.9103	1.1484
H	5.4439	-0.7842	-0.0119
H	5.5737	0.1265	-1.5099
H	4.4763	2.1034	-0.4136
H	4.3716	1.2143	1.0994

H	2.8935	-0.5063	-0.0050
H	2.9917	0.3805	-1.5238
H	1.8781	2.3630	-0.4498
H	1.8164	1.5002	1.0916
H	-1.5956	-0.5323	-0.2051
H	-1.6876	0.4739	-1.6311
H	-3.1565	2.1190	-0.3913
H	-3.0504	1.1341	1.0514
H	-4.1598	-0.7824	-0.1698
H	-4.2803	0.2117	-1.6145
H	-5.7248	1.8540	-0.3688
H	-5.5902	0.8751	1.0841
H	-6.7048	-1.0469	-0.1070
H	-6.8477	-0.0647	-1.5578
H	-8.2838	1.5817	-0.3050
H	-8.1315	0.6098	1.1511
H	-9.2525	-1.3204	-0.0198
H	-9.4102	-0.3463	-1.4743
H	-10.8388	1.3040	-0.2162
H	-10.6751	0.3362	1.2416
H	-11.8013	-1.5987	0.0835
H	-11.9683	-0.6295	-1.3732
H	-13.3914	1.0236	-0.1115
H	-13.2209	0.0581	1.3471
H	-14.3509	-1.8791	0.1969
H	-14.5231	-0.9130	-1.2612
H	-15.9425	0.7423	0.0025
H	-15.7685	-0.2220	1.4615
H	-16.9010	-2.1603	0.3157
H	-17.0755	-1.1959	-1.1433
H	-18.4940	0.4607	0.1209
H	-18.3189	-0.5030	1.5803
H	-19.4518	-2.4401	0.4370
H	-19.6261	-1.4774	-1.0224
H	-21.7586	-1.4656	0.2976
H	-21.0834	0.1720	0.2308
H	-20.9080	-0.7978	1.7021

17chain2

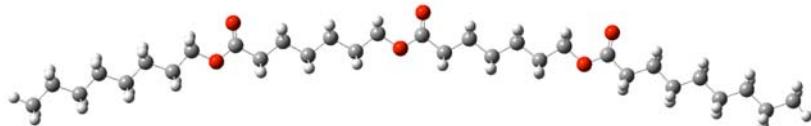


C	20.5442	2.1915	-0.1061
C	19.4544	1.1239	-0.2551
C	18.0354	1.6733	-0.0557
C	16.9378	0.6114	-0.2048
C	15.5193	1.1616	-0.0035
C	14.4216	0.0998	-0.1540
C	13.0043	0.6512	0.0512
C	11.9063	-0.4100	-0.1029
C	10.4930	0.1498	0.1102
C	9.4187	-0.9150	-0.0543

O	8.1365	-0.2857	0.1687
C	7.0527	-1.0837	0.0348
C	5.7754	-0.3074	0.3008
C	4.5087	-1.1314	0.0588
C	3.2234	-0.3405	0.3332
C	1.9469	-1.1504	0.0701
C	0.6557	-0.3637	0.3320
C	-0.6194	-1.1717	0.0557
C	-1.9117	-0.3801	0.2961
C	-3.1848	-1.1898	0.0147
C	-4.4729	-0.3820	0.2242
C	-5.7221	-1.2053	-0.0532
O	-6.8679	-0.3433	0.1288
C	-8.0772	-0.9120	-0.0818
C	-9.1906	0.1000	0.1200
C	-10.5877	-0.4899	-0.0865
C	-11.7019	0.5491	0.0926
C	-13.1095	-0.0290	-0.1069
C	-14.2269	1.0100	0.0571
C	-15.6358	0.4337	-0.1379
C	-16.7520	1.4751	0.0191
C	-18.1617	0.8997	-0.1721
C	-19.2777	1.9418	-0.0190
C	-20.6825	1.3578	-0.2073
O	7.1186	-2.2559	-0.2553
O	-8.2243	-2.0716	-0.3913
H	21.5454	1.7674	-0.2549
H	20.5208	2.6470	0.8933
H	20.4126	2.9992	-0.8389
H	19.6341	0.3131	0.4673
H	19.5276	0.6617	-1.2515
H	17.8567	2.4862	-0.7775
H	17.9623	2.1357	0.9416
H	17.1181	-0.2018	0.5160
H	17.0110	0.1505	-1.2027
H	15.3393	1.9754	-0.7237
H	15.4459	1.6217	0.9947
H	14.6023	-0.7154	0.5643
H	14.4928	-0.3582	-1.1533
H	12.8232	1.4673	-0.6659
H	12.9313	1.1068	1.0512
H	12.0886	-1.2285	0.6109
H	11.9755	-0.8616	-1.1049
H	10.2995	0.9637	-0.6031
H	10.4096	0.5891	1.1144
H	9.5412	-1.7361	0.6635
H	9.4284	-1.3554	-1.0593
H	5.7916	0.5960	-0.3254
H	5.8181	0.0589	1.3374
H	4.5386	-2.0313	0.6879
H	4.5090	-1.4953	-0.9780
H	3.2115	0.5682	-0.2898
H	3.2235	0.0113	1.3774
H	1.9558	-2.0570	0.6954
H	1.9514	-1.5046	-0.9727

H	0.6516	0.5453	-0.2904
H	0.6465	-0.0135	1.3763
H	-0.6221	-2.0752	0.6856
H	-0.6029	-1.5310	-0.9854
H	-1.9086	0.5220	-0.3358
H	-1.9323	-0.0195	1.3365
H	-3.1990	-2.0815	0.6608
H	-3.1538	-1.5666	-1.0196
H	-4.4748	0.4986	-0.4339
H	-4.5167	-0.0011	1.2546
H	-5.8091	-2.0622	0.6267
H	-5.7337	-1.5988	-1.0777
H	-9.0079	0.9385	-0.5680
H	-9.0817	0.5255	1.1282
H	-10.7346	-1.3229	0.6145
H	-10.6463	-0.9335	-1.0897
H	-11.5464	1.3787	-0.6156
H	-11.6312	0.9951	1.0975
H	-13.2685	-0.8522	0.6072
H	-13.1774	-0.4822	-1.1083
H	-14.0677	1.8312	-0.6598
H	-14.1559	1.4662	1.0573
H	-15.7969	-0.3842	0.5821
H	-15.7056	-0.0266	-1.1362
H	-16.5917	2.2914	-0.7030
H	-16.6804	1.9376	1.0164
H	-18.3241	0.0851	0.5517
H	-18.2339	0.4349	-1.1683
H	-19.1179	2.7535	-0.7452
H	-19.2047	2.4081	0.9755
H	-21.4564	2.1282	-0.0971
H	-20.8885	0.5710	0.5311
H	-20.7971	0.9111	-1.2044

17chain3

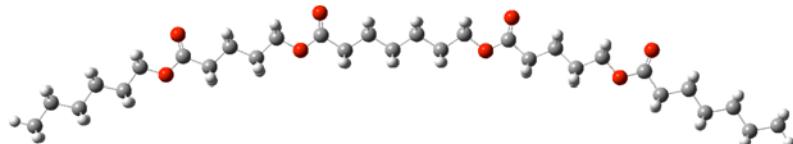


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C	-16.7483	0.8181	-0.0283
C	-15.2966	1.3084	0.0552
C	-14.2639	0.1852	-0.1100
C	-12.8130	0.6796	-0.0276
C	-11.8115	-0.4556	-0.1799
O	-10.4831	0.1090	-0.0940
C	-9.4604	-0.7713	-0.1770
C	-8.1232	-0.0574	-0.0872
C	-6.9317	-1.0179	-0.0941
C	-5.5815	-0.2928	-0.0361
C	-4.3850	-1.2539	-0.0349

C	-3.0303	-0.5336	0.0066
C	-1.8633	-1.5098	0.0145
O	-0.6403	-0.7392	0.0382
C	0.5074	-1.4543	0.0532
C	1.7171	-0.5366	0.0656
C	3.0440	-1.2984	0.1026
C	4.2646	-0.3699	0.0852
C	5.5970	-1.1309	0.1209
C	6.8217	-0.2068	0.0807
C	8.1290	-0.9845	0.1207
O	9.2131	-0.0316	0.0482
C	10.4614	-0.5527	0.0805
C	11.5071	0.5423	-0.0291
C	12.9404	0.0193	0.0919
C	13.9928	1.1231	-0.0723
C	15.4334	0.6079	0.0474
C	16.4937	1.7027	-0.1316
C	17.9341	1.1871	-0.0124
C	18.9958	2.2794	-0.1980
C	20.4315	1.7556	-0.0788
O	0.5411	-2.6630	0.0534
O	10.6870	-1.7368	0.1764
O	-9.6138	-1.9634	-0.3097
H	-21.2931	2.1820	0.1740
H	-20.1528	3.3349	-0.5417
H	-20.1543	3.0626	1.2082
H	-19.3965	0.9453	-0.9064
H	-19.4016	0.6733	0.8294
H	-17.6253	2.4364	1.1116
H	-17.6197	2.7085	-0.6250
H	-16.9084	0.3185	-0.9968
H	-16.9157	0.0462	0.7396
H	-15.1358	1.8103	1.0222
H	-15.1256	2.0764	-0.7154
H	-14.4257	-0.3183	-1.0759
H	-14.4346	-0.5810	0.6624
H	-12.6402	1.1814	0.9351
H	-12.6255	1.4299	-0.8089
H	-11.9169	-0.9683	-1.1444
H	-11.9268	-1.2121	0.6064
H	-8.1308	0.5667	0.8178
H	-8.0665	0.6512	-0.9269
H	-6.9821	-1.6459	-0.9937
H	-7.0218	-1.7097	0.7547
H	-5.5399	0.3408	0.8639
H	-5.4954	0.3943	-0.8928
H	-4.4334	-1.8938	-0.9295
H	-4.4672	-1.9336	0.8273
H	-2.9690	0.1045	0.8998
H	-2.9318	0.1338	-0.8614
H	-1.8606	-2.1519	-0.8755
H	-1.8853	-2.1684	0.8918
H	1.6196	0.1404	0.9266
H	1.6550	0.1117	-0.8207
H	3.0858	-1.9878	-0.7515

H	3.0694	-1.9348	0.9977
H	4.2170	0.3206	0.9420
H	4.2325	0.2639	-0.8151
H	5.6370	-1.8304	-0.7283
H	5.6344	-1.7542	1.0278
H	6.7954	0.4928	0.9283
H	6.8001	0.4067	-0.8313
H	8.2143	-1.6840	-0.7208
H	8.2302	-1.5701	1.0431
H	11.2890	1.2998	0.7372
H	11.3529	1.0526	-0.9916
H	13.0999	-0.7659	-0.6593
H	13.0638	-0.4739	1.0660
H	13.8236	1.9093	0.6807
H	13.8616	1.6117	-1.0511
H	15.5981	-0.1844	-0.6996
H	15.5669	0.1276	1.0294
H	16.3284	2.4959	0.6149
H	16.3593	2.1819	-1.1144
H	18.0988	0.3911	-0.7560
H	18.0708	0.7113	0.9718
H	18.8327	3.0743	0.5459
H	18.8590	2.7542	-1.1816
H	21.1655	2.5600	-0.2157
H	20.6377	0.9848	-0.8338
H	20.6103	1.3061	0.9074

17chain4

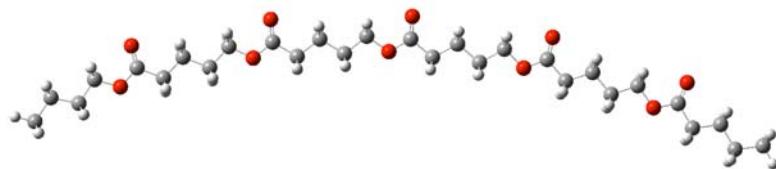


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C	17.3188	2.5293	-0.0057
C	16.4603	1.2574	-0.0210
C	14.9541	1.5478	0.0377
C	14.1181	0.2768	0.0146
O	12.7261	0.6655	0.0712
C	11.8261	-0.3412	0.0292
C	10.4092	0.2006	0.1019
C	9.3455	-0.8917	-0.0305
C	7.9208	-0.3291	0.0535
C	6.8662	-1.4180	-0.0807
O	5.5710	-0.7823	-0.0002
C	4.4999	-1.6036	-0.0887
C	3.2069	-0.8121	-0.0062
C	1.9581	-1.6968	-0.0241
C	0.6587	-0.8840	0.0323
C	-0.6030	-1.7577	0.0169
C	-1.8988	-0.9368	0.0699
C	-3.1422	-1.8135	0.0489
O	-4.2937	-0.9408	0.1068

C	-5.5014	-1.5463	0.0713
C	-6.6182	-0.5204	0.1493
C	-8.0119	-1.1424	0.0345
C	-9.1247	-0.0907	0.1268
C	-10.5112	-0.7063	0.0046
O	-11.4715	0.3693	0.0892
C	-12.7732	0.0158	-0.0238
C	-13.6699	1.2371	0.0669
C	-15.1601	0.9048	-0.0403
C	-16.0489	2.1533	0.0242
C	-17.5476	1.8407	-0.0812
C	-18.4380	3.0892	-0.0267
C	-19.9341	2.7721	-0.1314
O	12.1289	-1.5090	-0.0524
O	4.5862	-2.8022	-0.2204
O	-5.6491	-2.7436	-0.0083
O	-13.1435	-1.1245	-0.1787
H	20.7478	3.2970	-0.0941
H	19.4977	4.1149	0.8598
H	19.4397	4.1720	-0.9094
H	19.1120	1.6124	0.7843
H	19.0535	1.6699	-0.9711
H	17.0336	3.1707	-0.8545
H	17.0913	3.1110	0.9015
H	16.7445	0.6162	0.8280
H	16.6873	0.6764	-0.9285
H	14.6602	2.1820	-0.8107
H	14.7155	2.1152	0.9486
H	14.3389	-0.3763	0.8684
H	14.2858	-0.3090	-0.8978
H	10.2972	0.9655	-0.6795
H	10.3054	0.7409	1.0543
H	9.5039	-1.6447	0.7530
H	9.4879	-1.4195	-0.9832
H	7.7609	0.4191	-0.7362
H	7.7739	0.1923	1.0103
H	6.9462	-2.1678	0.7162
H	6.9444	-1.9483	-1.0381
H	3.1990	-0.0994	-0.8441
H	3.2457	-0.1918	0.9006
H	1.9996	-2.3972	0.8214
H	1.9724	-2.3214	-0.9273
H	0.6256	-0.1847	-0.8180
H	0.6547	-0.2571	0.9380
H	-0.5729	-2.4549	0.8684
H	-0.5998	-2.3845	-0.8882
H	-1.9391	-0.2425	-0.7815
H	-1.9148	-0.3176	0.9781
H	-3.1746	-2.5014	0.9033
H	-3.2018	-2.4209	-0.8629
H	-6.4481	0.2277	-0.6378
H	-6.5051	0.0254	1.0975
H	-8.1349	-1.8976	0.8222
H	-8.0855	-1.6887	-0.9156
H	-9.0015	0.6624	-0.6648

H	-9.0585	0.4493	1.0823
H	-10.7119	-1.4295	0.8051
H	-10.6445	-1.2301	-0.9503
H	-13.3615	1.9366	-0.7239
H	-13.4429	1.7522	1.0116
H	-15.4333	0.2068	0.7629
H	-15.3416	0.3627	-0.9783
H	-15.7652	2.8465	-0.7838
H	-15.8560	2.6938	0.9647
H	-17.8344	1.1532	0.7301
H	-17.7409	1.2964	-1.0191
H	-18.1510	3.7749	-0.8385
H	-18.2433	3.6330	0.9104
H	-20.5420	3.6848	-0.0873
H	-20.2599	2.1153	0.6865
H	-20.1677	2.2620	-1.0758

17chain5

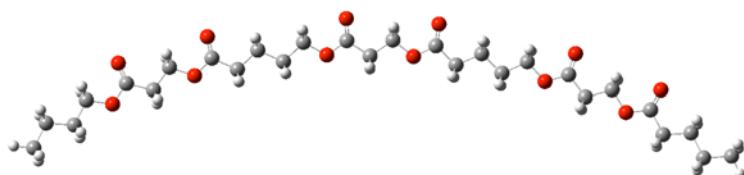


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C	17.1682	2.4915	0.0211
C	16.3920	1.1833	-0.0021
O	14.9821	1.5023	0.0458
C	14.1369	0.4492	0.0056
C	12.6919	0.9125	0.0692
C	11.6944	-0.2422	-0.0494
C	10.2373	0.2313	0.0284
C	9.2590	-0.9281	-0.0913
O	7.9211	-0.3862	-0.0118
C	6.9147	-1.2856	-0.0839
C	5.5651	-0.5948	0.0025
C	4.3931	-1.5784	-0.0329
C	3.0331	-0.8720	0.0339
C	1.8781	-1.8622	-0.0007
O	0.6477	-1.1052	0.0560
C	-0.4930	-1.8300	0.0272
C	-1.7103	-0.9240	0.0849
C	-3.0289	-1.7006	0.0595
C	-4.2527	-0.7767	0.1045
C	-5.5569	-1.5603	0.0717
O	-6.6427	-0.6074	0.1194
C	-7.8894	-1.1288	0.0774
C	-8.9360	-0.0307	0.1444
C	-10.3653	-0.5632	0.0185
C	-11.4139	0.5529	0.1079
C	-12.8316	0.0153	-0.0243
O	-13.7348	1.1397	0.0563
C	-15.0520	0.8510	-0.0620

C	-15.8904	2.1132	0.0258
C	-17.3933	1.8470	-0.0864
C	-18.2315	3.1298	-0.0201
C	-19.7374	2.8665	-0.1310
O	14.5022	-0.7011	-0.0682
O	7.0879	-2.4760	-0.2043
O	-0.5179	-3.0368	-0.0376
O	-8.1171	-2.3136	0.0009
O	-15.4767	-0.2699	-0.2189
H	20.5628	3.3840	-0.0425
H	19.2748	4.1561	0.8993
H	19.2289	4.2065	-0.8709
H	18.9895	1.6411	0.8274
H	18.9428	1.6924	-0.9290
H	16.8537	3.1091	-0.8324
H	16.8994	3.0519	0.9280
H	16.6396	0.5441	0.8550
H	16.5930	0.6030	-0.9114
H	12.5382	1.6587	-0.7232
H	12.5555	1.4591	1.0138
H	11.8978	-0.9745	0.7432
H	11.8691	-0.7726	-0.9952
H	10.0295	0.9573	-0.7707
H	10.0570	0.7536	0.9789
H	9.3939	-1.6628	0.7122
H	9.3708	-1.4610	-1.0439
H	5.5033	0.1270	-0.8250
H	5.5515	0.0121	0.9190
H	4.4928	-2.2868	0.8006
H	4.4609	-2.1839	-0.9464
H	2.9269	-0.1715	-0.8070
H	2.9602	-0.2709	0.9516
H	1.9082	-2.5569	0.8480
H	1.8828	-2.4653	-0.9172
H	-1.6468	-0.2194	-0.7568
H	-1.6291	-0.3043	0.9895
H	-3.0507	-2.3998	0.9062
H	-3.0596	-2.3261	-0.8427
H	-4.2347	-0.0803	-0.7461
H	-4.2305	-0.1590	1.0138
H	-5.6455	-2.2444	0.9250
H	-5.6504	-2.1618	-0.8409
H	-8.7108	0.7031	-0.6424
H	-8.7959	0.5081	1.0930
H	-10.5396	-1.3122	0.8024
H	-10.4664	-1.1010	-0.9339
H	-11.2429	1.2996	-0.6809
H	-11.3221	1.0851	1.0656
H	-13.0759	-0.6975	0.7733
H	-12.9866	-0.4992	-0.9809
H	-15.5478	2.7979	-0.7640
H	-15.6434	2.6170	0.9716
H	-17.6987	1.1587	0.7137
H	-17.5958	1.3157	-1.0265
H	-17.9190	3.8131	-0.8248

H	-18.0203	3.6578	0.9226
H	-20.3116	3.8002	-0.0792
H	-20.0875	2.2139	0.6800
H	-19.9859	2.3740	-1.0806

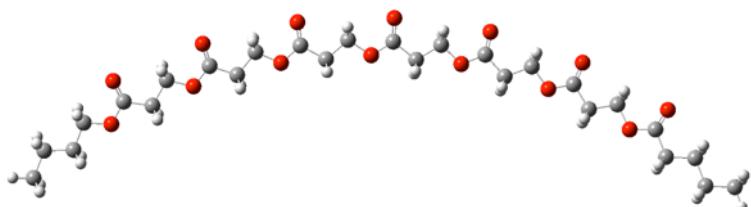
17chain6



C	-18.8367	4.3547	-0.1879
C	-18.2060	2.9584	-0.1492
C	-16.6727	3.0006	-0.0861
C	-16.0577	1.6100	-0.0498
O	-14.6193	1.7665	0.0076
C	-13.9004	0.6270	0.0329
C	-12.4148	0.9267	0.0935
C	-11.5847	-0.3483	0.0774
O	-10.2021	0.0642	0.1378
C	-9.2869	-0.9321	0.0991
C	-7.8780	-0.3711	0.1753
C	-6.8023	-1.4516	0.0421
C	-5.3832	-0.8749	0.1289
C	-4.3215	-1.9560	-0.0092
O	-3.0281	-1.3117	0.0740
C	-1.9567	-2.1241	-0.0268
C	-0.6663	-1.3324	0.0656
C	0.5527	-2.2393	-0.0156
O	1.7093	-1.3788	0.0682
C	2.9104	-1.9985	-0.0069
C	4.0426	-0.9918	0.0919
C	5.4235	-1.6408	-0.0274
C	6.5609	-0.6157	0.0673
C	7.9279	-1.2724	-0.0567
O	8.9253	-0.2278	0.0312
C	10.2093	-0.6289	-0.0699
C	11.1551	0.5527	0.0235
C	12.6097	0.1142	-0.0615
O	13.4043	1.3163	0.0105
C	14.7473	1.1373	-0.0380
C	15.4716	2.4691	0.0316
C	16.9951	2.3247	0.0226
C	17.7217	3.6745	0.0717
C	19.2477	3.5313	0.0641
O	-14.3858	-0.4808	0.0108
O	-9.5755	-2.1021	0.0175
O	-2.0282	-3.3223	-0.1736
O	3.0390	-3.1927	-0.1346
O	10.5466	-1.7807	-0.2183
O	15.2692	0.0516	-0.1280
H	-19.9312	4.2956	-0.2333
H	-18.4962	4.9206	-1.0653

H	-18.5704	4.9364	0.7046
H	-18.5207	2.3894	-1.0369
H	-18.5933	2.4050	0.7194
H	-16.3486	3.5580	0.8043
H	-16.2762	3.5437	-0.9559
H	-16.3134	1.0228	-0.9405
H	-16.3856	1.0370	0.8266
H	-12.2085	1.5120	0.9992
H	-12.1478	1.5748	-0.7512
H	-11.7540	-0.9347	-0.8314
H	-11.8136	-0.9954	0.9302
H	-7.7825	0.1678	1.1293
H	-7.7742	0.3965	-0.6044
H	-6.9381	-1.9786	-0.9120
H	-6.9539	-2.2079	0.8236
H	-5.2412	-0.3562	1.0878
H	-5.2295	-0.1231	-0.6584
H	-4.3941	-2.4827	-0.9687
H	-4.3947	-2.7087	0.7854
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H	-0.6493	-0.5884	-0.7417
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H	0.5755	-2.9670	0.8021
H	3.9352	-0.4562	1.0463
H	3.8896	-0.2314	-0.6872
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H	5.5318	-2.4018	0.7569
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H	6.4573	0.1412	-0.7234
H	8.0463	-1.7961	-1.0133
H	8.1071	-2.0029	0.7418
H	10.9636	1.0894	0.9618
H	10.9167	1.2602	-0.7817
H	12.8213	-0.4128	-0.9975
H	12.8820	-0.5581	0.7585
H	15.1246	2.9963	0.9321
H	15.1254	3.0821	-0.8136
H	17.2986	1.7685	-0.8748
H	17.3036	1.7028	0.8743
H	17.4095	4.2269	0.9715
H	17.4071	4.2909	-0.7847
H	19.7419	4.5104	0.0971
H	19.5932	3.0130	-0.8404
H	19.5967	2.9518	0.9293

17chain7



C 18.1362 5.0927 -0.3997

C	17.6220	3.6589	-0.2290
C	16.0893	3.5730	-0.2237
C	15.5955	2.1442	-0.0557
O	14.1472	2.1716	-0.0628
C	13.5344	0.9791	0.0650
C	12.0259	1.1399	0.0466
C	11.3229	-0.2052	0.1495
O	9.9036	0.0711	0.1330
C	9.0948	-1.0075	0.1933
C	7.6366	-0.5911	0.1770
C	6.7133	-1.8005	0.1817
O	5.3634	-1.2832	0.1846
C	4.3793	-2.2067	0.1545
C	3.0163	-1.5423	0.1719
C	1.8954	-2.5655	0.0639
O	0.6580	-1.8200	0.1138
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C	-1.6971	-1.6554	0.0659
C	-2.9802	-2.4511	-0.1218
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C	-5.3081	-2.0115	-0.1618
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C	-7.7620	-1.4759	-0.1990
O	-8.6607	-0.3559	-0.0404
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C	-10.8121	0.6169	0.0150
C	-12.2978	0.3323	-0.1509
O	-12.9773	1.5865	0.0629
C	-14.3282	1.5529	-0.0520
C	-14.9227	2.9269	0.1947
C	-16.4492	2.9502	0.0875
C	-17.0412	4.3426	0.3393
C	-18.5701	4.3701	0.2336
O	14.1175	-0.0745	0.1800
O	9.4918	-2.1472	0.2543
O	4.5726	-3.3989	0.1211
O	-0.4920	-3.7458	-0.1598
O	-5.5384	-3.1783	-0.3747
O	-10.4104	-1.7348	-0.4159
O	-14.9469	0.5499	-0.3163
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H	17.7891	5.5295	-1.3455
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H	18.0211	3.0278	-1.0372
H	15.6869	3.9829	-1.1610
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H	15.9348	1.7002	0.8885
H	15.9393	1.4916	-0.8678
H	11.7341	1.6632	-0.8731
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H	1.9453	-3.1313	-0.8717
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H	-7.9960	-2.2432	0.5459
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H	-10.6064	1.0312	1.0108
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H	-14.5874	3.2654	1.1859
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18chain0



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H	1.0825	-1.9275	-0.8787

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H	-1.0914	-8.3473	0.8787
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H	1.0771	-9.6324	-0.8787
H	-1.0921	-10.9163	-0.8787
H	-1.0921	-10.9163	0.8787
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H	1.0769	-12.2005	-0.8787
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H	-1.0815	-21.1923	0.8785
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H	1.0799	-22.5134	-0.8854

19chain0

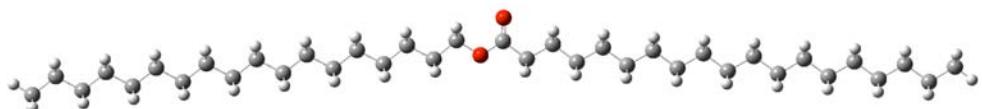


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C	18.6218	0.3876	0.0001
C	17.3372	-0.4520	0.0001
C	16.0536	0.3892	0.0002
C	14.7685	-0.4498	0.0003
C	13.4853	0.3921	0.0003
C	12.1998	-0.4464	0.0004
C	10.9169	0.3960	0.0004
C	9.6311	-0.4420	0.0005
C	8.3485	0.4008	0.0005
C	7.0625	-0.4367	0.0005
C	5.7801	0.4064	0.0005
C	4.4939	-0.4309	0.0005

C	3.2117	0.4125	0.0005
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C	0.6432	0.4188	0.0004
C	-0.6432	-0.4183	0.0004
C	-1.9253	0.4252	0.0003
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C	-5.7801	-0.4059	0.0001
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C	-13.4852	-0.3920	-0.0004
C	-14.7685	0.4497	-0.0004
C	-16.0535	-0.3894	-0.0005
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C	-18.6218	-0.3880	-0.0007
C	-19.9059	0.4524	-0.0007
C	-21.1901	-0.3876	-0.0008
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H	-19.9059	1.1168	-0.8794
H	-19.9059	1.1167	0.8781
H	-21.1911	-1.0521	0.8780
H	-21.1910	-1.0521	-0.8796
H	-22.4745	1.1152	-0.8793
H	-22.4746	1.1151	0.8777
H	-24.6521	0.2329	-0.0009
H	-23.7991	-1.0441	0.8845
H	-23.7990	-1.0440	-0.8864

19chain1



C	-18.3814	-0.9169	-0.0003
C	-17.1619	0.0148	-0.0005
C	-15.8194	-0.7288	-0.0001

C	-14.6010	0.2042	-0.0003
C	-13.2575	-0.5377	0.0001
C	-12.0406	0.3973	0.0000
C	-10.6958	-0.3422	0.0004
C	-9.4810	0.5956	0.0004
C	-8.1344	-0.1407	0.0007
C	-6.9226	0.8009	0.0006
C	-5.5743	0.0681	0.0009
C	-4.3668	1.0154	0.0007
C	-3.0194	0.2802	0.0009
C	-1.8411	1.2429	0.0007
O	-0.6267	0.4592	0.0008
C	0.5294	1.1616	-0.0002
C	1.7285	0.2305	-0.0002
C	3.0660	0.9746	-0.0002
C	4.2746	0.0301	-0.0001
C	5.6187	0.7709	-0.0001
C	6.8364	-0.1629	-0.0001
C	8.1782	0.5821	-0.0002
C	9.3991	-0.3476	-0.0002
C	10.7391	0.4006	-0.0003
C	11.9620	-0.5265	-0.0003
C	13.3008	0.2239	-0.0004
C	14.5250	-0.7016	-0.0003
C	15.8630	0.0502	-0.0004
C	17.0880	-0.8742	-0.0002
C	18.4256	-0.1218	-0.0002
O	0.5752	2.3701	-0.0011
C	-19.7233	-0.1721	-0.0006
C	-20.9434	-1.1027	-0.0002
C	19.6508	-1.0459	0.0000
C	20.9884	-0.2939	0.0001
C	-22.2852	-0.3580	-0.0005
C	-23.4984	-1.2948	-0.0001
C	22.2135	-1.2180	0.0004
C	23.5455	-0.4593	0.0004
H	-18.3332	-1.5792	0.8787
H	-18.3331	-1.5797	-0.8788
H	-17.2105	0.6778	0.8780
H	-17.2104	0.6772	-0.8794
H	-15.7705	-1.3916	-0.8787
H	-15.7707	-1.3911	0.8788
H	-14.6504	0.8670	0.8782
H	-14.6502	0.8665	-0.8792
H	-13.2075	-1.2004	-0.8785
H	-13.2078	-1.1999	0.8791
H	-12.0911	1.0600	0.8785
H	-12.0909	1.0595	-0.8789
H	-10.6444	-1.0047	-0.8783
H	-10.6447	-1.0043	0.8793
H	-9.5330	1.2581	0.8789
H	-9.5328	1.2577	-0.8785
H	-8.0812	-0.8029	-0.8781
H	-8.0814	-0.8026	0.8796
H	-6.9764	1.4630	0.8793

H	-6.9763	1.4628	-0.8782
H	-5.5179	-0.5933	-0.8779
H	-5.5180	-0.5929	0.8800
H	-4.4239	1.6766	0.8796
H	-4.4239	1.6762	-0.8784
H	-2.9468	-0.3738	-0.8797
H	-2.9468	-0.3734	0.8819
H	-1.8438	1.8937	0.8843
H	-1.8439	1.8934	-0.8831
H	1.6402	-0.4315	-0.8740
H	1.6402	-0.4316	0.8735
H	3.1084	1.6376	0.8747
H	3.1085	1.6375	-0.8752
H	4.2242	-0.6325	-0.8789
H	4.2241	-0.6323	0.8788
H	5.6674	1.4334	0.8784
H	5.6674	1.4333	-0.8786
H	6.7878	-0.8253	-0.8789
H	6.7878	-0.8252	0.8788
H	8.2257	1.2449	0.8784
H	8.2256	1.2448	-0.8789
H	9.3522	-1.0103	-0.8789
H	9.3523	-1.0102	0.8787
H	10.7852	1.0635	0.8783
H	10.7852	1.0633	-0.8791
H	11.9164	-1.1894	-0.8790
H	11.9165	-1.1892	0.8785
H	13.3460	0.8868	0.8782
H	13.3459	0.8866	-0.8792
H	14.4803	-1.3645	-0.8790
H	14.4803	-1.3643	0.8785
H	15.9076	0.7133	0.8782
H	15.9076	0.7130	-0.8792
H	17.0437	-1.5372	-0.8789
H	17.0436	-1.5370	0.8786
H	18.4698	0.5412	0.8784
H	18.4700	0.5410	-0.8791
H	-19.7713	0.4902	-0.8795
H	-19.7713	0.4908	0.8780
H	-20.8965	-1.7653	0.8788
H	-20.8965	-1.7659	-0.8788
H	19.6065	-1.7090	-0.8786
H	19.6063	-1.7087	0.8789
H	21.0338	0.3692	0.8787
H	21.0340	0.3689	-0.8788
H	-22.3325	0.3034	-0.8792
H	-22.3325	0.3040	0.8778
H	-24.4410	-0.7326	-0.0003
H	-23.4987	-1.9448	0.8855
H	-23.4987	-1.9454	-0.8853
H	22.1687	-1.8799	-0.8780
H	22.1685	-1.8797	0.8789
H	24.4004	-1.1476	0.0006
H	23.6366	0.1846	0.8858
H	23.6368	0.1844	-0.8851

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