Supporting Information

A force field for poly(oxymethylene) dimethyl ethers (OMEn)

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1. Dihedral potential with Fourier equation

Some simulation codes use the Fourier equation instead of the Ryckaert-Bellemans (RB) equation discussed in the main text. We thus provide the equivalents of our dihedral parameters if the Fourier equation is used instead. The dihedral potential using the Fourier equation with six coefficients a_i is 1:

$$u_{\mathrm{t}} = a_0 + \sum_{i=1}^{5} a_i \left[1 + (-1)^{i+1} \cos(i\theta)\right] \tag{1}$$

The a_i coefficients for OME for the Fourier equation are given in Table S1. The dihedral angle in the RB equation φ is related to the angle θ in the Fourier equation by 2:

$$\varphi = \theta - 180^\circ \tag{2}$$

Table S1: Parameters for the dihedral potential using the Fourier equation.

a_i / K	CH_3-O-CH_2-O (edge)	CH_2-O-CH_2-O (center)
a_0	1037.95	1112.16
a_1	225.21	525.59
a_2	−866.08	−1060.64
a_3	917.08	725.12
a_4	−81.66	−146.37
a_5	53.16	51.24

2. Numerical values of liquid densities at 1 bar from *NPT* simulations

The liquid densities at 1 bar for OMEn (n = 1 - 4), calculated using NPT simulations with MedeA-Gibbs [1] are given in Table S2.

Table S2: Liquid densities at 1 bar for OMEn (n = 1 - 4).

T / K	ρ^{liq} / kg m^{-3}
	OME1
293.05	850.69±1.15
333.16	797.92±2.39
363.15	755.73±1.38
	OME2
293.15	966.02±2.30
333.15	920.34±2.81
363.15	881.52±2.53
	OME3
293.15	1017.5±3.17
333.15	975.24±1.67
942.35	942.35±2.74
	OME4
293.15	1053.0±7.32
333.15	1018.9±4.00
363.15	993.46±3.11

3. Numerical values of VLE properties from GEMC simulations

VLE properties of OME1-OME4 modelled with the present force field, calculated using Gibbs Ensemble Monte Carlo simulations with MedeA-Gibbs [1] are given in Table S3.

Table S3: VLE properties for OME1-OME4.

T / K	p^{s} / bar	ρ^{liq} / kg m^{-3}	ρ^{vap} / kg m^{-3}
		OME1	
336.455	2.179±0.073	794.76±0.968	6.276±0.219
360.490	4.071±0.110	759.59±1.402	11.300±0.376
384.520	7.042±0.107	723.34±0.641	19.129±0.312
408.553	11.563±0.104	683.97±0.532	31.605±0.466
432.585	17.979±0.238	638.52±1.523	50.690±0.877
442.200	21.253±0.241	618.69±1.482	61.127±0.864
		OME2	
386.540	1.237±0.032	850.37±1.267	3.895±0.046
414.150	2.549±0.051	814.25±1.295	8.411±0.209
441.760	5.057±0.152	773.59±1.072	16.556±0.680
469.370	8.630±0.193	727.34±2.425	28.112±0.891
496.980	14.414±0.226	678.29±1.694	45.799±1.110
508.024	17.120±0.278	652.33±2.041	55.977±1.718
		OME3	
452.550	2.029±0.061	831.53±0.853	7.908±0.294
482.720	3.819±0.148	789.59±2.034	14.498±0.862
512.890	6.630±0.128	740.11±1.315	24.730±0.413
543.060	11.620±0.214	690.99±2.920	45.799±1.110
		OME4	
485.175	1.005±0.026	858.07±1.677	4.244±0.116
517.520	2.252±0.063	821.65±2.256	9.470±0.326
549.865	4.480±0.138	769.15±1.756	18.816±0.802
582.210	7.809±0.206	715.17±0.970	33.648±1.442

4. Comparison between two independent MC codes

In addition to the GEMC results computed with MedeA-Gibbs [1], which are discussed in the main text, for several state-points we also calculated the VLE properties of OME1-OME4 with Cassandra [2]. Excellent agreement was observed between the two simulation codes, as illustrated in Figure S1.

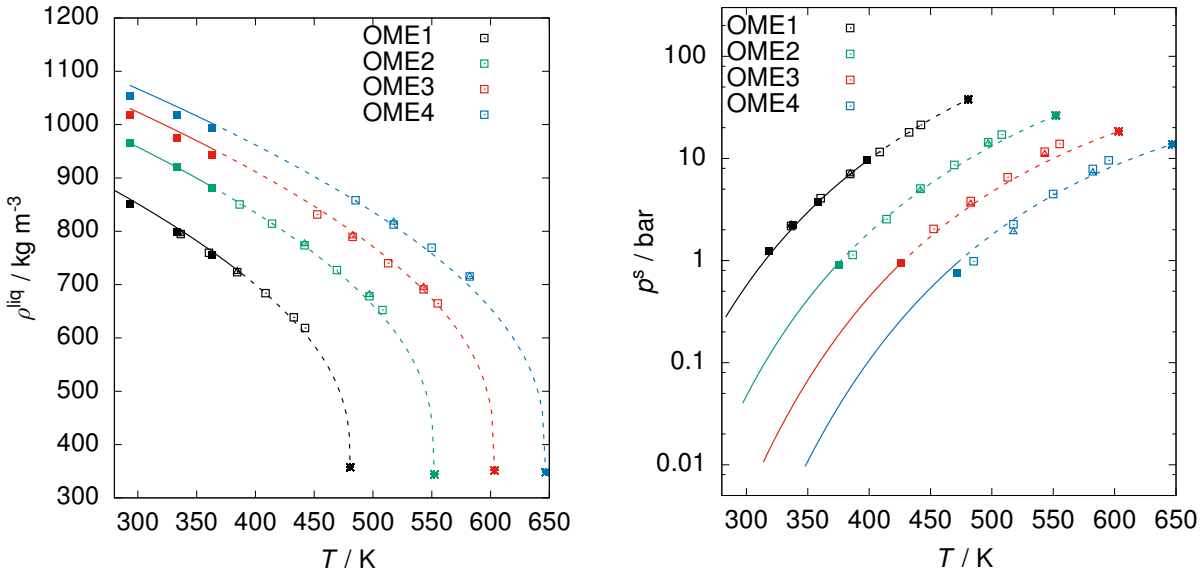

Figure S1: Liquid densities (left) and saturated vapour pressures (right) for OME1-OME4 as a function of temperature. Full lines are correlations of experimental data and dashed lines are extrapolations of these correlations. Filled squares indicate the molecular simulation results obtained with MedeA-Gibbs, at temperatures that were considered for parametrisation. Open squares indicate the molecular simulation results obtained with MedeA-Gibbs, at temperatures that were not considered for parametrisation. Triangles indicate the molecular simulation results obtained with Cassandra. Error bars are within symbol size.

5. Numerical results for solubility from BPE-MC simulations

The numerical results for the pressures in vapour phase for CO_2-OMEn mixtures at 353.15 K, obtained with BPE-MC simulations with MedeA-Gibbs [1] are given in Table S4

Table S4: Solubilities of CO_2 in OMEn for $n = 2$ - 4

x_{CO_2}	p/bar
	OME2
0.064	5.6709±0.4166
0.150	13.083±0.2655
0.280	26.921±0.2492
	OME3
0.030	2.5757±0.0321
0.078	7.2016±0.0530
0.122	10.152±0.3517
0.264	25.559±0.8138
	OME4
0.034	2.7402±0.1413
0.088	7.9732±0.3603
0.192	15.700±0.6535
0.294	27.961±0.8630

6. Shear viscosity

The numerical values of the shear viscosity and density for OME1-OME4 modelled with the present force field are provided in Table S5.

Table S5: Shear viscosity for OME1-OME4.

T / K	ρ^{liq} / kg m^{-3}	η / mPa s
	OME1	
293.15	851.181±0.025	0.2954±0.0151
303.15	838.642±0.029	0.2564±0.0136
313.15	825.579±0.024	0.2265±0.0115
323.15	812.746±0.028	0.2026±0.0103
	OME2	
298.15	960.930±0.033	0.5914±0.0333
303.15	955.111±0.024	0.5585±0.0273
308.15	949.402±0.038	0.5288±0.0253
313.15	943.536±0.042	0.4959±0.0255
318.15	937.635±0.060	0.4646±0.0215
323.15	931.690±0.038	0.4350±0.0193
	OME3	
298.15	1014.860±0.040	0.9125±0.0336
303.15	1009.340±0.031	0.8547±0.0306
308.15	1003.880±0.028	0.8011±0.0270
313.15	998.372±0.027	0.7515±0.0260
318.15	992.858±0.021	0.7103±0.0245
323.15	987.366±0.038	0.6671±0.0197
	OME4	
298.15	1067.770±0.036	1.7227±0.0497
303.15	1062.650±0.041	1.5934±0.0460
308.15	1057.520±0.052	1.4124±0.0435
313.15	1052.280±0.045	1.3385±0.0415
318.15	1047.110±0.045	1.2445±0.0394
323.15	1041.990±0.038	1.1229±0.0376

7. Quantum-Mechanical Calculations

7.1. Bond Lengths and Partial Charges

This section explains the procedure to calculate the bond lengths and the partial charges. The procedure is divided into three subsequent steps: As the first step, a DFT calculation with the 6-311G** Basis set was carried out for obtaining the polarisability α and the permanent dipolar moment μ_0 for each molecule. As

the second step, the Clausius-Mossotti-Debye equation 3

$$\frac{4}{3}\pi\frac{N_A}{V_m}\left(\alpha+\frac{\mu_0^2}{3k_BT}\right)=\frac{\epsilon_r-1}{\epsilon_r+2} \tag{3}$$

was applied in order to calculate the dielectric constant ϵ_r using the reference data [5] for temperature T and molar volume V_m given in Table S6.

Table S6: DFT Results of the first calculation.

Molecule	T / K	V_m / cm^3	α / Å^3	μ_0 / D	ϵ_r
OME1	293.15	88.56	7.29	0.0632	2.650
OME2	298.15	110.55	9.79	0.5078	4.471
OME3	298.15	132.98	12.30	0.0053	1.913
OME4	298.15	155.75	14.85	0.4914	3.407
OME5	298.15	178.32	17.42	0.1214	2.039

As the third step, the dielectric constants were used in a DFT calculation combined with the COSMO [6] solvation model to calculate the partial charges, the bond lengths and the angles. The RESP Method [7] uses 4 layers of spherical isosurfaces with a scaling factor of 1.4 VDW radii for the first shell. The step for each layer is 0.2 VDW radii with a distance of 0.8 Å for each point in the single layer.

In the next subsection of the supporting information the details about the Quantum-Chemical calculations for OMEs, i.e. bond lengths, angles and point charges for the united-atom model are shown. For each OMEn (with n = 1 to 5), the atom coordinates corresponding to the lowest energy configuration are provided including the center of mass and the Z-Matrix.

7.2. Angle Conformational Analysis

In this section, the results about the angle conformational analysis are provided for each angle type. The Quantum-chemical calculations were carried out using Hartree-Fock method with 6-311G** basis set. The angle bending is modelled using a harmonic potential:

$$u_\mathrm{b}=k_\mathrm{b}(\theta-\theta_0)^2/2 \tag{4}$$

where u_b is the bending energy, k_b is the bending constant, and θ_0 and θ are the equilibrium and the bending angle, respectively.

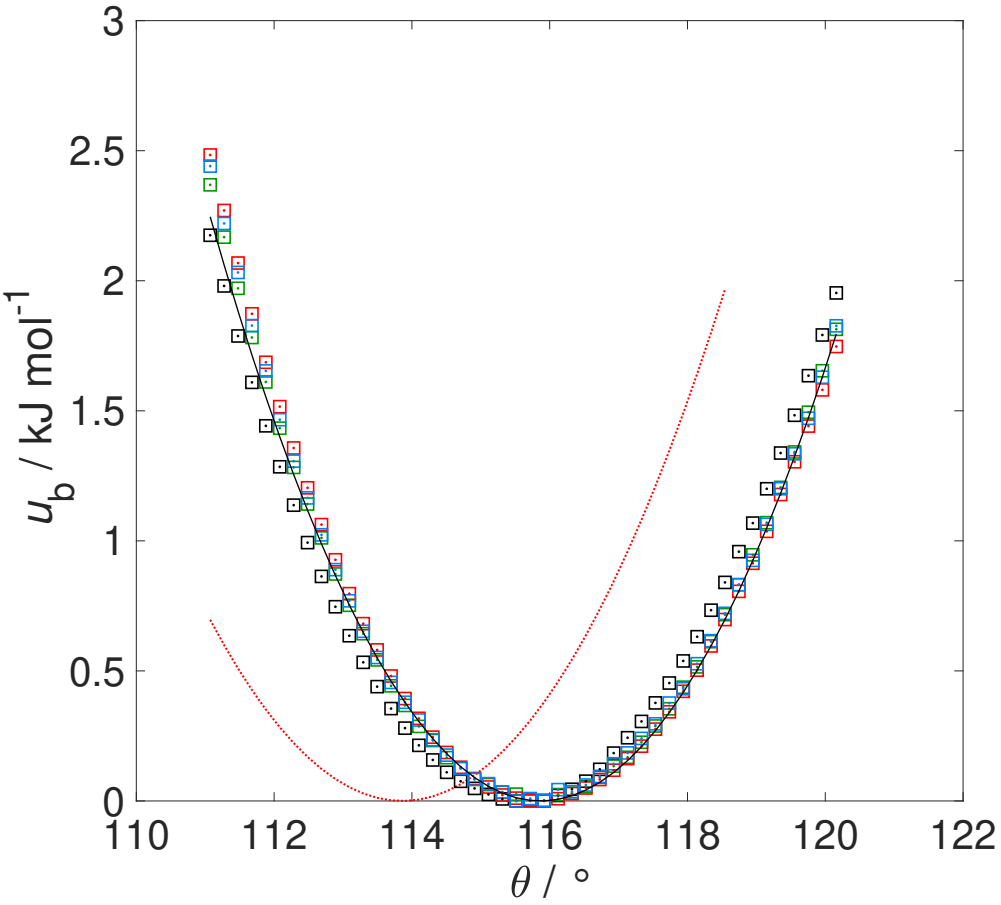

Figure S2: Angle conformational analysis obtained from QM calculations for the CH_3-O-CH_2 angle type. OME1 (black), OME2 (green), OME3 (red) and OME4 (blue). The solid black line (-) represents the fitted harmonic function (eq. 4) for all the OMEs QM calculation and the dotted red line (- - -) is the harmonic potential function from Dasgupta et al. [8].

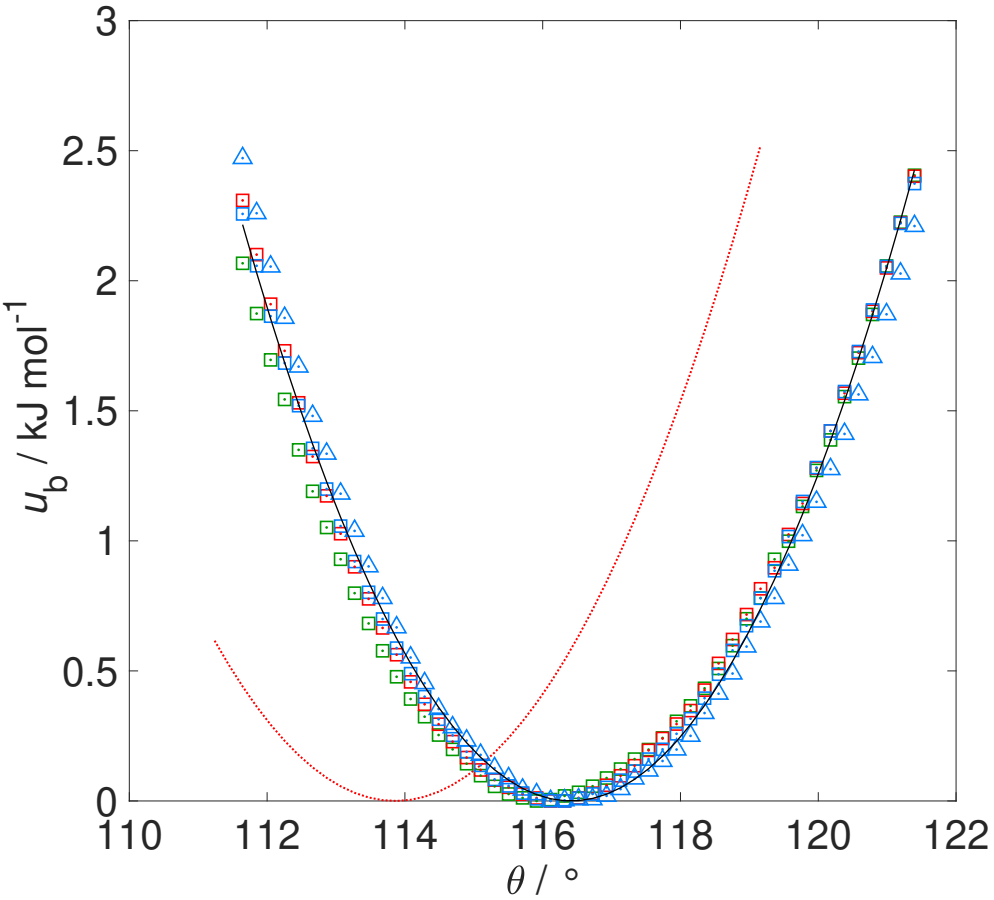

Figure S3: Angle conformational analysis obtained from QM calculations for the CH_2-O-CH_2 angle type. Squares indicate edge angles and triangles indicate central angles. OME1 (black), OME2 (green), OME3 (red) and OME4 (blue). The solid black line (-) represents the fitted harmonic function (eq. 4) for all the OMEs QM calculation and the dotted red line (- - -) is the harmonic potential function from Dasgupta et al. [8].

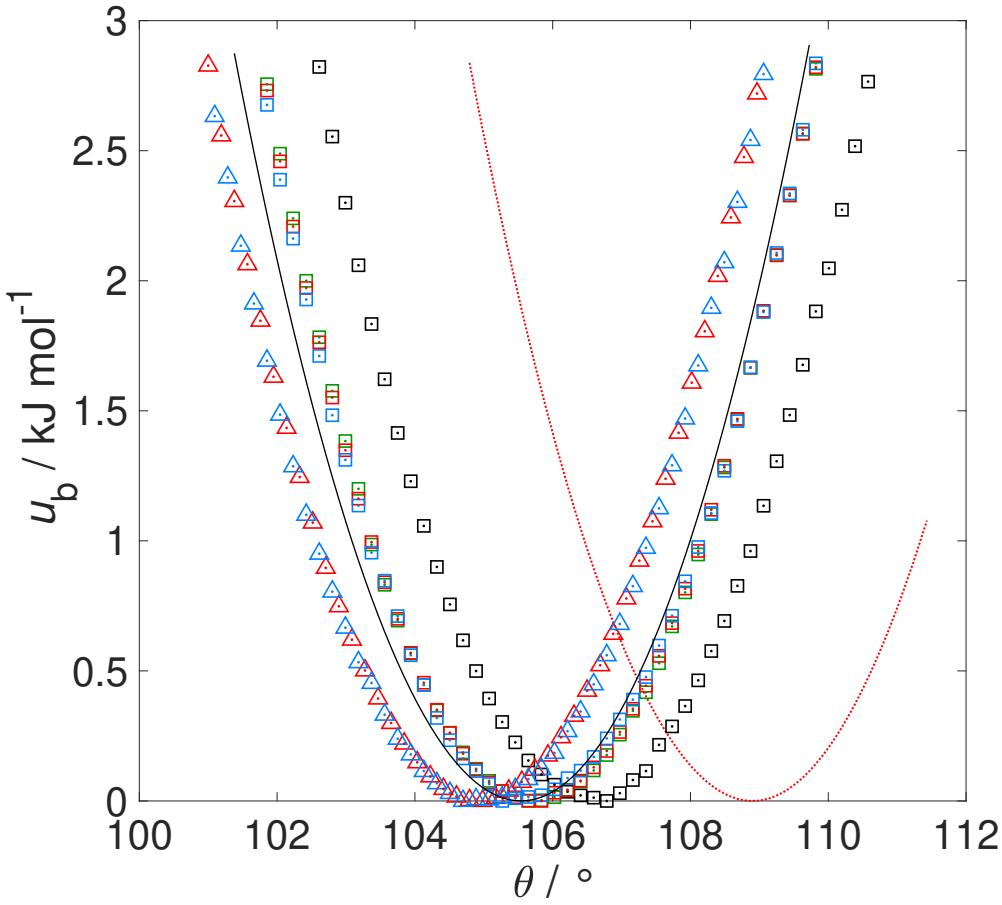

Figure S4: Angle conformational analysis obtained from QM calculations for the O-CH_2-O angle type. Squares indicate edge angles and triangles indicate central angles. OME1 (black), OME2 (green), OME3 (red) and OME4 (blue). The solid black line (-) represents the fitted harmonic function (eq. 4) for all the OMEs QM calculation and the dotted red line (- - -) is the harmonic potential function from Dasgupta et al. [8].

7.3. OME1

In this section the full atom and center of mass coordinates for OME1 are shown in table S7. The table S8 represents the Z-Matrix for equilibrium geometry of united-atom model, and related partial charges are shown in table S9.

Table S7: Full atom coordinates and center of mass (CM) for equilibrium geometry of OME1.

Atom	x/Å	y/Å	z/Å	Group	x_{CM}/Å	y_{CM}/Å	z_{CM}/Å
C	1.856	0.553	0.308				
H	2.312	-0.161	1.004	CH_3	1.903	0.588	0.354
H	1.311	1.309	0.878				
H	2.638	1.034	-0.277				
O	1.004	-0.122	-0.616	O	1.004	-0.122	-0.616
C	0.000	-0.890	-0.003				
H	0.423	-1.515	0.790	CH_2	0.000	-0.980	-0.004
H	-0.422	-1.510	-0.801				
O	-1.006	-0.128	0.615	O	-1.006	-0.128	0.615
C	-1.854	0.557	-0.304				
H	-1.305	1.313	-0.870	CH_3	-1.901	0.592	-0.350
H	-2.315	-0.150	-1.004				
H	-2.633	1.039	0.285				

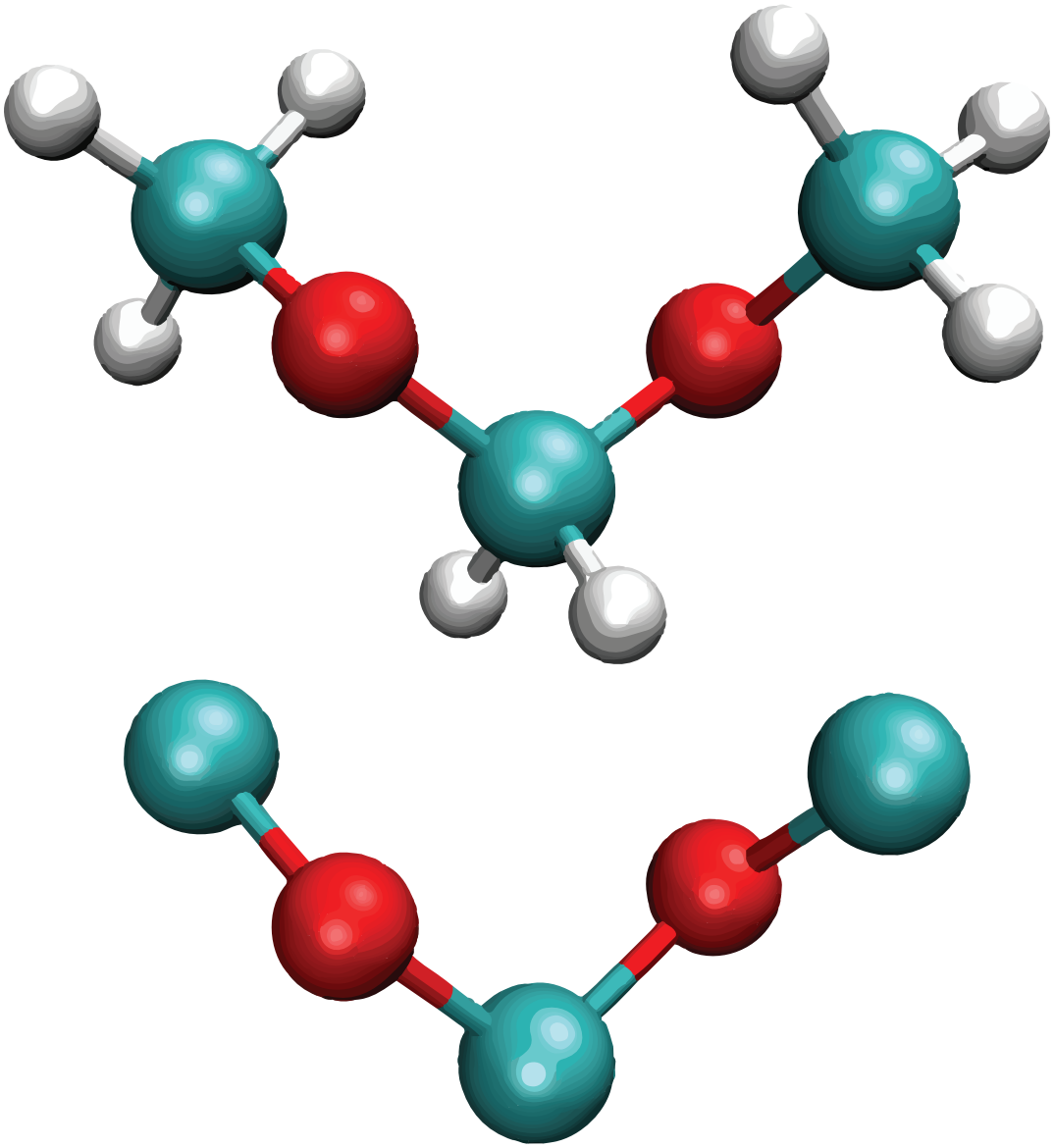

Figure S5: Equilibrium geometry of OME1. Top: full atom representation, bottom: united-atom model.

Table S8: Z-Matrix for equilibrium geometry of OME1 using united-atom model.

Group	ID	Bonds / Å	ID	Angles / °	ID	Dihedrals / °
CH_3						
O	1	1.500				
CH_2	2	1.456	1	114.811		
O	3	1.456	2	108.100	1	71.900
CH_3	4	1.500	3	114.804	2	71.600

Table S9: Point Charges for OME1.

Atom	Charge	Group	Total Charge
C	0.0265	CH_3	0.2195
H	0.0491		
H	0.0772		
H	0.0667		
O	-0.3455	O	-0.3455
C	-0.0342	CH_2	0.2539
H	0.1436		
H	0.1445		
O	-0.3469	O	-0.3469
C	0.0312	CH_3	0.2189
H	0.0742		
H	0.0489		
H	0.0646		

7.4. OME2

In this section the full atom and center of mass coordinates for OME2 are shown in table S10. The table S11 represents the Z-Matrix for equilibrium geometry of united-atom model, and related partial charges are shown in table S12.

Table S10: Full atom coordinates and center of mass (CM) for equilibrium geometry of OME2.

Atom	x/Å	y/Å	z/Å	Group	x_{CM}/Å	y_{CM}/Å	z_{CM}/Å
C	-2.870	-0.359	0.267				
H	-3.273	0.431	0.912	CH_3	-2.922	-0.386	0.312
H	-2.437	-1.146	0.889				
H	-3.672	-0.776	-0.340				
O	-1.903	0.177	-0.638	O	-1.903	0.177	-0.638
C	-0.848	0.851	-0.007				
H	-1.227	1.580	0.715	CH_2	-0.835	0.939	-0.012
H	-0.289	1.347	-0.802				
O	-0.003	-0.008	0.742	O	-0.003	-0.008	-0.742
C	0.838	-0.835	-0.047				
H	0.275	-1.288	-0.864	CH_2	0.824	-0.922	-0.056
H	1.213	-1.601	0.638				
O	1.897	-0.137	-0.644	O	1.897	-0.137	-0.644
C	2.888	0.314	0.281				
H	2.483	1.061	0.968	CH_3	2.941	0.337	0.327
H	3.688	0.759	-0.307				
H	3.286	-0.528	0.859				

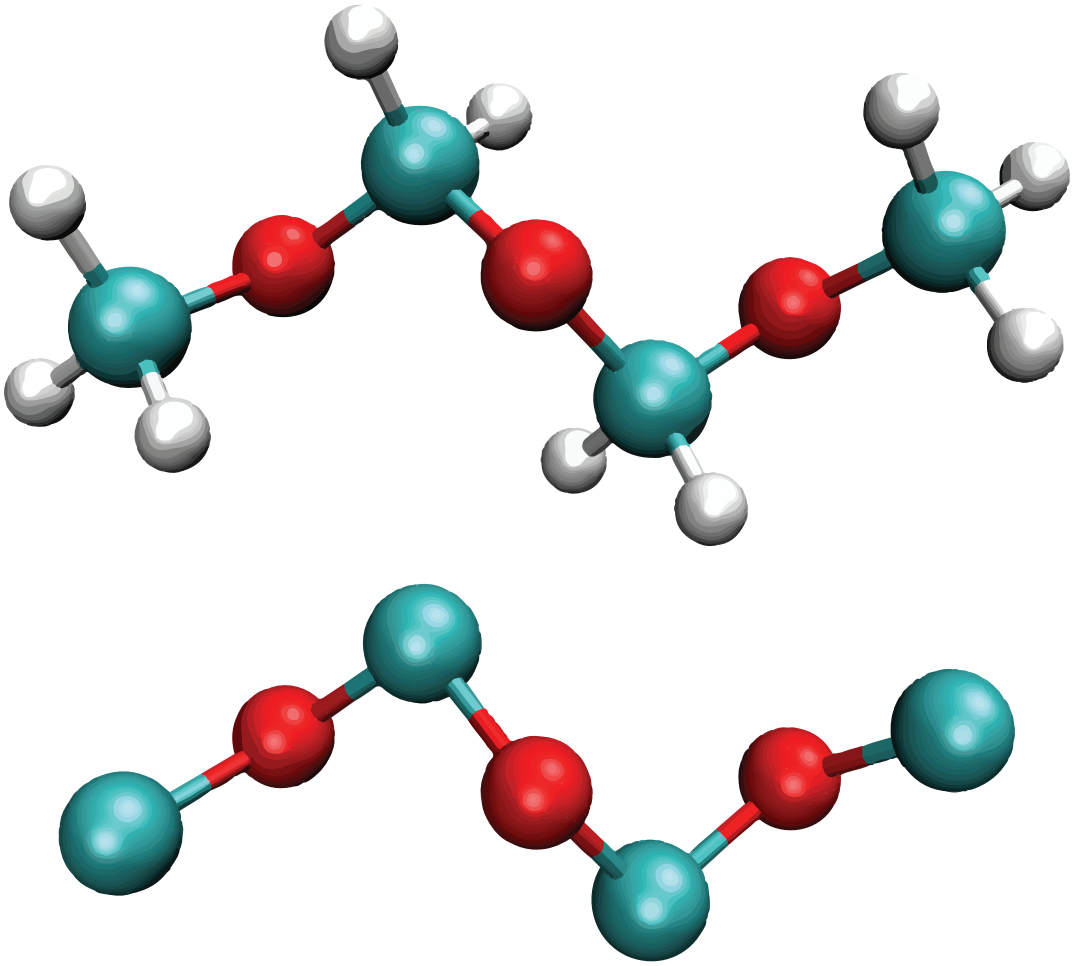

Figure S6: Equilibrium geometry of OME2. Top: full atom representation, bottom: united-atom model.

Table S11: Z-Matrix for equilibrium geometry of OME2 using united-atom model.

Group	ID	Bonds / Å	ID	Angles / °	ID	Dihedrals / °
CH_3						
O	1	1.502				
CH_2	2	1.454	1	115.008		
O	3	1.469	2	107.424	1	69.100
CH_2	4	1.469	3	116.161	2	71.000
O	5	1.453	4	107.375	3	71.700
CH_3	6	1.502	5	114.999	4	70.900

Table S12: Point Charges for OME2.

Atom	Charge	Group	Total Charge
C	-0.0110	CH_3	0.2097
H	0.0632		
H	0.0669		
H	0.0906		
O	-0.4134	O	-0.4134
C	0.2150	CH_2	0.4040
H	0.0907		
H	0.0983		
O	-0.4083	O	-0.4083
C	0.2338	CH_2	0.4140
H	0.0956		
H	0.0846		
O	-0.4090	O	-0.4090
C	-0.0395	CH_3	0.2029
H	0.0762		
H	0.0997		
H	0.0665		

7.5. OME3

In this section the full atom and center of mass coordinates for OME3 are shown in table S13. The table S14 represents the Z-Matrix for equilibrium geometry of united-atom model, and related partial charges are shown in table S15.

Table S13: Full atom coordinates and center of mass (CM) for equilibrium geometry of OME3.

Atom	x/Å	y/Å	z/Å	Group	x_{CM}/Å	y_{CM}/Å	z_{CM}/Å
C	-3.731	-0.612	0.333				
H	-3.189	-1.237	1.048	CH_3	-3.779	-0.642	0.381
H	-4.450	-1.223	-0.211				
H	-4.263	0.178	0.876				
O	-2.850	-0.049	-0.637	O	-2.850	-0.049	-0.637
C	-1.894	0.821	-0.098				
H	-1.413	1.306	-0.948	CH_2	-1.893	0.909	-0.112
H	-2.361	1.560	0.560				
O	-0.933	0.164	0.714	O	-0.933	0.164	-0.714
C	0.000	-0.618	-0.005				
H	-0.501	-1.232	-0.753	CH_2	0.000	-0.707	-0.005
H	0.500	-1.241	0.738				
O	0.934	0.169	-0.715	O	0.934	0.169	-0.715
C	1.894	0.821	0.102				
H	2.363	1.563	-0.551	CH_2	1.893	0.909	0.117
H	1.412	1.301	0.954				
O	2.848	-0.052	0.639	O	2.848	-0.052	0.639
C	3.731	-0.611	-0.333				
H	3.190	-1.233	-1.050	CH_3	3.779	-0.641	-0.381
H	4.449	-1.223	0.210				
H	4.263	0.181	-0.872				

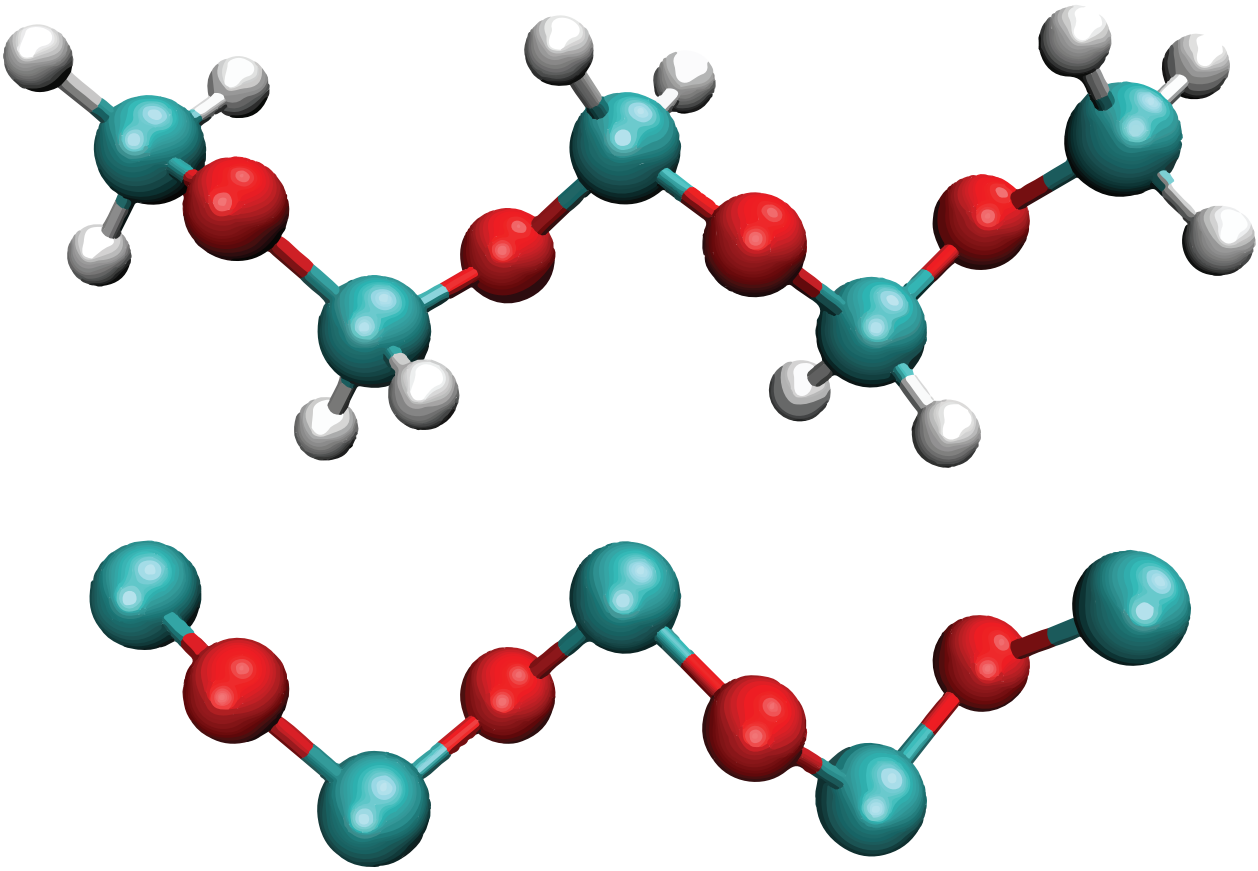

Figure S7: Equilibrium geometry of OME3. Top: full atom representation, bottom: united-atom model.

Table S14: Z-Matrix for equilibrium geometry of OME3 using united-atom model.

Group	ID	Bonds / Å	ID	Angles / °	ID	Dihedrals / °
CH_3						
O	1	1.500				
CH_2	2	1.452	1	115.014		
O	3	1.469	2	107.436	1	69.500
CH_2	4	1.465	3	116.231	2	70.700
O	5	1.465	4	106.765	3	70.500
CH_2	6	1.469	5	116.278	4	70.300
O	7	1.452	6	107.456	5	70.600
CH_3	8	1.500	7	115.025	6	69.400

Table S15: Point Charges for OME3.

Atom	Charge	Group	Total Charge
C	0.0054	CH_3	0.1941
H	0.0537		
H	0.0802		
H	0.0548		
O	-0.3720	O	-0.3720
C	0.1694	CH_2	0.3476
H	0.0763		
H	0.1019		
O	-0.4398	O	-0.4398
C	0.4858	CH_2	0.5368
H	0.0267		
H	0.0243		
O	-0.4472	O	-0.4472
C	0.2219	CH_2	0.3713
H	0.0866		
H	0.0628		
O	-0.3781	O	-0.3781
C	-0.0252	CH_3	0.1873
H	0.0586		
H	0.0908		
H	0.0631		

7.6. OME4

In this section the full atom and center of mass coordinates for OME4 are shown in table S16. The table S17 represents the Z-Matrix for equilibrium geometry of united-atom model, and related partial charges are shown in table S18.

Table S16: Full atom coordinates and center of mass (CM) for equilibrium geometry of OME4.

Atom	x/Å	y/Å	z/Å	Group	x_{CM}/Å	y_{CM}/Å	z_{CM}/Å
C	4.736	-0.430	-0.285				
H	5.464	-1.044	0.242	CH_3	4.778	-0.452	-0.333
H	5.241	0.440	-0.722				
H	4.276	-1.017	-1.084				
O	3.768	-0.017	0.680	O	3.768	-0.017	0.680
C	2.796	0.854	0.174				
H	2.256	1.244	1.037	CH_2	2.790	0.941	0.195
H	3.253	1.667	-0.398				
O	1.900	0.227	-0.734	O	1.900	0.227	-0.734
C	0.987	-0.666	-0.127				
H	0.538	-1.231	-0.944	CH_2	0.992	-0.754	-0.136
H	1.496	-1.331	0.571				
O	-0.001	0.003	0.633	O	-0.001	-0.003	0.633
C	-0.989	0.665	-0.134				
H	-1.498	1.336	0.558	CH_2	-0.993	0.753	-0.144
H	-0.538	1.223	-0.956				
O	-1.901	-0.233	-0.735	O	-1.901	-0.233	-0.735
C	-2.796	-0.855	0.177				
H	-3.256	-1.670	-0.390	CH_2	-2.790	-0.941	0.198
H	-2.255	-1.241	1.041				
O	-3.766	0.020	0.681	O	-3.766	0.020	0.681
C	-4.734	0.431	-0.286				
H	-4.273	1.009	-1.090	CH_3	-4.786	0.453	-0.333
H	-5.458	1.053	0.239				
H	-5.245	-0.439	-0.714				

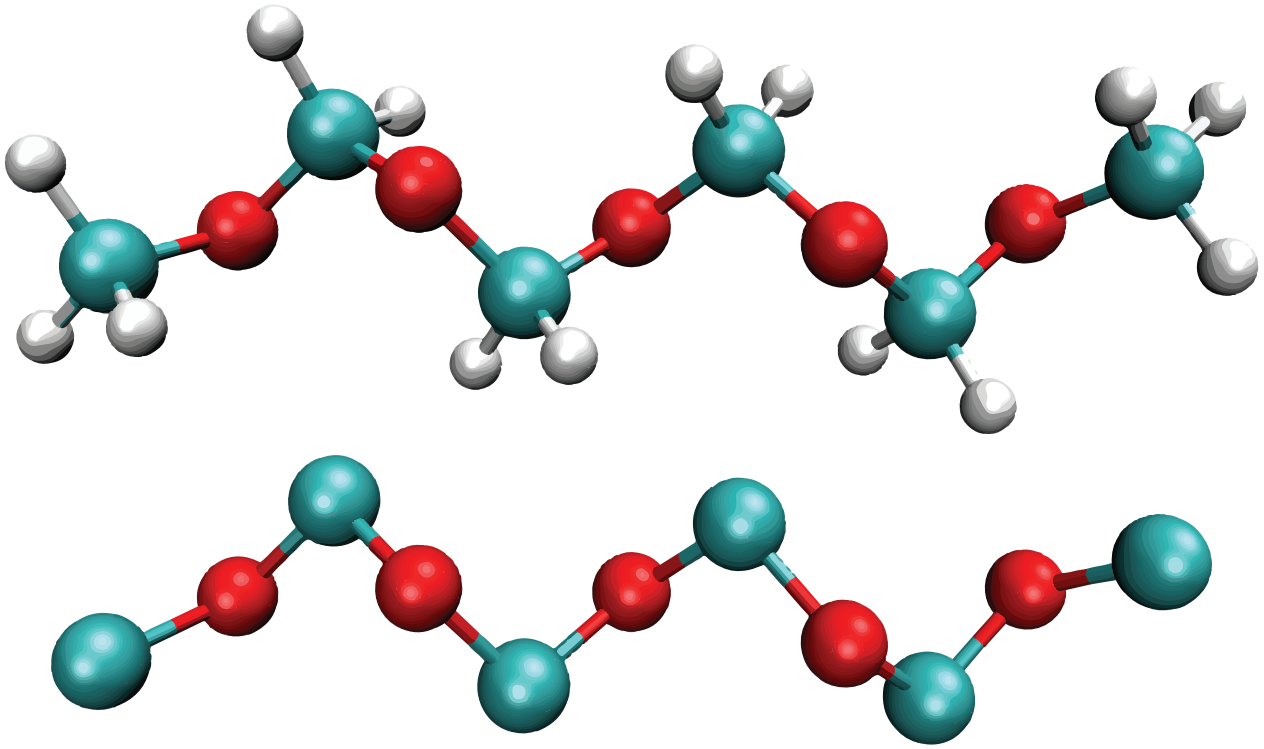

Figure S8: Equilibrium geometry of OME4. Top: full atom representation, bottom: united-atom model.

Table S17: Z-Matrix for equilibrium geometry of OME4 using united-atom model.

Group	ID	Bonds / Å	ID	Angles / °	ID	Dihedrals / °
CH_3						
O	1	1.502				
CH_2	2	1.452	1	115.003		
O	3	1.471	2	107.395	1	71.000
CH_2	4	1.465	3	116.279	2	70.000
O	5	1.466	4	106.722	3	69.600
CH_2	6	1.466	5	116.415	4	71.800
O	7	1.465	6	106.752	5	71.800
CH_2	8	1.471	7	116.309	6	69.500
O	9	1.452	8	107.390	7	69.800
CH_3	10	1.502	9	114.998	8	70.900

Table S18: Point Charges for OME4.

Atom	Charge	Group	Total Charge
C	-0.0867	CH_3	0.1839
H	0.1037		
H	0.0852		
H	0.0817		
O	-0.3428	O	-0.3428
C	0.1024	CH_2	0.3186
H	0.0922		
H	0.1240		
O	-0.4268	O	-0.4268
C	0.4672	CH_2	0.5197
H	0.0112		
H	0.0413		
O	-0.4840	O	-0.4840
C	0.3818	CH_2	0.4808
H	0.0675		
H	0.0315		
O	-0.4171	O	-0.4171
C	0.1243	CH_2	0.3296
H	0.1181		
H	0.0872		
O	-0.3532	O	-0.3532
C	-0.0513	CH_3	0.1912
H	0.0759		
H	0.0924		
H	0.0742		

7.7. OME5

In this section the full atom and center of mass coordinates for OME5 are shown in table S19. The table S20 represents the Z-Matrix for equilibrium geometry of united-atom model, and related partial charges are shown in table S21.

Table S19: Full atom coordinates and center of mass (CM) for equilibrium geometry of OME5.

Atom	x/Å	y/Å	z/Å	Group	x_{CM}/Å	y_{CM}/Å	z_{CM}/Å
C	5.650	0.558	0.476				
H	5.100	0.974	1.324	CH_3	5.697	0.575	0.531
H	6.368	1.292	0.114				
H	6.183	-0.343	0.801				
O	4.777	0.261	-0.613	O	4.777	0.261	-0.613
C	3.822	-0.720	-0.320				
H	3.351	-0.979	-1.270	CH_2	3.821	-0.802	-0.356
H	4.288	-1.600	0.134				
O	2.850	-0.288	0.621	O	2.850	-0.288	0.621
C	1.897	0.614	0.098				
H	1.425	1.085	0.961	CH_2	1.898	0.701	0.114
H	2.371	1.359	-0.541				
O	0.934	-0.032	-0.713	O	0.934	-0.032	0.713
C	-0.001	-0.814	0.004				
H	0.499	-1.428	0.754	CH_2	-0.001	-0.903	0.005
H	-0.500	-1.437	-0.737				
O	-0.935	-0.023	0.712	O	-0.935	-0.023	0.712
C	-1.898	0.613	-0.107				
H	-2.372	1.366	0.524	CH_2	-1.898	0.701	-0.124
H	-1.427	1.075	-0.975				
O	-2.850	-0.295	-0.618	O	-2.850	-0.295	-0.618
C	-3.821	-0.717	0.327				
H	-4.289	-1.600	-0.119	CH_2	-3.821	-0.799	0.363
H	-3.350	-0.968	1.279				
O	-4.776	0.267	0.612	O	-4.776	0.267	0.612
C	-5.649	0.554	-0.480				
H	-5.100	0.962	-1.332	CH_3	-5.696	-0.570	-0.534
H	-6.367	1.290	-0.123				
H	-6.183	-0.350	-0.796				

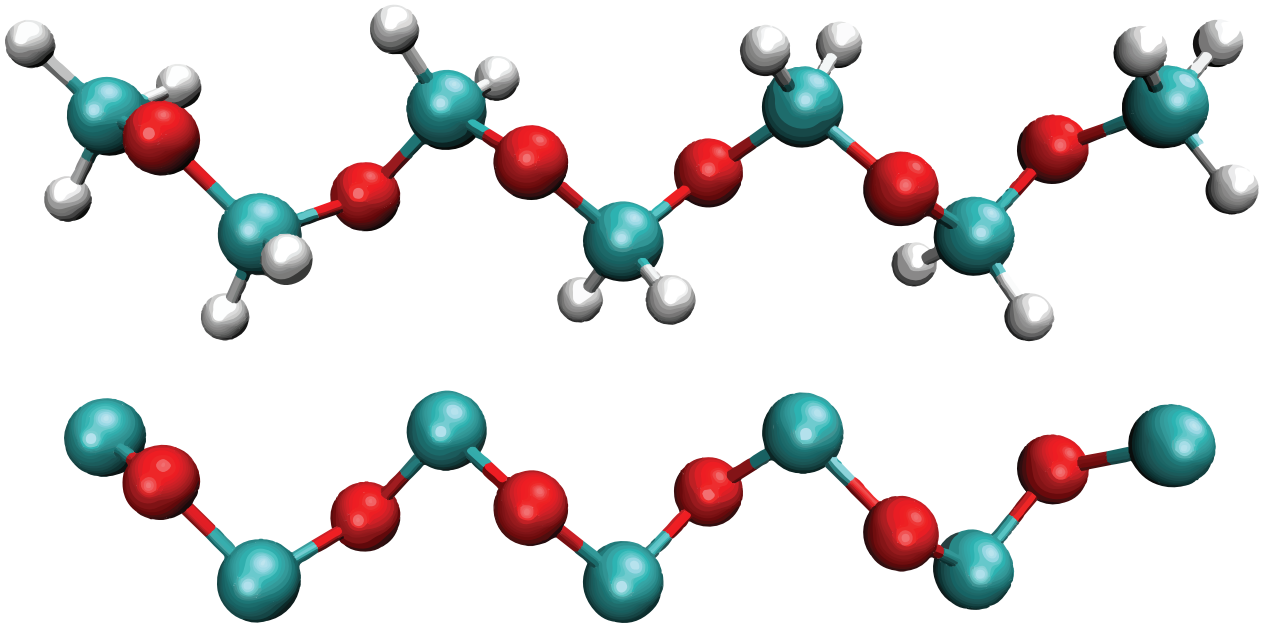

Figure S9: Equilibrium geometry of OME5. Top: full atom representation, bottom: united-atom model.

Table S20: Z-Matrix for equilibrium geometry of OME5 using united-atom model.

Group	ID	Bonds / Å	ID	Angles / °	ID	Dihedrals / °
CH_3						
O	1	1.501				
CH_2	2	1.452	1	114.907		
O	3	1.470	2	107.250	1	69.800
CH_2	4	1.464	3	115.872	2	72.600
O	5	1.467	4	106.545	3	73.900
CH_2	6	1.466	5	116.069	4	70.900
O	7	1.465	6	106.640	5	71.000
CH_2	8	1.467	7	116.094	6	71.100
O	9	1.464	8	106.539	7	70.900
CH_2	10	1.470	9	115.911	8	73.800
O	11	1.452	10	107.261	9	72.400
CH_3	12	1.501	11	114.884	10	69.800

Table S21: Point Charges for OME5.

Atom	Charge	Group	Total Charge
C	-0.0455	CH_3	0.1855
H	0.0698		
H	0.0912		
H	0.0700		
O	-0.3301	O	-0.3301
C	0.0376	CH_2	0.2808
H	0.1115		
H	0.1317		
O	-0.3701	O	-0.3701
C	0.3910	CH_2	0.4677
H	0.0223		
H	0.0544		
O	-0.4730	O	-0.4730
C	0.4516	CH_2	0.4823
H	0.0169		
H	0.0138		
O	-0.4780	O	-0.4780
C	0.3761	CH_2	0.4638
H	0.0646		
H	0.0231		
O	-0.3686	O	-0.3686
C	0.0549	CH_2	0.2908
H	0.1253		
H	0.1106		
O	-0.3404	O	-0.3404
C	-0.0343	CH_3	0.1893
H	0.0685		
H	0.0890		
H	0.0661		

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