

Electronic Supplementary Material

Low-viscosity oligoether esters (OEEs) as high-efficiency lubricating oils: Insight on their structure–lubricity relationship

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Table S1 Names of OEEs and synthetic raw materials.

Name	Alcohols used	Acids used	Ester abbreviations
Diethylene glycol dioctanoate	Diethylene glycol	Octanoic acid	2g-2c8
Diethylene glycol di(2-ethylhexanoate)	Diethylene glycol	2-ethylhexanoic acid	2g-2ci8
Triethylene glycol dioctanoate	Triethylene glycol	Octanoic acid	3g-2c8
Triethylene glycol bis(2-ethylhexanoate)	Triethylene glycol	2-ethylhexanoic acid	3g-2ci8
Tetraethylene glycol dibutyrate	Tetraethylene glycol	butyric acid	4g-2c4
Tetraethylene glycol dihexanoate	Tetraethylene glycol	hexanoic acid	4g-2c6
Tetraethylene glycol dioctanoate	Tetraethylene glycol	Octanoic acid	4g-2c8
Tetraethylene glycol di(2-ethylhexanoate)	Tetraethylene glycol	2-ethylhexanoic acid	4g-2ci8
Tetraethylene glycol didecanoate	Tetraethylene glycol	Decanoic acid	4g-2c12
Hexaethylene glycol dioctanoate	Hexaethylene glycol	Octanoic acid	6g-2c8
Hexaethylene glycol di(2-ethylhexanoate)	Hexaethylene glycol	2-ethylhexanoic acid	6g-2ci8

Details of the synthesis process of OEEs.

In a similar series of esterification reactions, we have detailed the preparation reaction of diethylene glycol diisooctanoate (2g-2ci8). 2-ethylhexanoic acid (100 g, 0.336 mol), diethylene glycol (500 g, 0.14 mol), and p-toluenesulfonic acid (15 g, 0.0168 mol) were mixed in a 1 L round-bottom flask equipped with a water separator and a spherical condenser and stirred in an oil bath at 120 °C for 4 hours. At the end of the reaction, the heating power was disconnected and the reaction mixture was waited until it cooled to room temperature (RT) before proceeding to the next step. The crude product was directed into a separatory funnel and extracted and washed with ethyl acetate and water, respectively. Then the excess isooctanoic acid was removed by saturated sodium bicarbonate. Finally, the pure product was obtained by removing ethyl acetate by distillation under reduced pressure.

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Table S2 Value of 13 molecular descriptors.

TDB1v	TDB1p	DPSA-1	FNSA-2	RNCG	GRAVH-2	RDF140m	RDF145p	L3e	Di	VI	TDB6i	TDB3p
292.8573	2.0213	508.0564	-0.58205	0.17218	46.50448	0.41101	6.18558	0.36284	1.82228	219.634	988.2628	2.94137
292.8573	2.0213	373.1941	-0.69284	0.17241	46.50448	1.80726	7.08739	0.96153	1.50894	227.2	889.2422	3.1062
292.1676	1.99965	539.9252	-0.68296	0.14689	49.45031	0.41321	4.15555	0.36196	1.89982	251.331	993.2573	2.95003
292.1676	1.99965	469.2612	-0.69232	0.14706	49.45031	2.00458	3.02881	0.57616	1.39854	300.1954	912.4958	3.10914
290.7996	2.01915	836.5511	-0.71685	0.11187	58.58327	0.60965	5.95416	0.3785	1.77097	670.129	982.0488	2.96828
293.1535	1.91054	369.9591	-0.76523	0.14983	44.98889	0.20801	0.7684	0.32912	1.74299	158.6227	1013.533	2.9321
292.234	1.95296	512.4352	-0.75724	0.13809	48.74423	0.30955	2.48702	0.34803	1.80225	239.0113	1011.727	2.94775
291.6049	1.98199	623.7167	-0.72282	0.12808	52.23026	0.41013	4.58569	0.36124	1.79536	345.4694	997.2974	2.95727
291.6049	1.98199	551.1281	-0.79805	0.12821	52.23026	1.5023	3.55418	0.84473	1.49253	365.9687	913.491	3.09523
290.7421	1.95492	740.377	-0.9036	0.10196	57.38757	0.41014	4.73566	0.36014	1.77469	493.2551	1003.433	2.96871
290.7421	1.95492	725.1814	-0.88036	0.10205	57.38757	1.50231	3.70415	0.77051	1.47383	528.1547	930.8445	3.08733

¹H and ¹³C chemical shift of each oligoether esters.

2g-2ci8: ¹H NMR (400 MHz, CDCl₃) δ: 4.22–4.21 (m, 4H), 3.68–3.66 (m, 4H), 2.32–2.24 (m, 2H), 1.67–1.54 (m, 4H), 1.54–1.40 (m, 4H), 1.34–1.19 (m, 8H), 0.90–0.85 (m, 12H). ¹³C NMR (100 MHz, CDCl₃) δ: 176.17, 69.07, 62.89, 47.11, 31.56, 29.44, 25.29, 22.49, 13.79, 11.63.

2g-2c8: ¹H NMR (400 MHz, CDCl₃) δ: 4.20–4.25 (m, 4H), 3.70–3.66 (m, 4H), 2.35–2.28 (m, 4H), 1.66–1.56 (m, 4H), 1.34–1.23 (m, 16H), 0.88–0.84 (m, 6H). ¹³C NMR (100 MHz, CDCl₃) δ: 173.87, 77.07, 69.08, 63.23, 33.90, 32.78, 29.36, 25.29, 22.62, 14.32.

3g-2ci8: ¹H NMR (400 MHz, CDCl₃) δ: 4.24–4.21(m, 4H), 3.69–3.66 (m, 4H), 3.62 (s, 4H), 2.31–2.24 (m, 2H), 1.61–1.43 (m, 8H), 1.31–1.21 (m, 8H), 0.89–0.85 (m, 12H). ¹³C NMR (100 MHz, CDCl₃) δ: 176.11, 70.36, 69.15, 62.83, 46.99, 31.50, 29.37, 25.23, 22.42, 13.72, 11.57.

3g-2c8: ¹H NMR (400 MHz, CDCl₃) δ: 4.23–4.20(m, 4H), 3.69–3.64 (m, 4H), 3.62 (s, 4H), 2.32–2.29(m, 4H), 1.64–1.56 (m, 4H), 1.32–1.22 (m, 16H), 0.89–0.84 (m, 6H). ¹³C NMR (100 MHz, CDCl₃) δ: 173.75, 77.23, 76.91, 76.62, 70.58, 69.23, 63.32, 34.16, 31.55, 28.65, 25.01, 22.53, 24.79, 22.62, 14.00.

4g-2c4: ¹H NMR (400 MHz, CDCl₃) δ: 4.23–4.18(m, 4H), 3.68–3.65 (m, 4H), 3.63 (s, 8H), 2.31–2.28 (m, 4H), 1.67–1.60 (m, 4H), 0.96–0.90 (m, 4H). ¹³C NMR (100 MHz, CDCl₃) δ: 173.44, 77.67, 70.62, 69.02, 63.59, 36.09, 18.31, 13.77.

4g-2c6: ¹H NMR (400 MHz, CDCl₃) δ: 4.21–4.18(m, 4H), 3.70–3.65 (m, 4H), 3.63 (s, 8H), 2.32–2.26 (m, 4H), 1.63–1.55 (m, 4H), 1.31–1.25 (m, 8H), 0.88–0.84 (m, 6H). ¹³C NMR (100 MHz, CDCl₃) δ: 173.75, 77.07, 70.64, 69.02, 60.97, 34.21, 31.21, 24.44, 22.18, 13.90.

4g-2c8: ¹H NMR (400 MHz, CDCl₃) δ: 4.21–4.18(m, 4H), 3.68–3.65 (m, 4H), 3.62 (s, 8H), 2.31–2.28 (m, 4H), 1.63–1.56 (m, 4H), 1.27–1.25 (m, 16H), 0.87–0.83 (m, 12H). ¹³C NMR (100 MHz, CDCl₃) δ: 173.85, 70.67, 69.32, 63.41, 34.30, 31.74, 29.16, 29.01, 25.00, 22.72, 14.12.

4g-2ci8: ¹H NMR (400 MHz, CDCl₃) δ: 4.23–4.20(m, 4H), 3.67–3.65 (m, 4H), 3.61 (s, 8H), 2.30–2.23 (m, 2H), 1.63–1.54 (m, 4H), 1.52–1.40 (m, 4H), 1.31–1.19 (m, 8H), 0.88–0.83 (m, 12H). ¹³C NMR (100 MHz, CDCl₃) δ: 176.37, 70.76, 70.66, 69.39, 63.13, 47.27, 31.78, 29.65, 25.51, 22.70, 14.01, 11.85.

4g-2c12: ^1H NMR (400 MHz, CDCl_3) δ : 4.23–4.20(m, 4H), 3.69–3.67 (m, 4H), 3.64 (s, 8H), 2.33–2.29 (m, 4H), 1.63–1.59 (m, 4H), 1.27–1.25 (m, 32H), 0.89–0.85 (m, 12H). ^{13}C NMR (100 MHz, CDCl_3) δ : 173.93, 70.78, 70.72, 69.37, 63.46, 34.36, 32.04, 29.37, 29.60, 29.46, 29.28, 25.06, 22.81, 14.22.

6g-2ci8: ^1H NMR (400 MHz, CDCl_3) δ : 4.22–4.19(m, 4H), 3.67–3.64 (m, 4H), 3.61 (s, 16H), 2.29–2.22 (m, 2H), 1.64–1.37 (m, 8H), 1.31–1.17 (m, 8H), 0.87–0.83 (m, 12H). ^{13}C NMR (100 MHz, CDCl_3) δ : 176.36, 70.72, 70.67, 70.62, 69.36, 63.12, 47.24, 31.76, 29.63, 25.49, 22.68, 14.00, 11.84.

6g-2c8: ^1H NMR (400 MHz, CDCl_3) δ : 4.22–4.18(m, 4H), 3.69–3.65 (m, 4H), 3.63 (s, 16H), 2.32–2.27 (m, 4H), 1.63–1.56 (m, 4H), 1.31–1.23 (m, 16H), 0.88–0.84 (m, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ : 173.99, 77.42, 76.98, 76.65, 70.67, 70.62, 69.36, 63.35, 34.17, 31.56, 28.93, 24.83, 22.58, 14.00.