Supplemental Material

Review of the Influence of Oxygenated Additives on the Combustion Chemistry of Hydrocarbons

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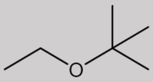
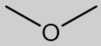
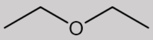
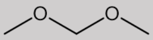
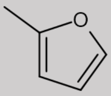
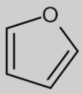
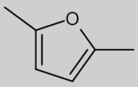
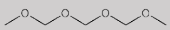
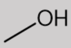
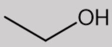
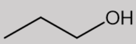
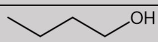
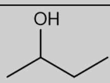
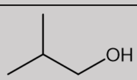
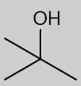
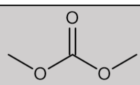
Table S1. The properties of the oxygenated fuels reviewed in this paper

Name	Formula	Structure	Density@ 298K (kg/m³)	Net heat value (MJ/kg)	Oxygen content (wt/%)
Ether					
Ethyl tert-butyl ether (ETBE)	$C_6H_{14}O$		739	35.9	15.7
Dimethyl ether (DME)	C_2H_6O		1.97(gas)	28.8	34.8
Diethyl ether (DEE)	$C_4H_{10}O$		714	33.9	21.6
Dimethoxy methane (DMM)	$C_3H_8O_2$		865	22.4	42.1
2-Methylfuran	C_5H_6O		913	31.2	19.5
Furan	C_4H_4O		942	30.7(*)	23.5
2,5-Dimethylfuran	C_6H_8O		890	33.7	16.7
OME3	$C_5H_{12}O_4$		1020	19.14	47.1
Alcohol					
Methanol	CH_4O		792	19.9	50
Ethanol	C_2H6_O		794	26.9	34.8
n-Propanol	C_3H_8O		804	30.6	26.7
1-Butanol	$C_4H_{10}O$		810	33.2	21.6
2-Butanol	$C_4H_{10}O$		806	32.7	21.6
iso-Butanol	$C_4H_{10}O$		802	33.1	21.6
tert-Butanol	$C_4H_{10}O$		789	29.8	21.6
Ester					
Dimethyl carbonate (DMC)	$C_3H_6O_3$		1070	15.8	53.3

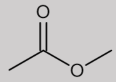
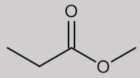
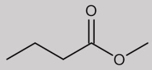
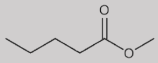
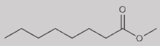
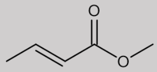
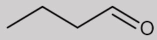
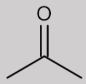
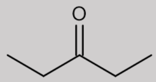
Methyl acetate	$C_3H_6O_2$		940	21.5	43.2
Methyl propanoate	$C_4H_8O_2$		920	25.6	36.4
Methyl butanoate	$C_5H_{10}O_2$		900	28.4	31.4
Methyl pentanoate	$C_6H_{12}O_2$		894	30.7	27.6
Methyl octanoate	$C_9H_{18}0_2$		875	35.0	20.3
Methyl crotonate	$C_5H_8O_2$		944	—	32
Ketone, aldehyde					
Butanal	C_4H_8O		810	34.45	22.2
Acetone	C_3H_6O		791	29.6	27.6
3-Pentanone	$C_5H_{10}O$		820	35.7	18.6

Table S1. Shock tube experimental data of blended fuels studied in literature

Shock tube					
Fuel composition	**Pressure**	**Temperature range [K]**	**Equivalence ratio(φ)**	**measure**	**Reference**
50% iso-octane/ 35% toluene/ 15% 1-hexene/ 0% ETBE	2 bar, 10 bar	1390-1880	1.0	IDT	Yahyaoui et al., Proceedings of the Combustion Institute 31 (2007) 385-391
47.5% iso-octane/ 33.25% toluene/ 14.25% 1-hexene/ 5% ETBE	2 bar, 10 bar	1390-1880	1.0	IDT	Yahyaoui et al., Proceedings of the Combustion Institute 31 (2007) 385-391
45% iso-octane/ 31.5% toluene/ 13.5% 1-hexene/ 10% ETBE	2 bar, 10 bar	1390-1880	1.0	IDT	Yahyaoui et al., Proceedings of the Combustion Institute 31 (2007) 385-391
14.5% n-heptane/ 44.5% iso-octane/ 41% ethanol	10 bar, 30 bar, 50 bar	690-1200	1.0	IDT	Fikri et al., Combustion and Flame 152 (2008) 276-281
17.5% n-heptane/ 55% toluene/ 19.5% iso-octane/ 8.0% diisobutylene	10 bar, 30 bar, 50 bar	690-1200	1.0	IDT	Fikri et al., Combustion and Flame 152 (2008) 276-281
40vol% ethanol/ 37.8vol% iso-octane/ 10.2vol% n-heptane/ 12vol% toluene	10 bar, 30 bar, 50 bar	690-1200	1.0	IDT	Cancino et al., Proceedings of the Combustion Institute 32 (2009) 501-508
0.273 mole% n-heptane/ 0.137 mole% dimethyl ether	20-30 atm	1500-1900	5.0	Soot yield	Hong et al., Fuel 88 (2009) 1901-1906
0.273 mole% n-heptane/ 0.068 mole% butanal	20-30 atm	1500-1900	5.0	Soot yield	Hong et al., Fuel 88 (2009) 1901-1906
0.273 mole% n-heptane/ 0.091 mole% acetone	20-30 atm	1500-1900	5.0	Soot yield	Hong et al., Fuel 88 (2009) 1901-1906
0.247 mole% n-heptane/ 0.091 mole% 3-pentanone	20-30 atm	1500-1900	5.0	Soot yield	Hong et al., Fuel 88 (2009) 1901-1906
25% ethanol/ 75% iso-octane by liquid volume	30 bar	720-1220 K	1.0	IDT	Cancino et al., Fuel 90 (2011) 1238-1244
30% iso-octane/ 25% toluene/ 22% n-heptane/ 13% di-iso-butylene/ 10% ethanol by liquid volume	10 bar, 30 bar	720-1220 K	1.0	IDT	Cancino et al., Fuel 90 (2011) 1238-1244
100% methane/ 0% DME	1 bar, 5 bar, 10 bar	1134-2105	1.0	IDT	Tang et al., Energy Fuels 26 (2012) 6720-6728
99% methane/ 1% DME	1 bar, 5 bar, 10 bar	1134-2105	1.0	IDT	Tang et al., Energy Fuels 26 (2012) 6720-6728
95% methane/ 5% DME	1 bar, 5 bar, 10 bar	1134-2105	1.0	IDT	Tang et al., Energy Fuels 26 (2012) 6720-6728
90% methane/ 10% DME	1 bar, 5 bar, 10 bar	1134-2105	1.0	IDT	Tang et al., Energy Fuels 26 (2012) 6720-6728

Shock tube (continued)					
Fuel composition	**Pressure**	**Temperature range [K]**	**Equivalence ratio(φ)**	**measure**	**Reference**
80% methane/ 20% DME	1 bar, 5 bar, 10 bar	1134-2105	1.0	IDT	Tang et al., Energy Fuels 26 (2012) 6720-6728
50% methane/ 50% DME	1 bar, 5 bar, 10 bar	1134-2105	1.0	IDT	Tang et al., Energy Fuels 26 (2012) 6720-6728
0% methane/ 100% DME	1 bar, 5 bar, 10 bar	1134-2105	1.0	IDT	Tang et al., Energy Fuels 26 (2012) 6720-6728
0% DME/ 100% ethane	2 atm, 20 atm	1100-1500	0.5, 1.0, 2.0		Zhang et al., Energy Fuels 27 (2013) 6247-6254
20% DME/ 80% ethane	2 atm, 20 atm	1100-1500	0.5		Zhang et al., Energy Fuels 27 (2013) 6247-6254
50% DME/ 50% ethane	2 atm, 20 atm	1100-1500	0.5, 1.0		Zhang et al., Energy Fuels 27 (2013) 6247-6254
0% DME/ 100% propane	20 bar	1100-1500	0.5, 1.0, 2.0	IDT	Hu et al., Energy Fuels 27 (2013) 4007-4013
20% DME/ 80% propane	20 bar	1100-1500	1.0, 2.0	IDT	Hu et al., Energy Fuels 27 (2013) 4007-4013
50% DME/ 50% propane	20 bar	1100-1500	0.5, 1.0, 2.0	IDT	Hu et al., Energy Fuels 27 (2013) 4007-4013
80% DME/ 20% propane	20 bar	1100-1500	1.0, 2.0	IDT	Hu et al., Energy Fuels 27 (2013) 4007-4013
100% DME/ 0% propane	20 bar	1100-1500	0.5, 1.0, 2.0	IDT	Hu et al., Energy Fuels 27 (2013) 4007-4013
0% DME/ 100% n-butane	1.2atm, 5.3 atm	1200-1600	1.0	IDT	Hu et al., Energy Fuels 27, (2013) 530-536
30% DME/ 70% n-butane	1.2atm, 5.3 atm	1200-1600	1.0	IDT	Hu et al., Energy Fuels 27, (2013) 530-536
70% DME/ 30% n-butane	1.2atm, 5.3 atm	1200-1600	1.0	IDT	Hu et al., Energy Fuels 27, (2013) 530-536
100% DME/ 0% n-butane	1.2atm, 5.3 atm	1200-1600	1.0	IDT	Hu et al., Energy Fuels 27, (2013) 530-536
100% DME/ 0% n-butane	2 bar, 10 bar, 20 bar	1100-1600	0.5	IDT	Jiang et al., Energy Fuels 27 (2013) 6238-6246
80% DME/ 20% n-butane	2 bar, 10 bar, 20 bar	1100-1600	0.5	IDT	Jiang et al., Energy Fuels 27 (2013) 6238-6246
60% DME/ 40% n-butane	2 bar, 10 bar, 20 bar	1100-1600	0.5	IDT	Jiang et al., Energy Fuels 27 (2013) 6238-6246
40% DME/ 60% n-butane	2 bar, 10 bar, 20 bar	1100-1600	0.5	IDT	Jiang et al., Energy Fuels 27 (2013) 6238-6246
0% DME/ 100% n-butane	2 bar, 10 bar, 20 bar	1100-1600	0.5	IDT	Jiang et al., Energy Fuels 27 (2013) 6238-6246

Shock tube (continued)					
Fuel composition	**Pressure**	**Temperature range [K]**	**Equivalence ratio(φ)**	**measure**	**Reference**
100% LPG/ 0% DME	10 atm	1100-1500	1.0	IDT	Xu et al., Energy Fuels 28 (2014) 7168-7177
90% LPG/ 10% DME	10 atm	1100-1500	1.0	IDT	Xu et al., Energy Fuels 28 (2014) 7168-7177
70% LPG/ 30% DME	5 atm, 10 atm, 15 atm	1100-1500	0.5, 1.0, 1.5	IDT	Xu et al., Energy Fuels 28 (2014) 7168-7177
50% LPG/ 50% DME	10 atm	1100-1500	1.0	IDT	Xu et al., Energy Fuels 28 (2014) 7168-7177
70% propane/ 30% DME	10 atm	1100-1500	1.0	IDT	Xu et al., Energy Fuels 28 (2014) 7168-7177
0% n-butanol/ 100% DME	10 bar	1150-1650	1.0	IDT	Geng et al., Energy Fuels 28 (2014) 4206-4215
20% n-butanol/ 80% DME	10 bar	1150-1650	1.0	IDT	Geng et al., Energy Fuels 28 (2014) 4206-4215
40% n-butanol/ 60% DME	6 bar,10 bar,15 bar	1150-1650	0.5, 1.0, 1.5	IDT	Geng et al., Energy Fuels 28 (2014) 4206-4215
60% n-butanol/ 40% DME	10 bar	1150-1650	1.0	IDT	Geng et al., Energy Fuels 28 (2014) 4206-4215
100 mole% methane/ 0 mole% dimethyl ether	7-41 atm	600-1600	0.3, 0.5, 1.0, 2.0	IDT	Burke et al., Combustion and Flame 162 (2015) 50-59
80 mole% methane/ 20 mole% dimethyl ether	7-41 atm	600-1600	0.3, 0.5, 1.0, 2.0	IDT	Burke et al., Combustion and Flame 162 (2015) 315-330
60 mole% methane/ 40 mole% dimethyl ether	7-41 atm	600-1600	0.3, 0.5, 1.0, 2.0	IDT	Burke et al., Combustion and Flame 162 (2015) 315-330
0 mole% methane/ 100 mole% dimethyl ether	7-41 atm	600-1600	0.3, 0.5, 1.0, 2.0	IDT	Burke et al., Combustion and Flame 162 (2015) 315-330
90% (21.9% n-heptane / 28.7% iso-octane / 49.4% toluene)/ 10% (68.8% 2-butanol/ 31.2% tert-butanol)	20, 40 bar	800-1200	1.0	IDT	AlRamadan et al., Combustion and Flame 162 (2015) 3971-3979
80% (21.9% n-heptane / 28.7% iso-octane / 49.4% toluene)/ 20% (68.8% 2-butanol/ 31.2% tert-butanol)	20, 40 bar	800-1200	1.0	IDT	AlRamadan et al., Combustion and Flame 162 (2015) 3971-3979
90% (22.9% n-heptane / 48.3% iso-octane / 28.8% toluene)/ 10% (68.8% 2-butanol/ 31.2% tert-butanol)	20, 40 bar	800-1200	1.0	IDT	AlRamadan et al., Combustion and Flame 162 (2015) 3971-3979

80% (22.9% n-heptane / 48.3% iso-octane / 28.8% toluene)/ 20% (68.8% 2-butanol/ 31.2% tert-butanol)	20, 40 bar	800-1200	1.0	IDT	AlRamadan et al., Combustion and Flame 162 (2015) 3971-3979
Shock tube (continued)					
Fuel composition	**Pressure**	**Temperature range [K]**	**Equivalence ratio(φ)**	**measure**	**Reference**
2 oxygenated gasolines – Haltermann gasoline (17 mole% ethanol) Coryton gasoline (8 mole% ethanol)	10, 20, 40 bar	650-1250	0.45, 0.9, 1.8	IDT	Lee et al., Combustion and Flame 186 (2017) 114-128 (see also table for RCM)
Multi-component surrogate mixtures HG-KAUST, HG-TPRF, HG-TPRFE (see Ref. for details)	10, 20, 40 bar	650-1250	0.45, 0.9, 1.8	IDT	Lee et al., Combustion and Flame 186 (2017) 114-128 (see also table for RCM)
Multi-component surrogate mixture CG-KAUST, CG-TPRF, CG-TPRFE (see Ref. for details)	10, 20, 40 bar	650-1250	0.45, 0.9, 1.8	IDT	Lee et al., Combustion and Flame 186 (2017) 114-128 (see also table for RCM)
0 mole% dimethoxy methane/ 100 mole% n-heptane	2 atm, 10 atm	1100-1600	0.5, 1.0, 2.0	IDT	Hu et al., Fuel 189 (2017) 350-357
20 mole% dimethoxy methane/ 80 mole% n-heptane	2 atm, 10 atm	1100-1600	0.5, 1.0, 2.0	IDT	Hu et al., Fuel 189 (2017) 350-357
80 mole% dimethoxy methane/ 20 mole% n-heptane	2 atm, 10 atm	1100-1600	0.5, 1.0, 2.0	IDT	Hu et al., Fuel 189 (2017) 350-357
100 mole% dimethoxy methane/ 0 mole% n-heptane	2 atm, 10 atm	1100-1600	0.5, 1.0, 2.0	IDT	Hu et al., Fuel 189 (2017) 350-357
0 mole% Dimethyl ether/ 100 mole% n-pentane	2 atm,10 atm, 20 atm	1100-1600	0.5	IDT	Jiang et al., Fuel 191 (2017) 77-86
50 mole% Dimethyl ether/ 50 mole% n-pentane	2 atm,10 atm, 20 atm	1100-1600	0.5	IDT	Jiang et al., Fuel 191 (2017) 77-86
100 mole% Dimethyl ether/ 0 mole% n-pentane	2 atm,10 atm, 20 atm	1100-1600	0.5	IDT	Jiang et al., Fuel 191 (2017) 77-86
100 mole% Dimethyl ether/ 0 mole% n-butane	2 atm, 10 atm	650-1400	0.5, 1.0	IDT	Jiang et al., Fuel 203 (2017) 316-329
50 mole% Dimethyl ether/ 50 mole% n-butane	2 atm, 10 atm	650-1400	0.5, 1.0	IDT	Jiang et al., Fuel 203 (2017) 316-329
0 mole% Dimethyl ether/ 100 mole% n-butane	2 atm, 10 atm	650-1400	0.5, 1.0	IDT	Jiang et al., Fuel 203 (2017) 316-329

50 mole% 2-methylfuran/ 50 mole% n-heptane	10, 20 bar	672-1207	0.5, 1.0, 1.5	IDT	Tripathi et al., Combustion and Flame 196 (2018), 54-70 (see also table for RCM)
100 mole% n-heptane/ 0 mole% dimethyl carbonate	2 atm, 10 atm	1100-1600	0.5, 1.0, 2.0	IDT	Gao et al., Combustion Science and Technology 190 (5) (2018) 933-948
Shock tube (continued)					
Fuel composition	**Pressure**	**Temperature range [K]**	**Equivalence ratio(φ)**	**measure**	**Reference**
80 mole% n-heptane/ 20 mole% dimethyl carbonate	2 atm, 10 atm	1100-1600	0.5, 1.0, 2.0	IDT	Gao et al., Combustion Science and Technology 190 (5) (2018) 933-948
20 mole% n-heptane/ 80 mole% dimethyl carbonate	2 atm, 10 atm	1100-1600	0.5, 1.0, 2.0	IDT	Gao et al., Combustion Science and Technology 190 (5) (2018) 933-948
0 mole% n-heptane/ 100 mole% dimethyl carbonate	2 atm, 10 atm	1100-1600	0.5, 1.0, 2.0	IDT	Gao et al., Combustion Science and Technology 190 (5) (2018) 933-948
0 mole% ethanol/ 100 mole% methane	3 atm		0.5, 1.0	IDT	Zheng et al., Journal of Engineering for Gas Turbines and Power 141 (2019) 121015
50 mole% ethanol/ 50 mole% methane	3 atm		0.5 1.0	IDT	Zheng et al., Journal of Engineering for Gas Turbines and Power 141 (2019) 121015
100 mole% ethanol/ 0 mole% methane	3 atm		0.5, 1.0	IDT	Zheng et al., Journal of Engineering for Gas Turbines and Power 141 (2019) 121015
50 mole% n-propanol/ 50 mole% methane	3 atm		0.5, 1.0	IDT	Zheng et al., Journal of Engineering for Gas Turbines and Power 141 (2019) 121015
50 mole% methyl propanoate/ 50 mole% methane	3 atm		0.5, 1.0	IDT	Zheng et al., Journal of Engineering for Gas Turbines and Power 141 (2019) 121015
95 mole% methane/ 5 mole% dimethoxy methane	30 bar	600-1500	2, 10	IDT, species	Herzler et al., Combustion and Flame 216 (2020) 293-299
80 mole% methane/ 20 mole% dimethoxy methane	30 bar	600-1500	2, 10	IDT, species	Herzler et al., Combustion and Flame 216 (2020) 293-299
0 mole% dimethyl ether/ 100 mole% n-heptane	0.8 atm, 4.5 atm, 10 atm	1171-1571	1.0	IDT	Lu et al., Fuel 264 (2020) 116812
20 mole% dimethyl ether/ 80 mole% n-heptane	0.8 atm, 4.5 atm, 10 atm	1171-1571	1.0	IDT	Lu et al., Fuel 264 (2020) 116812
50 mole% dimethyl ether/ 50 mole% n-heptane	0.8 atm, 4.5 atm, 10 atm	1171-1571	1.0	IDT	Lu et al., Fuel 264 (2020) 116812
80 mole% dimethyl ether/ 20	0.8 atm, 4.5	1171-1571	1.0	IDT	Lu et al., Fuel 264 (2020)

mole% n-heptane	atm, 10 atm				116812
85 mole% dimethyl ether/ 15 mole% n-heptane	0.8 atm, 4.5 atm, 10 atm	1171-1571	1.0	IDT	Lu et al., Fuel 264 (2020) 116812
95 mole% dimethyl ether/ 5 mole% n-heptane	0.8 atm, 4.5 atm, 10 atm	1171-1571	1.0	IDT	Lu et al., Fuel 264 (2020) 116812
Shock tube (continued)					
Fuel composition	**Pressure**	**Temperature range [K]**	**Equivalence ratio(φ)**	**measure**	**Reference**
100 mole% dimethyl ether/ 0 mole% n-heptane	0.8 atm, 4.5 atm, 10 atm	1171-1571	1.0	IDT	Lu et al., Fuel 264 (2020) 116812
(55% iso-octane/ 25% toluene/ 15% n-heptane/ 5% 1-hexene)	4-60 atm	968-1361	0.5, 1.0	IDT	Cooper et al., Fuel 275 (2020) 118016
50% (55% iso-octane/ 25% toluene/ 15% n-heptane/ 5% 1-hexene)/ 50% ethanol	25 atm	968-1361	0.5	IDT	Cooper et al., Fuel 275 (2020) 118016
15% (55% iso-octane/ 25% toluene/ 15% n-heptane/ 5% 1-hexene)/ 85% ethanol	25 atm	968-1361	0.5	IDT	Cooper et al., Fuel 275 (2020) 118016
50% (55% iso-octane/ 25% toluene/ 15% n-heptane/ 5% 1-hexene)/ 50% methyl acetate	25 atm	968-1361	0.5	IDT	Cooper et al., Fuel 275 (2020) 118016
15% (55% iso-octane/ 25% toluene/ 15% n-heptane/ 5% 1-hexene)/ 85% methyl acetate	25 atm	968-1361	0.5	IDT	Cooper et al., Fuel 275 (2020) 118016
33.3 mole% dimethyl ether/ 33.3 mole% hydrogen/ 33.3 mole% methane	33 bar	700-1150	0.5, 1.0, 2.0	IDT	Vinkeloe et al., Energy Fuels 34 (2020) 2246-2259
0 mole% iso-butane/ 100 mole% dimethyl ether	2 atm, 10 atm	1091-1797	0.5, 1.0, 2.0	IDT	Jiang et al., Fuel 287 (2021) 119486
50 mole% iso-butane/ 50 mole% dimethyl ether	2 atm, 10 atm	1091-1797	0.5, 1.0, 2.0	IDT	Jiang et al., Fuel 287 (2021) 119486
100 mole% iso-butane/ 0 mole% dimethyl ether	2 atm, 10 atm	1091-1797	1.0, 2.0	IDT	Jiang et al., Fuel 287 (2021) 119486

Table S2. JSR/Flow reactor experimental data of blended fuels studied in literature

JSR/flow reactor					
Fuel composition	**Pressure**	**Temperature range [K]**	**Equivalence ratio(φ)**	**measure**	**Reference**
Neat 95% indane	1 atm	950-1350	0.5,1.0	species	Dagaut et al., Energy Fuels 15 (2001) 372-376
95% indane/ 5% dimethoxymethane	1 atm	950-1350	1.0	species	Dagaut et al., Energy Fuels 15 (2001) 372-376
80% kerosene Jet A-1/ 20% rapsed oil methyl ester	10 atm	740-1200	0.5, 0.75, 1.0, 1.5	species	Dagaut et al., Journal of Physical Chemistry A 111 (2007) 3992-4000
5 mole% ethyl tert-butyl ether/ 47.5 mole% iso-octane/ 33.25 mole% toluene/ 14.25 mole% 1-hexene	10 bar	800-1130	1.0	species	Yahyaoui et al., Proceedings of the Combustion Institute 31 (2007) 385-391
0% ethyl tert-butyl ether/ 50 mole% iso-octane/ 35 mole% toluene/ 15 mole% 1-hexene	10bar	800-1130	1.0	species	Yahyaoui et al., Proceedings of the Combustion Institute 31 (2007) 385-391
10 mole% ethyl tert-butyl ether/ 45 mole% iso-octane/ 31.5 mole% toluene/ 13.5 mole% 1-hexene	10 bar	800-1100	1.0	species	Yahyaoui et al., Proceedings of the Combustion Institute 31 (2007) 385-391
85% 1-butanol/ iso-octane/ toluene/ 1-hexene	10 atm	770-1220	0.3, 0.6, 1.0, 2.0	species	Dagaut et al., Fuel 87 (2008) 3313-3321
85% ethanol/ toluene/ iso-octane/ 1-hexene	10 atm	770-1220	0.3, 0.6, 1.0, 2.0	species	Dagaut et al., Energy Fuels 22 (2008) 3499-3505
20 mole% 1-butanol/ 80 mole% n-heptane	10 atm	530-1070	0.5, 1.0	species	Dagaut et al., Energy Fuels 23 (2009) 3527-3535
50 mole% 1-butanol/ 50 mole% n-heptane	10 atm	530-1070	0.5, 1.0	species	Dagaut et al., Energy Fuels 23 (2009) 3527-3535
85% methanol/ toluene/ iso-octane/ 1-hexene	10 atm	770-1140	0.35, 0.6, 1.0, 2.0	species	Togbé et al., Energy Fuels 23 (2009) 1936-1941
50 mole% methyl octanoate/ 50 mole % 1-butanol	10 atm	560-1190	0.5, 1.0	species	Togbé et al., Energy Fuels 24 (2010), 3906-3916
80 mole % methyl octanoate/ 20 mole % 1-butanol	10 atm	560-1190	0.5, 1.0	species	Togbé et al., Energy Fuels 24 (2010), 3906-3916
90% methyl octanoate/ 10% 1-butanol	10 atm	560-1190	0.5, 1.0, 2.0	species	Togbé et al., Energy Fuels 24 (2010), 3906-3916
20 mole% ethanol/ 80 mole% n-heptane	10 atm	530-1070	0.5, 1.0	species	Dagaut et al., Fuel 89 (2010) 280-286
50 mole% ethanol/ 50 mole% n-heptane	10 atm	530-1070	0.5, 1.0	species	Dagaut et al., Fuel 89 (2010) 280-286

JSR/ flow reactor (continued)					
Fuel composition	**Pressure**	**Temperature range [K]**	**Equivalence ratio(φ)**	**measure**	**Reference**
25% iso-octane/ 75% ethanol	10 atm	770-1190	1.0	species	Dagaut et al., Combustion Science and Technology 184 (2012) 1025-1038
50% iso-octane/ 50% ethanol	10 atm	770-1190	1.0	species	Dagaut et al., Combustion Science and Technology 184 (2012) 1025-1038
75% iso-octane/ 25% ethanol	10 atm	770-1190	1.0	species	Dagaut et al., Combustion Science and Technology 184 (2012) 1025-1038
25% iso-octane/ 75% 1-butanol	10 atm	770-1190	1.0	species	Dagaut et al., Combustion Science and Technology 184 (2012) 1025-1038
50% iso-octane/ 50% 1-butanol	10 atm	770-1190	1.0	species	Dagaut et al., Combustion Science and Technology 184 (2012) 1025-1038
75% iso-octane/ 25% 1-butanol	10 atm	770-1190	1.0	species	Dagaut et al., Combustion Science and Technology 184 (2012) 1025-1038
50mole% 1-butanol/ 50 mole% n-heptane	10 bar	770-1070	0.3	species	Saisirirat et al., Proceedings of the Combuszion Institute 33 (2011) 3007-3014
50 mole % ethanol/ 50 mole% n-heptane	10 bar	770-1070	0.3	species	Saisirirat et al., Proceedings of the Combuszion Institute 33 (2011) 3007-3014
Bio-Diesel (B30)	10 atm	560-1030	0.25, 0.5, 1.0, 1.5	species	Ramirez et al., Proceedings of the Combustion Institute 33 (2011) 375-382
49 mole% n-decane/ 21 mole% 1-methylnaphthalene/ 30 mole% methyl octanoate	6 atm, 10 atm	560-1030	0.25, 0.5, 1.0, 1.5	species	Ramirez et al., Proceedings of the Combustion Institute 33 (2011) 375-382
neat n-pentane	970 mbar	450-930	0.7	species	Jin et al., Combustion and Flame 193 (2018) 36–53
neat dimethyl ether	970 mbar	450-930	0.7	species	Jin et al., Combustion and Flame 193 (2018) 36–53
neat ethanol	970 mbar	450-930	0.7	species	Jin et al., Combustion and Flame 193 (2018) 36–53
75 mole% n-pentane/ 25 mole% dimethyl ether (flow reactor)	970 mbar	450-930	0.7	species	Jin et al., Combustion and Flame 193 (2018) 36–53
50 mole% n-pentane/ 50	970 mbar	450-930	0.7	species	Jin et al., Combustion and

mole% dimethyl ether (flow reactor)					Flame 193 (2018) 36–53
JSR/ flow reactor (continued)					
Fuel composition	**Pressure**	**Temperature range [K]**	**Equivalence ratio(φ)**	**measure**	**Reference**
75 mole% n-pentane/ 25 mole % ethanol (flow reactor)	970 mbar	450-930	0.7	species	Jin et al., Combustion and Flame 193 (2018) 36–53
50 mole % n-pentane/ 50 mole % ethanol (flow reactor)	970 mbar	450-930	0.7	species	Jin et al., Combustion and Flame 193 (2018) 36–53
ethanol/ acetylene (flow reactor) 16 different conditions 0-200 ppm ethanol	10-40 bar	575-1075	λ =0.7, 1, 20		Marrodán et al., Energy Fuels 32 (2018) 10078-10087
Neat iso-octane	10 bar	930	0.058	species	Yuan et al., Combustion and Flame 199 (2019) 96–113
Neat ethanol	10 bar	930	0.058	species	Yuan et al., Combustion and Flame 199 (2019) 96–113
Neat toluene	10 bar	930	0.058	species	Yuan et al., Combustion and Flame 199 (2019) 96–113
50% Iso-octane/ 50% ethanol (flow reactor)	10 bar	900	0.058	species	Yuan et al., Combustion and Flame 199 (2019) 96–113
80% Iso-octane/ 20% ethanol (flow reactor)	10 bar	900	0.058	species	Yuan et al., Combustion and Flame 199 (2019) 96–113
90% Iso-octane/ 10% ethanol (flow reactor)	10 bar	900	0.058	species	Yuan et al., Combustion and Flame 199 (2019) 96–113
15.4% Ethanol/ 84.6% toluene (flow reactor)	10 bar	900	0.058	species	Yuan et al., Combustion and Flame 199 (2019) 96–113
35.4% Ethanol/ 64.6% toluene (flow reactor)	10 bar	900	0.058	species	Yuan et al., Combustion and Flame 199 (2019) 96–113
62.2% Ethanol/ 37.8% toluene (flow reactor)	10 bar	900	0.058	species	Yuan et al., Combustion and Flame 199 (2019) 96–113
34.1% iso-octane/ 65.9% toluene (flow reactor)	10 bar	900	0.058	species	Yuan et al., Combustion and Flame 199 (2019) 96–113
60.8% iso-octane/ 39.2% toluene (flow reactor)	10 bar	900	0.058	species	Yuan et al., Combustion and Flame 199 (2019) 96–113
82.3% iso-octane/ 17.7% toluene (flow reactor)	10 bar	900	0.058	species	Yuan et al., Combustion and Flame 199 (2019) 96–113
91% iso-octane/ 9% n-heptene	10 bar	900	0.058	species	Yuan et al., Combustion and Flame 199 (2019) 96–113

(flow reactor)					
JSR/ flow reactor (continued)					
Fuel composition	**Pressure**	**Temperature range [K]**	**Equivalence ratio(φ)**	**measure**	**Reference**
53.2% iso-octane/ 17.0% n-heptene/ 29.8% toluene (flow reactor)	10 bar	900	0.058	species	Yuan et al., Combustion and Flame 199 (2019) 96–113
45.5% iso-octane/ 4.5% n-heptane/ 50% ethanol (flow reactor)	10 bar	900	0.058	species	Yuan et al., Combustion and Flame 199 (2019) 96–113
26.6% iso-octane/ 8.5% n-heptane/ 14.9% toluene/ 50% ethanol (flow reactor)	10 bar	900	0.058	species	Yuan et al., Combustion and Flame 199 (2019) 96–113
Neat dimethyl ether (flow reactor)	50 bar	700-900K	∞ , 20.2,1,0.04	species	Hashemi et al., Combustion and Flame 205 (2019) 80-92
3.1mole% dimethyl ether/ 96.9 mole% methane (flow reactor)	100 bar	450-900	20, 1, 0.06	species	Hashemi et al., Combustion and Flame 205 (2019) 80-92
75 mole% dimethoxymethane/ 25 mole % n-heptane	1 atm	500-1100	0.5, 1.0, 2.0	species	Gao et al., Combustion and Flame 207 (2019) 20-35
50 mole% dimethoxymethane/ 50 mole % n-heptane	1 atm	500-1100	0.5, 1.0, 2.0	species	Gao et al., Combustion and Flame 207 (2019) 20-35
Neat n-heptane	1 atm	500-1100	0.5, 1.0, 2.0	species	Gao et al., Combustion and Flame 207 (2019) 20-35
Neat heptane	10 bar	550-900	0.058	Species (only CO)	Lu et al., Proceedings of the Combustion Institute 37 (2019) 649-656
Neat iso-octane	10 bar	550-900	0.058	Species (only CO)	Lu et al., Proceedings of the Combustion Institute 37 (2019) 649-656
Neat ethanol	10 bar	550-900	0.058	Species (only CO)	Lu et al., Proceedings of the Combustion Institute 37 (2019) 649-656
90% iso-octane/ 10% ethanol (flow reactor)	10 bar	550-900	0.058	Species (only CO)	Lu et al., Proceedings of the Combustion Institute 37 (2019) 649-656
80% iso-octane/ 20% ethanol (flow reactor)	10 bar	550-900	0.058	Species (only CO)	Lu et al., Proceedings of the Combustion Institute 37 (2019) 649-656

50% iso-octane/ 50% ethanol (flow reactor)	10 bar	550-900	0.058	Species (only CO)	Lu et al., Proceedings of the Combustion Institute 37 (2019) 649-656
100% iso-octane/ 0% ethanol (flow reactor)	10 bar	550-900	0.058	Species (only CO)	Lu et al., Proceedings of the Combustion Institute 37 (2019) 649-656
JSR/ flow reactor (continued)					
Fuel composition	**Pressure**	**Temperature range [K]**	**Equivalence ratio(φ)**	**measure**	**Reference**
15% iso-octane/ 85% ethanol (flow reactor)	10 bar	550-900	0.058	Species (only CO)	Lu et al., Proceedings of the Combustion Institute 37 (2019) 649-656
90% iso-octane/ 10% ethanol (flow reactor)	10 bar	650, 875	0.058	species	Lu et al., Combustion and Flame 214 (2020) 167-183
80% iso-octane/ 20% ethanol (flow reactor)	10 bar	650, 875	0.058	species	Lu et al., Combustion and Flame 214 (2020) 167-183
50% iso-octane/ 50% ethanol (flow reactor)	10 bar	650, 875	0.058	species	Lu et al., Combustion and Flame 214 (2020) 167-183
15% iso-octane/ 85% ethanol (flow reactor)	10 bar	650, 875	0.058	species	Lu et al., Combustion and Flame 214 (2020) 167-183
0% iso-octane/ 100% ethanol (flow reactor)	10 bar	550-900	0.058	Species (only CO)	Lu et al., Proceedings of the Combustion Institute 37 (2019) 649-656
50 mole% DEE/ 50 mole% n-pentane	2.5-10 bar	650	1.0	species	Tran et al., Z. Phys. Chem. 2020; 234(7–9): 1269–1293
Neat DEE	5	400-1100	1.0	species	Tran et al., Z. Phys. Chem. 2020; 234(7–9): 1269–1293
Neat pentane	5,10	500-1100	1.0	species	Tran et al., Z. Phys. Chem. 2020; 234(7–9): 1269–1293
4.065 mole% methane/ 0.406 mole% ethane/ 0.045 mole% propane/ 0.238 mole% dimethyl ether (flow reactor)	6 bar	473-973	2	species	Kaczmarek et al., Combustion and Flame 25 (2021) 86-103
3.813 mole% methane/ 0.381 mole% ethane/ 0.042 mole% propane/ 0.471 mole% dimethyl ether (flow reactor)	6 bar	473-973	2	species	Kaczmarek et al., Combustion and Flame 25 (2021) 86-103
7.004 mole% methane/ 0.700 mole% ethane/ 0.078 mole% propane/ 0.410 mole% dimethyl ether (flow reactor)	6 bar	473-973	10	species	Kaczmarek et al., Combustion and Flame 25 (2021) 86-103
6.613 mole% methane/ 0.661 mole% ethane/ 0.073 mole% propane/ 0.816 mole%	6 bar	473-973	10	species	Kaczmarek et al., Combustion and Flame 25 (2021) 86-103

dimethyl ether (flow reactor)					
7.700 mole% methane/ 0.770 mole% ethane/ 0.086 mole% propane/ 0.450 mole% dimethyl ether (flow reactor)	6 bar	473-973	20	species	Kaczmarek et al., Combustion and Flame 25 (2021) 86-103
7.281 mole% methane/ 0.728 mole% ethane/ 0.081 mole% propane/ 0.899 mole% dimethyl ether (flow reactor)	6 bar	473-973	20	species	Kaczmarek et al., Combustion and Flame 25 (2021) 86-103

Table S3. RCM experimental data of blended fuels studied in literature

RCM					
Fuel composition	**Pressure**	**Temperature range[K]**	**Equivalence ratio(φ)**	**measure**	**Reference**
20% n-butanol/80% n-heptane	9 atm	700 K	1.0	species	Karwat et al., Journal of Physical Chemistry A 116 (2012) 12406-12421
50% n-butanol/50% n-heptane	9 atm	700 K	1.0	species	Karwat et al., Journal of Physical Chemistry A 116 (2012) 12406-12421
20% n-butanol/80% n-heptane	15 bar, 20 bar, 30 bar	650-830 K	1.0	IDT	Yang et al., Energy Fuels 27 (2013) 7800-7808
40% n-butanol/60% n-heptane	15 bar, 20 bar, 30 bar	650-830 K	0.4, 1.0, 1.5	IDT	Yang et al., Energy Fuels 27 (2013) 7800-7808
60% n-butanol/40% n-heptane	15 bar, 20 bar, 30 bar	650-830 K	1.0	IDT	Yang et al., Energy Fuels 27 (2013) 7800-7808
100 mole% methane/0 mole% dimethyl ether	7, 20, 30 atm	600-1600	0.3, 0.5, 1.0, 2.0	IDT	Burke et al., Combustion and Flame 162 (2015) 315-330
80 mole% methane/20 mole% dimethyl ether	7, 20, 30 atm	600-1600	0.3, 0.5, 1.0, 2.0	IDT	Burke et al., Combustion and Flame 162 (2015) 315-330
60 mole% methane/40 mole% dimethyl ether	7, 20, 30 atm	600-1600	0.3, 0.5, 1.0, 2.0	IDT	Burke et al., Combustion and Flame 162 (2015) 315-330
0 mole% methane/100 mole% dimethyl ether	7, 20, 30 atm	600-1600	0.3, 0.5, 1.0, 2.0	IDT	Burke et al., Combustion and Flame 162 (2015) 315-330
20% n-butanol/80% n-heptane	20 bar	613-979 K	0.4, 1.0	IDT	Kumar et al., Combustion and Flame 162 (2015) 2466-2479
40% n-butanol/60% n-heptane	20 bar	613-979 K	0.4, 1.0	IDT	Kumar et al., Combustion and Flame 162 (2015) 2466-2479
60% n-butanol/40% n-heptane	20 bar	613-979 K	0.4, 1.0	IDT	Kumar et al., Combustion and Flame 162 (2015) 2466-2479
80% n-butanol/20% n-heptane	20 bar	613-979 K	0.4, 1.0	IDT	Kumar et al., Combustion and Flame 162 (2015) 2466-2479
20% n-butanol/80% iso-octane	20 bar	613-979 K	0.4, 1.0	IDT	Kumar et al., Combustion and Flame 162 (2015) 2466-2479
40% n-butanol/60% iso-octane	20 bar	613-979 K	0.4, 1.0	IDT	Kumar et al., Combustion and Flame 162 (2015) 2466-2479
60% n-butanol/40% iso-octane	20 bar	613-979 K	0.4, 1.0	IDT	Kumar et al., Combustion and Flame 162 (2015) 2466-2479
80% n-butanol/20% iso-octane	20 bar	613-979 K	0.4, 1.0	IDT	Kumar et al., Combustion and Flame 162 (2015) 2466-2479
20 vol% n-butanol/80% (18.38 vol% toluene/9.12 vol%	20 bar	678-858 K	1.0	IDT	Agbro et al., Fuel 187 (2017) 211-219

n-heptane/52.51 vol% iso-octane)					
RCM (continued)					
Fuel composition	**Pressure**	**Temperature range[K]**	**Equivalence ratio(φ)**	**measure**	**Reference**
2 oxygenated gasolines – Haltermann gasoline (17 mole% ethanol) Coryton gasoline (8 mole% ethanol)	10, 20, 40 bar	650-1250	0.45, 0.9, 1.8	IDT	Lee et al., Combustion and Flame 186 (2017) 114-128 (see also table for ST)
Multi-component surrogate mixtures HG-KAUST, HG-TPRF, HG-TPRFE (see Ref. for details)	10, 20, 40 bar	650-1250	0.45, 0.9, 1.8	IDT	Lee et al., Combustion and Flame 186 (2017) 114-128 (see also table for ST)
Multi-component surrogate mixture CG-KAUST, CG-TPRF, CG-TPRFE (see Ref. for details)	10, 20, 40 bar	650-1250	0.45, 0.9, 1.8	IDT	Lee et al., Combustion and Flame 186 (2017) 114-128 (see also table for ST)
20% Dimethyl ether/80% n-butane	16 bar, 30 bar	657-929 K	0.5	IDT	Wu et al., Fuel 225 (2018), 35-46
40% Dimethyl ether/60% n-butane	16 bar, 30 bar	641-920 K	0.5	IDT	Wu et al., Fuel 225 (2018), 35-46
60% Dimethyl ether/40% n-butane	12 bar, 16 bar, 24 bar, 30 bar	634-904 K	0.5	IDT	Wu et al., Fuel 225 (2018), 35-462018
80% Dimethyl ether/20% n-butane	16 bar, 30 bar	622-873 K	0.5	IDT	Wu et al., Fuel 225 (2018), 35-462018
100% Iso-octane/0% ethanol	10 atm	900-1080	1.0	IDT, species	Barraza-Botet et al., Combustion and Flame 188 (2018) 324-336
95% Iso-octane/5% ethanol	10 atm	900-1080	1.0	IDT, species	Barraza-Botet et al., Combustion and Flame 188 (2018) 324-336
89% Iso-octane/11% ethanol	10 atm	900-1080	1.0	IDT, species	Barraza-Botet et al., Combustion and Flame 188 (2018) 324-336
74% Iso-octane/ 26% ethanol	10 atm	900-1080	1.0	IDT, species	Barraza-Botet et al., Combustion and Flame 188 (2018) 324-336
50% Iso-octane/50% ethanol	10 atm	900-1080	1.0	IDT, species	Barraza-Botet et al., Combustion and Flame 188 (2018) 324-336
33% Iso-octane/67% ethanol	10 atm	900-1080	1.0	IDT, species	Barraza-Botet et al., Combustion and Flame 188

					(2018) 324-336
RCM (continued)					
Fuel composition	**Pressure**	**Temperature range**	**Equivalence ratio(φ)**	**measure**	**Reference**
0% Iso-octane/100% ethanol	10 atm	900-1080	1.0	IDT, species	Barraza-Botet et al., Combustion and Flame 188 (2018) 324-336
50 mole% 2-methylfuran/50 mole% n-heptane	10, 20 bar	672-1207	0.5, 1.0, 1.5	IDT	Tripathi et al., Combustion and Flame 196 (2018), 54-70 (see also table for ST)
70% Dimethyl ether/30% ethane	16 bar, 30 bar	624-913 K	0.5	IDT	Shi et al., Combustion Science and Technology 191 (2019) 1201-1218
50% Dimethyl ether/50% ethane	16 bar, 30 bar	624-913 K	0.5, 0.75, 1.0	IDT	Shi et al., Combustion Science and Technology 191 (2019) 1201-1218
40% Dimethyl ether/60% ethane	16 bar, 30 bar	624-913 K	0.5	IDT	Shi et al., Combustion Science and Technology 191 (2019) 1201-1218
30% Dimethyl ether/70% ethane	16 bar, 30 bar	624-913 K	0.5	IDT	Shi et al., Combustion Science and Technology 191 (2019) 1201-1218
100 mole% Dimethyl ether/0 mole% propane	30 bar	602-645 K	1.0	IDT	Dames et al., Combustion and Flame 168 (2016) 310-330
75 mole% Dimethyl ether/25 mole% propane	30 bar	624-679 K	1.0	IDT	Dames et al., Combustion and Flame 168 (2016) 310-330
50 mole% Dimethyl ether/50 mole% propane	30 bar	650-706 K	1.0	IDT	Dames et al., Combustion and Flame 168 (2016) 310-330
25 mole% Dimethyl ether/75 mole% propane	30 bar	673-719 K	1.0	IDT	Dames et al., Combustion and Flame 168 (2016) 310-330
10 mole% Dimethyl ether/90 mole% propane	30 bar	687-898 K	1.0	IDT	Dames et al., Combustion and Flame 168 (2016) 310-330
0 mole% Dimethyl ether/100 mole% propane	30 bar	689-906 K	0.5, 1.0, 2.0	IDT	Dames et al., Combustion and Flame 168 (2016) 310-330

Table S4. Premixed flames of blended fuels studied in literature

Premixed flames					
Fuel composition	**Pressure**	**C/O ratio**	**Equivalence ratio(φ)**	**measure**	**Reference**
86.4% ethylene +13.6% DMM	50 mbar	0.76	2.5	species	Renard et al., Proceedings of the Combustion Institute 29 (2002) 1277-1284
92.5% propene +7.5% ethanol	50 mbar	0.77	2.36	species	Kohse-Höinghaus et al., Proceedings of the Combustion Institute 31 (2007) 1119-1127
85% propene +15% ethanol	50 mbar	0.77	2.41	species	Kohse-Höinghaus et al., Proceedings of the Combustion Institute 31 (2007) 1119-1127
75% propene +25% DME	40 mbar	0.5	1.57	species	Wang et al., The Journal of Physical Chemistry A 112 (2008) 9255-9265
50% propene +50% DME	40 mbar	0.5	1.67	species	Wang et al., The Journal of Physical Chemistry A 112 (2008) 9255-9265
25% propene +75% DME	40 mbar	0.5	1.80	species	Wang et al., The Journal of Physical Chemistry A 112 (2008) 9255-9265
75% propene + 25% ethanol	40 mbar	0.5	1.57	species	Wang et al., The Journal of Physical Chemistry A 112 (2008) 9255-9265
50% propene + 50% ethanol	40 mbar	0.5	1.67	species	Wang et al., The Journal of Physical Chemistry A 112 (2008) 9255-9265
25% propene + 75% ethanol	40 mbar	0.5	1.80	species	Wang et al., The Journal of Physical Chemistry A 112 (2008) 9255-9265
50% ethylene +50% ethanol	30 torr	0.67	2.0	species	Korobeinichev et al., Proceedings of the Combustion Institute 33 (2011) 569-576
86.4% ethylene +13.6% DMM	50 mbar	0.76	2.5	species	Dias et al., Combustion and Flame 158 (2011) 848-859
91.6% ethylene +8.4% DEM	50 mbar	0.79	2.5	species	Dias et al., Combustion and Flame 158 (2011) 848-859

Premixed flames (continued)					
Fuel composition	**Pressure**	**C/O ratio**	**Equivalence ratio(φ)**	**measure**	**Reference**
90% ethylene +10% ethanol	4 atm	0.67	2.01	particles	Salamanca et al., Experimental Thermal and Fluid Science 43 (2012) 71-75
80% ethylene +20% ethanol	4 atm	0.67	2.01	particles	Salamanca et al., Experimental Thermal and Fluid Science 43 (2012) 71-75
70% ethylene +30% ethanol	4 atm	0.67	2.01	particles	Salamanca et al., Experimental Thermal and Fluid Science 43 (2012) 71-75
50% ethylene +50% ethanol	1 atm	0.57	1.7	species	Salamanca et al., Experimental Thermal and Fluid Science 43 (2012) 71-75
82% benzene + 18% ethanol	45 mbar	0.77	2	PAH; soot	Golea et al., J. Phys. Chem. A 116 (2012) 3625-3642
66% benzene + 34% ethanol	45 mbar	0.74	2	PAH; soot	Golea et al., J. Phys. Chem. A 116 (2012) 3625-3642
53% benzene + 47% ethanol	45 mbar	0.70	2	PAH; soot	Golea et al., J. Phys. Chem. A 116 (2012) 3625-3642
41% benzene + 59% ethanol	45 mbar	0.67	2	PAH; soot	Golea et al., J. Phys. Chem. A 116 (2012) 3625-3642
30% benzene + 70% ethanol	45 mbar	0.63	2	PAH; soot	Golea et al., J. Phys. Chem. A 116 (2012) 3625-3642
83.5% n-heptane + 16.5% DMM	30 torr	0.507	1.618	species	Chen et al., Combustion and Flame 159 (2012) 2324-2335
80% n-heptane + 20% DMC	30 torr	0.507	1.618	species	Chen et al., Combustion and Flame 159 (2012) 2324-2335
15.5% toluene + 26.3% n-heptane + 58.2% methanol	30 Torr	0.61	2.00	species	Xu et al., Combustion and flame 160 (2013) 1333-1344
15.5% toluene + 26.2% n-heptane + 58.3% methanol	30 Torr	0.618	2.00	species	Xu et al., Combustion and flame 160 (2013) 1333-1344
83.6% benzene + 16.4% ethanol	45 mbar	0.77	2	species	Dias et al., Combustion and Flame 161 (2014) 2297-2304
90% n-dodecane + 10% n-butanol	1 atm	0.35	1.1	species	Ghiassi et al., Combustion and Flame 161 (2014) 671-679
70% n-dodecane + 30% n-butanol	1 atm	0.35	1.1	species	Ghiassi et al., Combustion and Flame 161 (2014) 671-679
60% n-dodecane + 40% n-butanol	1 atm	0.35	1.1	species	Ghiassi et al., Combustion and Flame 161 (2014) 671-679
90% acetylene + 10% ethanol	40 mbar	0.9	2.4	species	Bierkandt et al., Proceedings of the Combustion Institute

					35 (2015) 803-811
Premixed flames (continued)					
Fuel composition	**Pressure**	**C/O ratio**	**Equivalence ratio(φ)**	**measure**	**Reference**
18.7% toluene + 31.4% n-heptane + 49.9% methyl pentanoate	1 atm	0.5687	1.71	species	Dmitriev et al., Combustion and Flame 162 (2015) 1964-1975
75% 1,3-butadiene +25% n-butanol	20 torr	0.5	1.45	species	Hansen et al., Proceedings of the Combustion Institute 35 (2015) 771-778
50% 1,3-butadiene +50% n-butanol	20 torr	0.5	1.53	species	Hansen et al., Proceedings of the Combustion Institute 35 (2015) 771-778
25% 1,3-butadiene +75% n-butanol	30 torr	0.5	1.62	species	Hansen et al., Proceedings of the Combustion Institute 35 (2015) 771-778
92.6% ethylene +7.4% DMF	1 atm	0.82	2.46	particles	Russo et al., Combustion and Flame 167 (2016) 268-273
94.8% ethylene +5.2% furan	1 atm	0.68	2.01	particles	Conturso et al., Fuel 175 (2016) 137-145
90.0% ethylene +11.0% furan	1 atm	0.68	2.01	particles	Conturso et al., Fuel 175 (2016) 137-145
94.8% ethylene +5.2% furan	1 atm	0.72	2.16	particles	Conturso et al., Fuel 175 (2016) 137-145
90.0% ethylene +11.0% furan	1 atm	0.73	2.16	particles	Conturso et al., Fuel 175 (2016) 137-145
94.8% ethylene +5.2% furan	1 atm	0.77	2.31	particles	Conturso et al., Fuel 175 (2016) 137-145
90.0% ethylene +11.0% furan	1 atm	0.78	2.31	particles	Conturso et al., Fuel 175 (2016) 137-145
94.8% ethylene +5.2% furan	1 atm	0.82	2.46	particles	Conturso et al., Fuel 175 (2016) 137-145
90.0% ethylene +11.0% furan	1 atm	0.83	2.46	particles	Conturso et al., Fuel 175 (2016) 137-145
95.9% ethylene +4.1% 2-methylfuran	1 atm	0.67	2.01	particles	Conturso et al., Fuel 175 (2016) 137-145
91.2% ethylene +8.8% 2-methylfuran	1 atm	0.68	2.01	particles	Conturso et al., Fuel 175 (2016) 137-145
95.9% ethylene +4.1% 2-methylfuran	1 atm	0.72	2.16	particles	Conturso et al., Fuel 175 (2016) 137-145
91.6% ethylene +8.4% 2-methylfuran	1 atm	0.73	2.16	particles	Conturso et al., Fuel 175 (2016) 137-145
95.9% ethylene +4.1% 2-methylfuran	1 atm	0.77	2.31	particles	Conturso et al., Fuel 175 (2016) 137-145

91.2% ethylene +8.8% 2-methylfuran	1 atm	0.77	2.31	particles	Conturso et al., Fuel 175 (2016) 137-145
Premixed flames (continued)					
Fuel composition	**Pressure**	**C/O ratio**	**Equivalence ratio(φ)**	**measure**	**Reference**
95.9% ethylene +4.1% 2-methylfuran	1 atm	0.82	2.46	particles	Conturso et al., Fuel 175 (2016) 137-145
91.2% ethylene +8.8% 2-methylfuran	1 atm	0.83	2.46	particles	Conturso et al., Fuel 175 (2016) 137-145
96.5% ethylene +3.5% 2,5-dimethylfuran	1 atm	0.67	2.01	particles	Conturso et al., Fuel 175 (2016) 137-145
92.4% ethylene +7.6% 2,5-dimethylfuran	1 atm	0.68	2.01	particles	Conturso et al., Fuel 175 (2016) 137-145
96.5% ethylene +3.5% 2,5-dimethylfuran	1 atm	0.72	2.16	particles	Conturso et al., Fuel 175 (2016) 137-145
92.4% ethylene +7.6% 2,5-dimethylfuran	1 atm	0.73	2.16	particles	Conturso et al., Fuel 175 (2016) 137-145
96.5% ethylene +3.5% 2,5-dimethylfuran	1 atm	0.77	2.31	particles	Conturso et al., Fuel 175 (2016) 137-145
92.4% ethylene +7.6% 2,5-dimethylfuran	1 atm	0.78	2.31	particles	Conturso et al., Fuel 175 (2016) 137-145
96.5% ethylene +3.5% 2,5-dimethylfuran	1 atm	0.82	2.46	particles	Conturso et al., Fuel 175 (2016) 137-145
92.4% ethylene +7.6% 2,5-dimethylfuran	1 atm	0.83	2.46	particles	Conturso et al., Fuel 175 (2016) 137-145
80% ethylene +20% ethanol	1 atm	0.76	2.46	particles	Sirignano et al., Energy & Fuels 31 (2017) 2370-2377
75% 1,3-butadiene +25% i-butanol	30 torr	0.5	1.45	species	Braun-Unkhoff et al., Proceedings of the Combustion Institute 36 (2017) 1311-1319
50% 1,3-butadiene +50% i-butanol	30 torr	0.5	1.53	species	Braun-Unkhoff et al., Proceedings of the Combustion Institute 36 (2017) 1311-1319
25% 1,3-butadiene +75% i-butanol	30 torr	0.5	1.62	species	Braun-Unkhoff et al., Proceedings of the Combustion Institute 36 (2017) 1311-1319
75% ethane + 25% DMM	40 mbar	0.5	1.81	species	Sun et al., Proceedings of the Combustion Institute 36 (2017) 449-457
50% ethane + 50% DMM	40 mbar	0.5	1.88	species	Sun et al., Proceedings of the Combustion Institute 36

					(2017) 449-457
25% ethane + 75% DMM	40 mbar	0.5	1.94	species	Sun et al., Proceedings of the Combustion Institute 36 (2017) 449-457
75% ethane + 25% DMC	40 mbar	0.5	1.79	species	Sun et al., Proceedings of the Combustion Institute 36 (2017) 449-457
50% ethane + 50% DMC	40 mbar	0.5	1.87	species	Sun et al., Proceedings of the Combustion Institute 36 (2017) 449-457
25% ethane + 75% DMC	40 mbar	0.5	1.93	species	Sun et al., Proceedings of the Combustion Institute 36 (2017) 449-457
80% methane + 20% methyl butanoate	40 Torr	0.29	1.00	species	Sylla et al., Fuel 207 (2017) 801-813
50% methane + 50% methyl butanoate	40 Torr	0.31	1.00	species	Sylla et al., Fuel 207 (2017) 801-813
92.3% ethylene +7.7% 2,5-dimethylfuran	1 atm	0.68	2.01	particles	Conturso et al., Proceedings of the Combustion Institute 36 (2017) 985-992
92.3% ethylene +7.7% 2,5-dimethylfuran	1 atm	0.73	2.16	particles	Conturso et al., Proceedings of the Combustion Institute 36 (2017) 985-992
92.3% ethylene +7.7% 2,5-dimethylfuran	1 atm	0.78	2.31	particles	Conturso et al., Proceedings of the Combustion Institute 36 (2017) 985-992
92.3% ethylene +7.3% 2,5-dimethylfuran	1 atm	0.83	2.46	particles	Conturso et al., Proceedings of the Combustion Institute 36 (2017) 985-992
50% iso-octane + 50% DME	40 mbar	0.47	1.53	species	Zeng et al., Combustion and Flame 184 (2017) 41-54
20% iso-octane + 80% DME	40 mbar	0.47	1.63	species	Zeng et al., Combustion and Flame 184 (2017) 41-54
50% iso-octane + 50% DEE	40 mbar	0.47	1.51	species	Zeng et al., Combustion and Flame 184 (2017) 41-54
20% iso-octane + 80% DEE	40 mbar	0.47	1.55	species	Zeng et al., Combustion and Flame 184 (2017) 41-54
50% n-butane + 50% DEE	40 mbar	0.52	1.75	species	Tran et al., Combustion and Flame 175 (2017) 47-59
50% n-butane + 50% n-butanol	40 mbar	0.52	1.75	species	Tran et al., Combustion and Flame 175 (2017) 47-59
85% benzene + 15% ethanol	40 mbar	0.70	1.80	species	Zhao et al., Combustion and Flame 197 (2018) 355-368
70% benzene + 30% ethanol	40 mbar	0.70	1.87	species	Zhao et al., Combustion and

					Flame 197 (2018) 355-368
50% benzene + 50% ethanol	40 mbar	0.70	2.01	species	Zhao et al., Combustion and Flame 197 (2018) 355-368
85% benzene + 15% DME	40 mbar	0.70	1.80	species	Zhao et al., Combustion and Flame 197 (2018) 355-368
70% benzene + 30% DME	40 mbar	0.70	1.87	species	Zhao et al., Combustion and Flame 197 (2018) 355-368
50% benzene + 50% DME	40 mbar	0.70	2.01	species	Zhao et al., Combustion and Flame 197 (2018) 355-368
83.3% toluene + 16.7% n-butanol	40 mbar	0.66	1.75	species	Li et al., Physical Chemistry Chemical Physics 20 (2018) 10628-10636
66.7% toluene + 33.3% n-butanol	40 mbar	0.63	1.75	species	Li et al., Physical Chemistry Chemical Physics 20 (2018) 10628-10636
50% toluene + 50% n-butanol	40 mbar	0.61	1.75	species	Li et al., Physical Chemistry Chemical Physics 20 (2018) 10628-10636
94.8% ethylene +5.2% n-butanol	1 atm	0.68	2.01	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
89.0% ethylene + 11.0% n-butanol	1 atm	0.68	2.01	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
94.8% ethylene +5.2% 2-butanol	1 atm	0.68	2.01	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
89.0% ethylene + 11.0% 2-butanol	1 atm	0.68	2.01	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
94.8% ethylene +5.2% i-butanol	1 atm	0.68	2.01	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
89.0% ethylene + 11.0% i-butanol	1 atm	0.68	2.01	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
94.8% ethylene +5.2% t-butanol	1 atm	0.68	2.01	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
89.0% ethylene + 11.0% t-butanol	1 atm	0.68	2.01	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
94.6% ethylene + 5.4% n-butanol	1 atm	0.72	2.16	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
89.1% ethylene + 10.9% n-butanol	1 atm	0.73	2.16	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
94.6% ethylene + 5.4% 2-butanol	1 atm	0.72	2.16	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
89.1% ethylene + 10.9% 2-butanol	1 atm	0.73	2.16	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
94.6% ethylene + 5.4% i-butanol	1 atm	0.72	2.16	particles	Russo et al., Combustion and Flame 199 (2019) 122-130

89.1% ethylene + 10.9% i-butanol	1 atm	0.73	2.16	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
Premixed flames (continued)					
Fuel composition	**Pressure**	**C/O ratio**	**Equivalence ratio(φ)**	**measure**	**Reference**
94.6% ethylene + 5.4% t-butanol	1 atm	0.72	2.16	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
89.1% ethylene + 10.9% t-butanol	1 atm	0.73	2.16	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
94.9% ethylene + 5.1% n-butanol	1 atm	0.77	2.31	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
88.6% ethylene + 11.4% n-butanol	1 atm	0.78	2.31	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
94.9% ethylene + 5.1% 2-butanol	1 atm	0.77	2.31	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
88.6% ethylene + 11.4% 2-butanol	1 atm	0.78	2.31	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
94.9% ethylene + 5.1% i-butanol	1 atm	0.77	2.31	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
88.6% ethylene + 11.4% i-butanol	1 atm	0.78	2.31	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
94.9% ethylene + 5.1% t-butanol	1 atm	0.77	2.31	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
88.6% ethylene + 11.4% t-butanol	1 atm	0.78	2.31	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
95.7% ethylene + 5.3% n-butanol	1 atm	0.82	2.46	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
88.8% ethylene + 11.2% n-butanol	1 atm	0.83	2.46	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
95.7% ethylene + 5.3% 2-butanol	1 atm	0.82	2.46	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
88.8% ethylene + 11.2% 2-butanol	1 atm	0.83	2.46	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
95.7% ethylene + 5.3% i-butanol	1 atm	0.82	2.46	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
88.8% ethylene + 11.2% i-butanol	1 atm	0.83	2.46	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
95.7% ethylene + 5.3% t-butanol	1 atm	0.82	2.46	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
88.8% ethylene + 11.2% t-butanol	1 atm	0.83	2.46	particles	Russo et al., Combustion and Flame 199 (2019) 122-130
50% ethylene + 50% MB	40 mbar	0.51	1.60	species	Salamanca et al., Proceedings of the Combustion Institute 37 (2019) 1725-1732

50% ethylene + 50% MC	40 mbar	0.53	1.60	species	Salamanca et al., Proceedings of the Combustion Institute 37 (2019) 1725-1732
50% 1-butene + 50% MB	40 mbar	0.51	1.60	species	Salamanca et al., Proceedings of the Combustion Institute 37 (2019) 1725-1732
50% 1-butene + 50% MC	40 mbar	0.53	1.60	species	Salamanca et al., Proceedings of the Combustion Institute 37 (2019) 1725-1732
50% i-butene + 50% MB	40 mbar	0.51	1.60	species	Salamanca et al., Proceedings of the Combustion Institute 37 (2019) 1725-1732
50% i-butene + 50% MC	40 mbar	0.53	1.60	species	Salamanca et al., Proceedings of the Combustion Institute 37 (2019) 1725-1732
50% n-heptane + 50% DME	40 mbar	0.47	1.54	species	Wullenkord et al. Combustion and Flame 212 (2020) 323-336
20% n-heptane + 80% DME	40 mbar	0.47	1.65	species	Wullenkord et al. Combustion and Flame 212 (2020) 323-336
80% n-heptane + 20% i-butanol	40 mbar	0.4	1.26	species	Braun-Unkhoff et al., Proceedings of the Combustion Institute (2020)
60% n-heptane + 40% i-butanol	40 mbar	0.4	1.26	species	Braun-Unkhoff et al., Proceedings of the Combustion Institute (2020)
40% n-heptane + 60% i-butanol	40 mbar	0.4	1.27	species	Braun-Unkhoff et al., Proceedings of the Combustion Institute (2020)
90.9% ethylene + 9.1% OME3	1 atm	0.63	2.01	particles	Ferraro et al., Fuel 286 (2021) 119353
90.9% ethylene + 9.1% OME3	1 atm	0.67	2.16	particles	Ferraro et al., Fuel 286 (2021) 119353
90.9% ethylene + 9.1% OME3	1 atm	0.71	2.31	particles	Ferraro et al., Fuel 286 (2021) 119353
90.9% ethylene + 9.1% OME3	1 atm	0.75	2.46	particles	Ferraro et al., Fuel 286 (2021) 119353