

Supporting Information for “Sooting tendencies of oxygenated hydrocarbons in laboratory-scale flames”

Charles S. McEnally and Lisa D. Pfefferle*

Department of Chemical Engineering and Center for Combustion Studies, Yale University, New Haven

CT 06520-8286

*e-mail: charles.mcenally@yale.edu, phone: 203-432-4059, fax: 203-432-4387

Supporting Information Summary

Number of Pages: 17

Number of Figures: 1

Number of Tables: 2

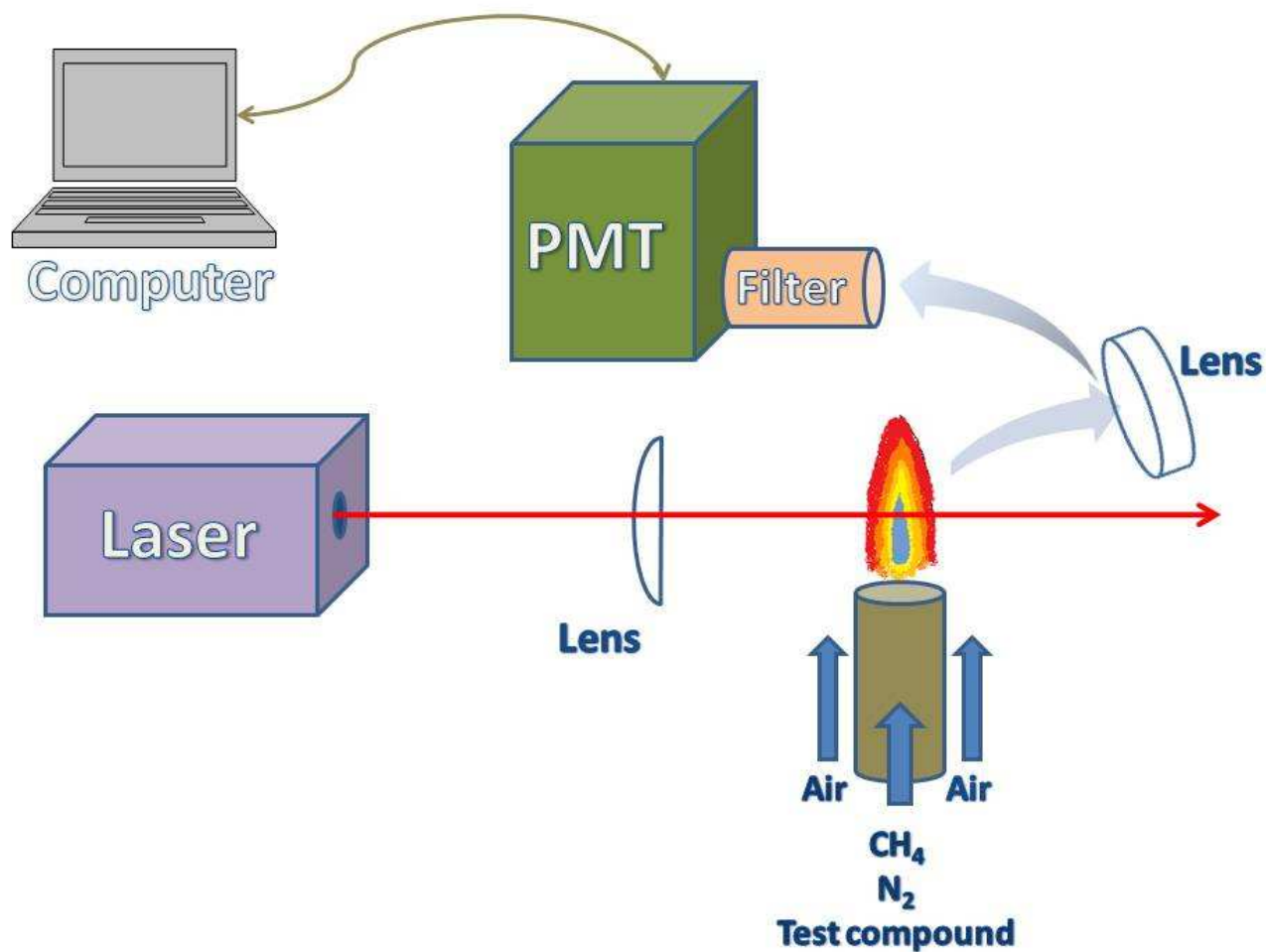


Figure S1. Diagram showing the experimental apparatus.

Table S1. Yield Sooting Indices measured for regular and oxygenated hydrocarbons and scaled such that YSI(n-hexane) = 0.0 and YSI(benzene) = 100.0.

Name (synonym)	Formula	CAS # ^a	YSI ^b
<i>Linear Alkanes</i>			
n-pentane	C ₅ H ₁₂	109-66-0	-8.9
n-hexane	C ₆ H ₁₄	110-54-3	0.0 ^c
2-methylpentane	C ₆ H ₁₄	107-83-5	9.8
3-methylpentane	C ₆ H ₁₄	96-14-0	12.2
2,2-dimethylbutane	C ₆ H ₁₄	75-83-2	20.2

2,3-dimethylbutane	C ₆ H ₁₄	79-29-8	21.1
n-heptane	C ₇ H ₁₆	142-82-5	8.7
2-methylhexane	C ₇ H ₁₆	591-76-4	18.6
3-methylhexane	C ₇ H ₁₆	589-34-4	19.6
2,2-dimethylpentane	C ₇ H ₁₆	590-35-2	26.5
2,3-dimethylpentane	C ₇ H ₁₆	565-59-3	29.6
2,4-dimethylpentane	C ₇ H ₁₆	108-08-7	29.9
3,3-dimethylpentane	C ₇ H ₁₆	562-49-2	26.9
2,2,3-trimethylbutane	C ₇ H ₁₆	464-06-2	38.7
n-octane	C ₈ H ₁₈	111-65-9	18.9
2-methylheptane	C ₈ H ₁₈	592-27-8	29.5
3-methylheptane	C ₈ H ₁₈	589-81-1	28.5
4-methylheptane	C ₈ H ₁₈	589-53-7	27.5
2,2-dimethylhexane	C ₈ H ₁₈	590-73-8	34.8
2,4-dimethylhexane	C ₈ H ₁₈	589-43-5	39.9
2,5-dimethylhexane	C ₈ H ₁₈	592-13-2	39.9
3,4-dimethylhexane	C ₈ H ₁₈	583-48-2	38.5
2,2,4-trimethylpentane (isooctane)	C ₈ H ₁₈	540-84-1	48.6
2,3,4-trimethylpentane	C ₈ H ₁₈	565-75-3	47.3
n-nonane	C ₉ H ₂₀	111-84-2	30.6
2,3-dimethylheptane	C ₉ H ₂₀	3074-71-3	46.3
n-decane	C ₁₀ H ₂₂	124-18-5	41.7
n-undecane	C ₁₁ H ₂₄	1120-21-4	53.3
n-dodecane	C ₁₂ H ₂₆	112-40-3	64.2
2,2,4,6,6-pentamethylheptane (isododecane)	C ₁₂ H ₂₆	13475-82-6	106.9
<i>Cyclic Alkanes</i>			
cyclopentane	C ₅ H ₁₀	287-92-3	14.0
cyclohexane	C ₆ H ₁₂	110-82-7	19.1

methylcyclopentane	C ₆ H ₁₂	96-37-7	30.9
cycloheptane	C ₇ H ₁₄	291-64-5	30.4
methylcyclohexane	C ₇ H ₁₄	108-87-2	36.0
ethylcyclopentane	C ₇ H ₁₄	1640-89-7	43.8
cyclooctane	C ₈ H ₁₆	292-64-8	42.4
ethylcyclohexane	C ₈ H ₁₆	1678-91-7	47.1
1,1-dimethylcyclohexane	C ₈ H ₁₆	590-66-9	58.2
cis 1,2-dimethylcyclohexane	C ₈ H ₁₆	2207-01-4	54.1
1,3-dimethylcyclohexane ^d	C ₈ H ₁₆	591-21-9	57.7
1,4-dimethylcyclohexane	C ₈ H ₁₆	589-90-2	57.7
propylcyclohexane	C ₉ H ₁₈	1678-92-8	60.3
isopropylcyclohexane	C ₉ H ₁₈	696-29-7	68.8
1,2,4-trimethylcyclohexane	C ₉ H ₁₈	2234-75-5	81.4
butylcyclohexane	C ₁₀ H ₂₀	1678-93-9	72.0

Alkenes

cis 2-pentene	C ₅ H ₁₀	627-20-3	14.7
2-methyl-2-butene	C ₅ H ₁₀	513-35-9	20.4
1-hexene	C ₆ H ₁₂	592-41-6	18.7
cis 2-hexene	C ₆ H ₁₂	7688-21-3	22.3
trans 2-hexene	C ₆ H ₁₂	4050-45-7	23.9
trans 3-hexene	C ₆ H ₁₂	13269-52-8	26.1
2-methyl-1-pentene	C ₆ H ₁₂	763-29-1	19.4
3-methyl-1-pentene	C ₆ H ₁₂	760-20-3	22.9
4-methyl-1-pentene	C ₆ H ₁₂	691-37-2	30.8
2-methyl-2-pentene	C ₆ H ₁₂	625-27-4	36.0
3-methyl-2-pentene	C ₆ H ₁₂	922-61-2	36.2
cis 4-methyl-2-pentene	C ₆ H ₁₂	691-38-3	36.8
2-ethyl-1-butene	C ₆ H ₁₂	760-21-4	23.6

2,3-dimethyl-1-butene	C ₆ H ₁₂	563-78-0	35.8
2,3-dimethyl-2-butene	C ₆ H ₁₂	563-79-1	49.7
3,3-dimethyl-1-butene	C ₆ H ₁₂	558-37-2	35.3
1-heptene	C ₇ H ₁₄	592-76-7	27.9
cis 2-heptene	C ₇ H ₁₄	6443-92-1	31.7
trans 3-heptene	C ₇ H ₁₄	14686-14-7	35.9
2-methyl-1-hexene	C ₇ H ₁₄	6094-02-6	29.1
4-methyl-1-hexene	C ₇ H ₁₄	3769-23-1	39.4
3-ethyl-2-pentene	C ₇ H ₁₄	816-79-5	45.7
4,4-dimethyl-1-pentene	C ₇ H ₁₄	762-62-9	48.1
2,3,3-trimethyl-1-butene	C ₇ H ₁₄	594-56-9	65.9
1-octene	C ₈ H ₁₆	111-66-0	39.8
trans 2-octene	C ₈ H ₁₆	13389-42-9	40.8
trans 3-octene	C ₈ H ₁₆	14919-01-8	44.1
trans 4-octene	C ₈ H ₁₆	14850-23-8	45.6
2-methyl-1-heptene	C ₈ H ₁₆	15870-10-7	40.7
2-methyl-2-heptene	C ₈ H ₁₆	627-97-4	53.0
2,3,4-trimethyl-2-pentene	C ₈ H ₁₆	565-77-5	87.9
2,4,4-trimethyl-1-pentene	C ₈ H ₁₆	107-39-1	59.2
2,4,4-trimethyl-2-pentene	C ₈ H ₁₆	107-40-4	91.4
1-nonene	C ₉ H ₁₈	124-11-8	52.8
1-decene	C ₁₀ H ₂₀	872-05-9	69.0
1-dodecene	C ₁₂ H ₂₄	112-41-4	93.0
<i>Cyclic Alkenes</i>			
cyclopentene	C ₅ H ₈	142-29-0	61.8
cyclohexene	C ₆ H ₁₀	110-83-8	23.7
1-methylcyclopentene	C ₆ H ₁₀	693-89-0	102.7
cycloheptene	C ₇ H ₁₂	628-92-2	71.6

Alkynes and Alkadienes

1-pentyne	C_5H_8	627-19-0	26.2
2-pentyne	C_5H_8	627-21-4	37.7
2-methyl-1,5-hexadiene	C_7H_{12}	4049-81-4	58.0
1-octyne	C_8H_{14}	629-05-0	67.8

Alcohols

methanol	CH_4O	67-56-1	-36.9
ethanol	C_2H_6O	64-17-5	-31.1
1-propanol	C_3H_8O	71-23-8	-22.0
2-propanol	C_3H_8O	67-63-0	-17.3
1-butanol -13.0	$C_4H_{10}O$	71-36-3	
2-butanol -8.6	$C_4H_{10}O$	78-92-2	
(R)-2-butanol -8.1	$C_4H_{10}O$	14898-79-4	
(S)-2-butanol -7.8	$C_4H_{10}O$	4221-99-2	
2-methyl-1-propanol -6.5	$C_4H_{10}O$	78-83-1	
tert-butanol -4.5	$C_4H_{10}O$	75-65-0	
1-pentanol -7.7	$C_5H_{12}O$	71-41-0	
2-pentanol -0.3	$C_5H_{12}O$	6032-29-7	
3-pentanol -2.0	$C_5H_{12}O$	584-02-1	
2-methyl-1-butanol 3.0	$C_5H_{12}O$	137-32-6	
2-methyl-2-butanol 3.9	$C_5H_{12}O$	75-85-4	

3-methyl-1-butanol 2.4	$C_5H_{12}O$	123-51-3
3-methyl-2-butanol 4.5	$C_5H_{12}O$	598-75-4
1-hexanol -0.6	$C_6H_{14}O$	111-27-3
2-hexanol 5.8	$C_6H_{14}O$	626-93-7
3-hexanol 5.5	$C_6H_{14}O$	623-37-0
2-methyl-1-pentanol 8.4	$C_6H_{14}O$	105-30-6
2-methyl-2-pentanol 9.4	$C_6H_{14}O$	590-36-3
3-methyl-1-pentanol 9.2	$C_6H_{14}O$	589-35-5
3-methyl-2-pentanol 11.4	$C_6H_{14}O$	565-60-6
4-methyl-1-pentanol 8.1	$C_6H_{14}O$	626-89-1
4-methyl-2-pentanol 18.1	$C_6H_{14}O$	108-11-2
2-ethyl-1-butanol 17.6	$C_6H_{14}O$	97-95-0
2,3-dimethyl-2-butanol 15.9	$C_6H_{14}O$	594-60-5
3,3-dimethyl-1-butanol 16.3	$C_6H_{14}O$	624-95-3
3,3-dimethyl-2-butanol 15.5	$C_6H_{14}O$	464-07-3
cyclohexanol 18.5	$C_6H_{12}O$	108-93-0
1-heptanol 6.7	$C_7H_{16}O$	111-70-6
2-heptanol 14.0	$C_7H_{16}O$	543-49-7
3-heptanol	$C_7H_{16}O$	589-82-2

12.6		
4-heptanol 12.6	$C_7H_{16}O$	589-55-9
2-methyl-2-hexanol 17.8	$C_7H_{16}O$	625-23-0
5-methyl-2-hexanol 22.3	$C_7H_{16}O$	627-59-8
3-ethyl-3-pentanol 15.7	$C_7H_{16}O$	597-49-9
2,2-dimethyl-3-pentanol 24.2	$C_7H_{16}O$	3970-62-5
2,4-dimethyl-3-pentanol 17.9	$C_7H_{16}O$	600-36-2
1-octanol 16.7	$C_8H_{18}O$	111-87-5
2-octanol 24.4	$C_8H_{18}O$	123-96-6
3-octanol 20.6	$C_8H_{18}O$	589-98-0
4-octanol 20.8	$C_8H_{18}O$	589-62-8
2-ethyl-1-hexanol 31.1	$C_8H_{18}O$	104-76-7
2-propyl-1-pentanol 31.2	$C_8H_{18}O$	58175-57-8
2,4,4-trimethyl-1-pentanol 44.4	$C_8H_{18}O$	16325-63-6
<i>Ethers</i>		
methyl propyl ether -19.2	$C_4H_{10}O$	557-17-5
diethyl ether -21.1	$C_4H_{10}O$	60-29-7
methyl butyl ether -11.4	$C_5H_{12}O$	628-28-4
methyl sec-butyl ether	$C_5H_{12}O$	6795-87-5

-2.8			
methyl tert-butyl ether 1.7	$C_5H_{12}O$	1634-04-4	
dipropyl ether -3.7	$C_6H_{14}O$	111-43-3	
diisopropyl ether 12.9	$C_6H_{14}O$	108-20-3	
methyl tert-amyl ether 12.0	$C_6H_{14}O$	994-05-8	
tert-butyl ethyl ether 11.7	$C_6H_{14}O$	637-92-3	
methyl cyclopentyl ether 49.6	$C_6H_{12}O$	5614-37-9	
dibutyl ether 12.9	$C_8H_{18}O$	142-96-1	
sec-butyl ether 36.6	$C_8H_{18}O$	6863-58-7	
isoamyl ether	$C_{10}H_{22}O$	544-01-4	51.6

Alkanones

2-propanone (acetone)	C_3H_6O	67-64-1	-26.9
2-butanone	C_4H_8O	78-93-3	-20.5
2-pentanone -14.4	$C_5H_{10}O$	107-87-9	
3-pentanone -14.4	$C_5H_{10}O$	96-22-0	
3-methyl-2-butanone -5.9	$C_5H_{10}O$	563-80-4	
2-hexanone -7.4	$C_6H_{12}O$	591-78-6	
3-hexanone -7.6	$C_6H_{12}O$	589-38-8	
2-methyl-3-pentanone 0.5	$C_6H_{12}O$	565-69-5	
3-methyl-2-pentanone -2.1	$C_6H_{12}O$	565-61-7	

4-methyl-2-pentanone 3.7	$C_6H_{12}O$	108-10-1	
3,3-dimethyl-2-butanone 15.8	$C_6H_{12}O$	75-97-8	
cyclohexanone 6.1	$C_6H_{10}O$	108-94-1	
2-heptanone 0.0	$C_7H_{14}O$	110-43-0	
3-heptanone 0.5	$C_7H_{14}O$	106-35-4	
4-heptanone -2.9	$C_7H_{14}O$	123-19-3	
2-methyl-3-hexanone 8.5	$C_7H_{14}O$	7379-12-6	
2,4-dimethyl-3-pentanone 18.9	$C_7H_{14}O$	565-80-0	
4,4-dimethyl-2-pentanone 19.2	$C_7H_{14}O$	590-50-1	
2-octanone 11.7	$C_8H_{16}O$	111-13-7	
3-octanone 8.8	$C_8H_{16}O$	106-68-3	
5-methyl-3-heptanone 20.3	$C_8H_{16}O$	541-85-5	
2-nonanone 22.9	$C_9H_{18}O$	821-55-6	
3-nonanone 19.6	$C_9H_{18}O$	925-78-0	
5-nonanone 17.7	$C_9H_{18}O$	502-56-7	
2,6-dimethyl-4-heptanone 39.4	$C_9H_{18}O$	108-83-8	
2,2,4,4-tetramethyl-3-pentanone 55.0	$C_9H_{18}O$	815-24-7	
2-decanone	$C_{10}H_{20}O$	693-54-9	33.4
3-decanone	$C_{10}H_{20}O$	928-80-3	30.7

Aldehydes

propanal (propionaldehyde)	C_3H_6O	123-38-6	-25.5
butanal	C_4H_8O	123-72-8	-19.9
isobutanal	C_4H_8O	78-84-2	-14.3
pentanal -14.4	$C_5H_{10}O$	110-62-3	
2-methylbutanal -11.9	$C_5H_{10}O$	96-17-3	
3-methylbutanal -3.8	$C_5H_{10}O$	590-86-3	
2,2-dimethylpropanal 0.4	$C_5H_{10}O$	630-19-3	
hexanal -5.7	$C_6H_{12}O$	66-25-1	
2-methylpentanal -4.3	$C_6H_{12}O$	123-15-9	
2-ethylbutanal -2.1	$C_6H_{12}O$	97-96-1	
3,3-dimethylbutanal 12.4	$C_6H_{12}O$	2987-16-8	
heptanal 5.3	$C_7H_{14}O$	111-71-7	
octanal 11.1	$C_8H_{16}O$	124-13-0	
2-ethylhexanal 9.6	$C_8H_{16}O$	123-05-7	
nonanal 20.7	$C_9H_{18}O$	124-19-6	
3,5,5-trimethylhexanal 49.5	$C_9H_{18}O$	5435-64-3	
decanal	$C_{10}H_{20}O$	112-31-2	34.8
2-butylhexanal	$C_{10}H_{20}O$	18459-51-3	27.6

Cyclic Ethers

1,3-dioxolane -31.1	C ₃ H ₆ O ₂	646-06-0	
tetrahydrofuran (oxolane)	C ₄ H ₈ O	109-99-9	-15.7
1,2-epoxybutane	C ₄ H ₈ O	106-88-7	-17.9
tetrahydropyran (oxane) -6.0	C ₅ H ₁₀ O	142-68-7	
2-methoxytetrahydropyran	C ₆ H ₁₂ O ₂	6581-66-4	-12.9

Esters and Carboxylic Acids

ethyl formate -32.9	C ₃ H ₆ O ₂	109-94-4	
methyl acetate -29.0	C ₃ H ₆ O ₂	79-20-9	
propyl formate -15.7	C ₄ H ₈ O ₂	110-74-7	
isopropyl formate -15.6	C ₄ H ₈ O ₂	625-55-8	
ethyl acetate -26.4	C ₄ H ₈ O ₂	141-78-6	
methyl propionate -23.9	C ₄ H ₈ O ₂	554-12-1	
butyric acid -19.0	C ₄ H ₈ O ₂	107-92-6	
isobutyric acid -17.9	C ₄ H ₈ O ₂	79-31-2	
butyl formate	C ₅ H ₁₀ O ₂	592-84-7	1.0
isobutyl formate	C ₅ H ₁₀ O ₂	542-55-2	0.0
tert-butyl formate	C ₅ H ₁₀ O ₂	762-75-4	-0.6
propyl acetate	C ₅ H ₁₀ O ₂	109-60-4	-9.3
isopropyl acetate	C ₅ H ₁₀ O ₂	108-21-4	-10.4
ethyl propionate	C ₅ H ₁₀ O ₂	105-37-3	-15.6
methyl butyrate	C ₅ H ₁₀ O ₂	623-42-7	-18.2
methyl isobutyrate	C ₅ H ₁₀ O ₂	547-63-7	-12.7

pentyl formate (amyl formate)	$C_6H_{12}O_2$	638-49-3	8.3
isopentyl formate (isoamyl formate)	$C_6H_{12}O_2$	110-45-2	12.1
butyl acetate	$C_6H_{12}O_2$	123-86-4	8.8
isobutyl acetate	$C_6H_{12}O_2$	110-19-0	6.9
sec-butyl acetate	$C_6H_{12}O_2$	105-46-4	7.0
tert-butyl acetate	$C_6H_{12}O_2$	540-88-5	3.6
propyl propionate	$C_6H_{12}O_2$	106-36-5	2.4
ethyl butyrate	$C_6H_{12}O_2$	105-54-4	-7.6
ethyl isobutyrate	$C_6H_{12}O_2$	97-62-1	-6.6
methyl pentanoate (methyl valerate)	$C_6H_{12}O_2$	624-24-8	-12.6
methyl isopentanoate (methyl isovalerate)	$C_6H_{12}O_2$	556-24-1	-3.1
methyl 2-methylbutyrate	$C_6H_{12}O_2$	868-57-5	-8.5
methyl trimethylacetate	$C_6H_{12}O_2$	598-98-1	0.7
2-ethylbutyric acid	$C_6H_{12}O_2$	88-09-5	-7.0
2,2-dimethylbutyric acid	$C_6H_{12}O_2$	595-37-9	-0.6
pentyl acetate	$C_7H_{14}O_2$	628-63-7	15.6
isopentyl acetate	$C_7H_{14}O_2$	123-92-2	20.6
butyl propionate	$C_7H_{14}O_2$	590-01-2	20.1
isobutyl propionate	$C_7H_{14}O_2$	540-42-1	16.7
tert-butyl propionate	$C_7H_{14}O_2$	20487-40-5	15.7
propyl butyrate	$C_7H_{14}O_2$	105-66-8	10.7
isopropyl butyrate	$C_7H_{14}O_2$	638-11-9	9.2
ethyl pentanoate (ethyl valerate)	$C_7H_{14}O_2$	539-82-2	-3.0
ethyl isopentanoate (ethyl isovalerate)	$C_7H_{14}O_2$	108-64-5	9.7
ethyl 2-methylbutyrate	$C_7H_{14}O_2$	7452-79-1	-1.6
methyl hexanoate	$C_7H_{14}O_2$	106-70-7	-5.7
methyl heptanoate	$C_8H_{16}O_2$	106-73-0	3.3
methyl octanoate	$C_9H_{18}O_2$	111-11-5	13.3

Other Multi-Oxygen Compounds

1,2-ethanediol (ethylene glycol) -34.4	$C_2H_6O_2$	107-21-1	
1,2-propanediol -25.9	$C_3H_8O_2$	57-55-6	
dimethyl carbonate -30.8	$C_3H_6O_3$	616-38-6	
dimethoxymethane (formaldehyde dimethyl acetal) -30.3	$C_3H_8O_2$	109-87-5	
1,1-dimethoxyethane (acetaldehyde dimethyl acetal)	$C_4H_{10}O_2$	534-15-6	-25.1
1,2-dimethoxyethane	$C_4H_{10}O_2$	110-71-4	-28.8
1-methoxy-2-propanol	$C_4H_{10}O_2$	107-98-2	-21.7
3-methoxy-1-propanol	$C_4H_{10}O_2$	1589-49-7	-19.3
2-ethoxyethanol	$C_4H_{10}O_2$	110-80-5	-22.8
trimethoxymethane	$C_4H_{10}O_3$	149-73-5	-27.2
2-hydroxy-methylpropionate -32.3	$C_4H_8O_3$	27871-49-4	
2,2-dimethoxypropane	$C_5H_{12}O_2$	77-76-9	-21.7
1-methoxy-2-butanol	$C_5H_{12}O_2$	53778-73-7	-16.4
1,2-dimethoxypropane	$C_5H_{12}O_2$	7778-85-0	-18.2
2-isopropoxyethanol	$C_5H_{12}O_2$	109-59-1	-7.5
diethoxymethane	$C_5H_{12}O_2$	462-95-3	-18.4
2-(2-methoxyethoxy)-ethanol (diethylene glycol methyl ether)	$C_5H_{12}O_3$	111-77-3	-23.8
1,1,1-trimethoxyethane	$C_5H_{12}O_3$	1445-45-0	-27.5
diethyl carbonate	$C_5H_{10}O_3$	105-58-8	-23.4
1,1-dimethoxy-2-propanone	$C_5H_{10}O_3$	6342-56-9	-24.2
tetramethoxymethane (tetramethylorthocarbonate)	$C_5H_{12}O_4$	1850-14-2	-24.1
2-butoxyethanol	$C_6H_{14}O_2$	111-76-2	-7.8
1-methoxy-2-(2-methoxyethoxy)ethane (diglyme)	$C_6H_{14}O_3$	111-96-6	-22.1
1,1-diethoxyethane (acetal)	$C_6H_{14}O_2$	105-57-7	-12.3
3-methoxy-3-methyl-1-butanol	$C_6H_{14}O_2$	56539-66-3	4.4

1-propoxy-2-propanol (propylene glycol propyl ether)	C ₆ H ₁₄ O ₂	1569-01-3	-7.1
1,2-diethoxyethane (ethylene glycol diethyl ether)	C ₆ H ₁₄ O ₂	629-14-1	-15.5
1-butoxy-2-propanol (propylene glycol butyl ether)	C ₇ H ₁₆ O ₂	5131-66-8	2.0
1-tert-butoxy-2-propanol	C ₇ H ₁₆ O ₂	57018-52-7	21.1
1,1-diethoxypropane (propionaldehyde diethyl acetal)	C ₇ H ₁₆ O ₂	4744-08-5	-4.7
dipropyl carbonate	C ₇ H ₁₄ O ₃	623-96-1	6.4

^amolecular identifier assigned by the American Chemical Society

^buncertainty = ± 2

^cYSI = 0.0 by definition

^dtest compounds are mixtures of geometric isomers, unless a specific isomer is listed

Table S2. Maximum carbon mass in aromatic species (M_C) calculated for the test flames using the method of Reference 11.

Name	YSI	M_C (mg/mole)
<i>Linear Alkanes</i>		
n-pentane	-8.9	2.813
n-hexane	0.0	2.922
2-methylpentane	9.8	3.056
3-methylpentane	12.2	3.056
2,3-dimethylbutane	21.1	3.190
n-heptane	8.7	3.030
2-methylhexane	18.6	3.165
3-methylhexane	19.6	3.165
2,3-dimethylpentane	29.6	3.299

2,4-dimethylpentane	29.9	3.299
n-octane	18.9	3.139
2-methylheptane	29.5	3.273
3-methylheptane	28.5	3.273
4-methylheptane	27.5	3.273
2,4-dimethylhexane	39.9	3.407
2,5-dimethylhexane	39.9	3.407
3,4-dimethylhexane	38.5	3.407
2,3,4-trimethylpentane	47.3	3.542
n-nonane	30.6	3.247
2,3-dimethylheptane	46.3	3.516
n-decane	41.7	3.356
n-undecane	53.3	3.464
n-dodecane	64.2	3.573

Alcohols

methanol	-36.9	2.317
ethanol	-31.1	2.426
1-propanol	-22.0	2.534
2-propanol	-17.3	2.669
1-butanol	-13.0	2.643
2-butanol	-8.6	2.777
2-methyl-1-propanol	-6.5	2.777
tert-butanol	-4.5	2.885
1-pentanol	-7.7	2.751
2-pentanol	-0.3	2.886
3-pentanol	-2.0	2.886
2-methyl-1-butanol	3.0	2.886
2-methyl-2-butanol	3.9	2.993

3-methyl-1-butanol	2.4	2.886
3-methyl-2-butanol	2.5	3.020
1-hexanol	-0.6	2.860
2-hexanol	5.8	2.994
3-hexanol	5.5	2.994
2-methyl-1-pentanol	8.4	2.994
3-methyl-1-pentanol	9.2	2.994
4-methyl-1-pentanol	8.1	2.994
2-ethyl-1-butanol	17.6	2.994
2-methyl-2-pentanol	9.4	3.102
3-methyl-2-pentanol	11.4	3.129
4-methyl-2-pentanol	18.1	3.129
2,3-dimethyl-2-butanol	15.9	3.236
1-heptanol	6.7	2.968
2-heptanol	14.0	3.103
3-heptanol	12.6	3.103
4-heptanol	12.6	3.103
2-methyl-2-hexanol	17.8	3.210
3-ethyl-3-pentanol	15.7	3.210
5-methyl-2-hexanol	22.3	3.237
2,4-dimethyl-3-pentanol	17.9	3.372
1-octanol	16.7	3.077
2-octanol	24.4	3.211
3-octanol	20.6	3.211
4-octanol	20.8	3.211
2-ethyl-1-hexanol	31.1	3.211
2-propyl-1-pentanol	31.2	3.211

Ethers

methyl propyl ether	-19.2	2.604
diethyl ether	-21.1	2.604
methyl butyl ether	-11.4	2.713
methyl sec-butyl ether	-2.8	2.847
methyl tert-butyl ether	1.7	2.955
dipropyl ether	-3.7	2.821
diisopropyl ether	12.9	3.090
methyl tert-amyl ether	12.0	3.063
ethyl tert-butyl ether	11.7	3.063
dibutyl ether	12.9	3.038
sec-butyl ether	36.6	3.307
isoamyl ether	51.6	3.524

6-Center Esters

propyl acetate	-9.3	2.616
butyl acetate	8.8	2.725
propyl propionate	2.4	2.725
pentyl acetate	15.6	2.833
isopentyl acetate	20.6	2.968
butyl propionate	20.1	2.833
propyl butyrate	10.7	2.833

Non-6-Center Esters and Carboxylic Acids

methyl acetate	-29.0	2.399
ethyl acetate	-26.4	2.508
methyl propionate	-23.9	2.508
isopropyl acetate	-10.4	2.751
ethyl propionate	-15.6	2.616
methyl butyrate	-18.2	2.616

methyl isobutyrate	-12.7	2.751
isobutyl acetate	6.9	2.859
ethyl butyrate	-7.6	2.725
ethyl isobutyrate	-6.6	2.859
methyl pentanoate	-12.6	2.725
methyl isopentanoate	-3.1	2.859
isobutyl propionate	16.7	2.968
tert-butyl propionate	15.7	3.075
isopropyl butyrate	9.2	2.968
ethyl pentanoate	-3.0	2.833
ethyl isopentanoate	9.7	2.968
ethyl 2methylbutyrate	-1.6	2.968
methyl hexanoate	-5.7	2.833
methyl heptanoate	3.3	2.942
methyl octanoate	13.3	3.050

Other Multi-Oxygen Compounds

1,2-ethanediol	-34.4	2.364
1,2-propanediol	-25.9	2.607
1,2-dimethoxyethane	-28.8	2.504
1-methoxy-2-propanol	-21.7	2.677
3-methoxy-1-propanol	-19.3	2.542
2-ethoxyethanol	-22.8	2.542
1-methoxy-2-butanol	-16.4	2.785
1,2-dimethoxypropane	-18.2	2.747
2-isopropoxyethanol	-7.5	2.685
2-(2-methoxyethoxy)-ethanol	-23.8	2.550
2-butoxyethanol	-7.8	2.759
1-methoxy-2-(2-methoxyethoxy)ethane	-22.1	2.620

3-methoxy-3-methyl-1-butanol	4.4	3.001
1-propoxy-2-propanol	-7.1	2.894
1,2-diethoxyethane	-15.5	2.721
1-butoxy-2-propanol	2.0	3.002
1-tert-butoxy-2-propanol	21.1	3.244