

Figure S1: The distillation curve of diesel fuel with the addition of 2.5% amyl nitrate performed under low-pressure conditions (900 Pa) in order to avoid thermolytic breakdown of amyl nitrate. Here we present temperature as T_k , the temperature measured directly in the liquid phase. The uncertainties are discussed in the text.

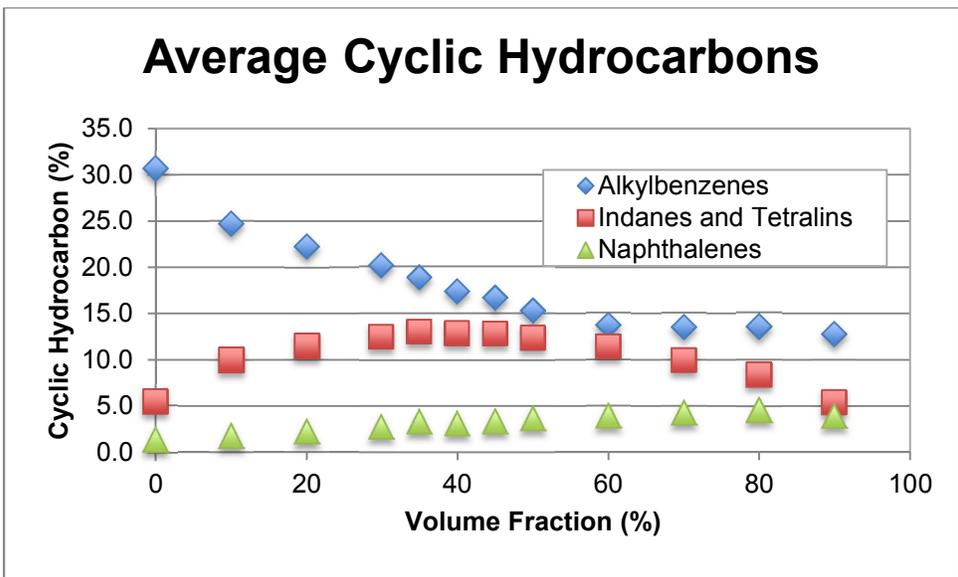
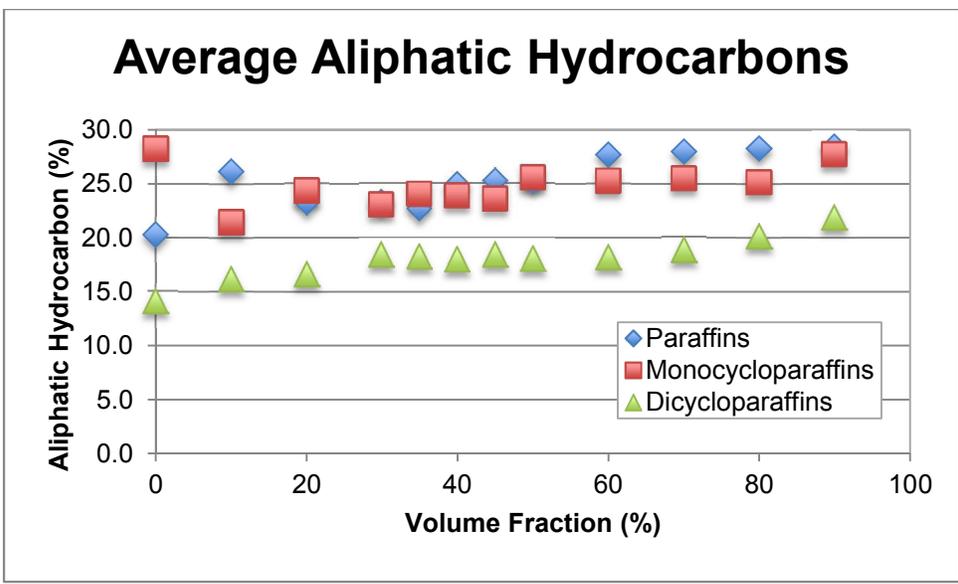
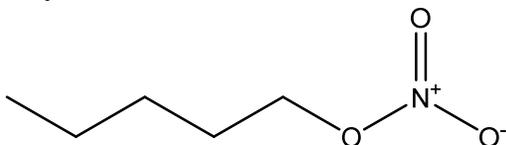


Figure S2: Average plots, of all the blends, of the hydrocarbon family types resulting from the moiety family analysis performed on CN improver blends and diesel fuels. The uncertainty is discussed in the text.

Table S1: Data on the CN improvers and the components of the CN improver PM-1 studied in this work. In this table INChI is the International Chemical Identifier, and RMM is the relative molecular mass.

amyl nitrate



CAS No. 1002-16-0

INChI = 1S/C5H11NO3/c1-2-3-4-5-9-6(7)8/h2-5H2,1H3

RMM = 133.1457

T_{boil} = 157.5 °C

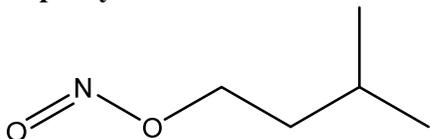
Density = 1.022 g/mL at 25 °C

Refractive index, n_D²⁰ = 1.42

Flash Point = 56.8 °C

Synonyms: *n*-amyl nitrate; pentyl nitrate; *n*-pentyl nitrate; 1-nitrooxypentane; 1-pentyl nitrate; nitric acid, pentyl ester

isopentyl nitrite



CAS No. 110-46-3

INChI = 1S/C5H11NO2/c1-2-3-4-5-8-6-7/h2-5H2,1H3

RMM = 117.15

T_{boil} = 96 °C - 99.0 °C

T_{autoignition} = 209 °C

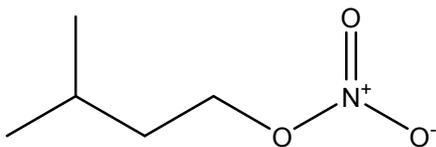
Density = 0.872 g/mL at 25 °C

Refractive index, n_D²⁰ = 1.3855-1.3875

Flash Point = 10 °C

Synonyms: amyl nitrite; 3-methylbutyl nitrite; isoamyl nitrite; nitramyl; pentyl nitrite; 3-methyl-1-nitrosooxybutane; pentyl alcohol nitrite; nitrous acid, pentyl ester; vaporole; aspiral; *poppers* (colloquial, street slang)

isoamyl nitrate



CAS No. 543-87-3

INChI = 1/C5H11NO3/c1-5(2)3-4-9-6(7)8/h5H,3-4H2,1-2H3

RMM = 133.1457

$T_{\text{boil}} = 147.6 \text{ }^{\circ}\text{C}$

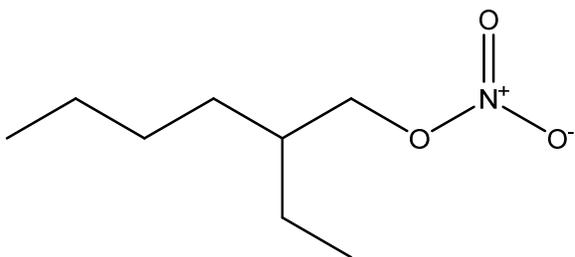
Density = 1.019 g/mL at 25 °C

Refractive index, $n_{\text{D}}^{\text{d}} = 1.418$

Flash Point = 51.7 °C

Synonyms: 3-methylbutyl nitrate; 1-butanol, 3-methyl, 1-nitrate; 1-butanol, 3-methyl, -nitrate; isopentyl alcohol nitrate; isopentyl nitrate

2-ethylhexyl nitrate



CAS No. 27247-96-7

INChI = 1/C8H17NO3/c1-3-5-6-8(4-2)7-12-9(10)11/h8H,3-7H2,1-2H3

RMM = 175.23

$T_{\text{boil}} = 210.9 \text{ }^{\circ}\text{C}$

$T_{\text{melt}} = 75.0 \text{ }^{\circ}\text{C}$

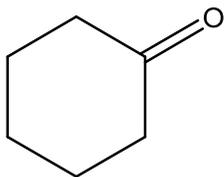
Density = 0.963 g/mL at 25 °C

Refractive index, $n_{\text{D}}^{\text{d}} = 1.432$

Flash Point = 168 °C

Synonyms: nitronal; ethylhexylnitrate; 2-ethylhexylnitrate; 2-ethylhexyl nitrat; 2-ethylhexyl-1-nitrate; 2-ethylhexylester nitric acid; salpetersaure-(2-ethylhexyl) ester; octyl nitrate (2-ethyl hexyl nitrate)

cyclohexanone



CAS No. 108-94-1

INChI = 1S/C6H10O/c7-6-4-2-1-3-5-6/h1-5H2

RMM = 98.15

T_{boil} = 155.65 °C

T_{melt} = -47 °C

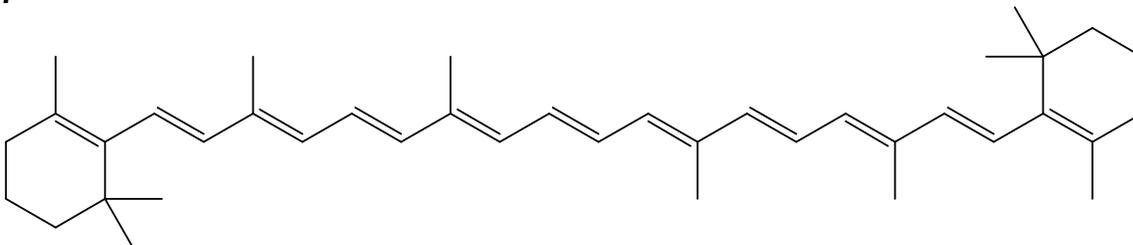
Density = 0.9478 g/mL at 25 °C

Refractive index, Na^d = 1.447

Flash Point = 44 °C

Synonyms: anon; caswellno270; cicloesanone; cykloheksanon; cykloheksanon(polish); epapesticidechemicalcode025902; hexanon; hytrol O

β-carotene



CAS No. 7235-40-7

INChI = 1/C40H56/c1-31(19-13-21-33(3)25-27-37-35(5)23-15-29-39(37,7)8)17-11-12-18-32(2)20-14-22-34(4)26-28-38-36(6)24-16-30-40(38,9)10/h11-14,17-22,25-28H,15-16,23-24,29-30H2,1-10H3/b12-11+,19-13+,20-14+,27-25+,28-26+,

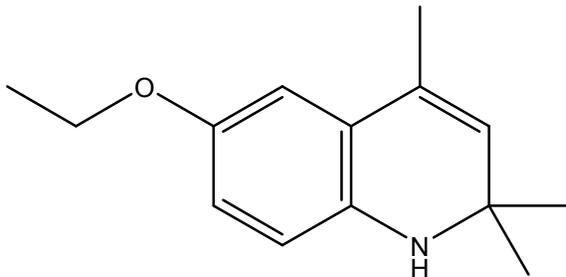
RMM = 536.87

Density = 0.94 g/mL at 25 °C

Flash Point = 103 °C

Synonyms: 1,3,3-trimethyl-2-[3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohex-1-en-1-yl)octadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl]cyclohex-1-ene; betacarotene; food orange 5; 1,1'-(3,7,12,16-Tetramethyl-1,3,5,7,9,11,13,15,17-octadecanonaene-1,18-diyl)bis[2,6,6-trimethylcyclohexene]

santoquin



CAS No. 91-53-2

INChI = 1/C14H19NO/c1-5-16-11-6-7-13-12(8-11)10(2)9-14(3,4)15-13/h6-9,15H,5H2,1-4H3

RMM = 217.31

T_{boil} = 123-125 °C

Density = 1.03 at 25 °C

Refractive index, Na^d = 1.57

Flash Point = 137 °C

Synonyms: 3-ethoxy-2,2,4-trimethyl-1H-quinoline; ethoxyquine; ethoxy quinolone; santoquine; niflex, antioxidant EC; antioxidantAW; antioxidantec; santoflex A; santoflex AW; Stop-Scald; amea100; antageaw; 6-ethoxy-2,2,4-trimethylquinoline; 6-ethoxy-1,2-dihydro-2,2,4-trimethylquinoline; anti-oxidizing quinoline; 1,2-dihydro-2,2,4-trimethyl-6-ethoxyquinoline; 2,2,4-trimethyl-6-ethoxy-1,2-dihydroquinoline; 6-ethoxy-1,2-dihydro-2,2,4-trimethyl-quinolin; 6-ethoxyl-2,2,4-trimethyl-1,2-dihydrquinoline; 1,2-dihydro-6-ethoxy-2,2,4-trimethylquinoline

Table S2: A summary of the distillate volume fraction analysis (also shown in histogram plot form in Figures 2-6) of the diesel fuel mixtures with the CN improving additives. The data shows the concentration, percent (mass/mass) with the propagated uncertainties of the sample and standards measurements given in parentheses next to the percent concentration.

Volume Fraction	diesel fuel + 500 ppm amyl nitrate	diesel fuel + 1000 ppm amyl nitrate	diesel fuel + 2000 ppm amyl nitrate
First Drop	0.0072% (0.0039)	0.0927% (0.0090)	0.0970% (0.0504)
0.10	0.0009% (0.0005)	0.0077% (0.0003)	0.0067% (0.0033)
0.20	0.0004% (0.0002)	0.0026% (0.0003)	0.0026% (0.0014)
0.30		0.0006% (0.0001)	0.0006% (0.0003)

Volume Fraction	diesel fuel + 500 ppm isoamyl nitrite	diesel fuel + 1000 ppm isoamyl nitrite	diesel fuel + 2000 ppm isoamyl nitrite
First Drop	0.0807% (0.0404)	0.3360% (0.0176)	1.3303% (0.1144)
0.10		0.0049% (0.0006)	0.0152% (0.0025)

Volume Fraction	diesel fuel + 500 ppm 2-ethylhexyl nitrate	diesel fuel + 1000 ppm 2-ethylhexyl nitrate	diesel fuel + 2000 ppm 2-ethylhexyl nitrate
First Drop	0.0549% (0.0155)	0.0552% (0.0168)	0.2652% (0.0144)
0.10	0.0192% (0.0130)	0.0189% (0.0029)	0.0783% (0.0057)
0.20	0.0120% (0.0071)	0.0120% (0.0109)	0.0085% (0.0052)

Volume Fraction	diesel fuel + 500 ppm isoamyl nitrate	diesel fuel + 1000 ppm isoamyl nitrate	diesel fuel + 2000 ppm isoamyl nitrate
First Drop	0.0862% (0.0081)	0.1211% (0.0072)	0.2934% (0.0186)
0.10	0.0412% (0.0037)	0.0283% (0.0053)	0.0293% (0.0060)
0.20	0.0156% (0.0012)	0.0095% (0.0025)	0.0271% (0.0049)
0.30			0.0041% (0.0006)

Volume Fraction	diesel fuel + 5000 ppm (0.5 %) (vol/vol) PM-1	diesel fuel + 25,000 ppm (2.5%) (vol/vol) PM-1	diesel fuel + 50,000 ppm (5%) (vol/vol) PM-1
2-ethylhexyl nitrate			
First Drop	1.3158% (0.0278)	4.1131% (0.1018)	4.1954% (0.1339)
0.10	0.9681% (0.0279)	4.1851% (0.0433)	7.3764% (0.1234)
0.20	0.6779% (0.0069)	2.6564% (0.0228)	4.3214% (0.1833)
0.30	0.2792% (0.0078)	1.2499% (0.0101)	

0.35	0.0966% (0.0028)	0.6092% (0.0061)	0.8515 (0.0336)
0.40	0.0543% (0.0003)	0.3215% (0.0054)	0.2336 (0.0084)
0.45	0.0230% (0.0007)	0.1363% (0.0095)	0.1259 (0.0037)
0.50	0.0092% (0.0002)	0.0740% (0.0008)	0.0853 (0.0038)
cyclohexanone			
First Drop	4.2221% (0.0934)	7.5508% (0.1429)	10.5556% (0.3724)
0.10	2.8437% (0.0510)	5.9622% (0.0633)	8.0960% (0.1493)
0.20	1.3664% (0.0178)	2.4457% (0.0097)	4.0508% (0.0885)
0.30	0.4474% (0.0149)	0.7271% (0.0038)	
0.35	0.2237% (0.0027)	0.2773% (0.0046)	0.5540% (0.0207)
0.40	0.0935% (0.0026)	0.1199% (0.0028)	0.1178% (0.0032)
0.45	0.0351% (0.0013)	0.0297% (0.0005)	0.0630% (0.0013)
0.50	0.0200% (0.0024)	0.0196% (0.0043)	0.0412% (0.0022)
santoquin			
First Drop	0.0003% (0.00002)		0.0010% (0.0003)
0.10	0.0015% (0.00025)		0.0101% (0.0016)
0.20	0.0023%(0.00002)		0.0256% (0.0009)
0.30	0.0034% (0.00023)		
0.35	0.0070% (0.00105)		0.0730% (0.0022)
0.40	0.0085% (0.00020)		0.1029% (0.0022)
0.45	0.0257% (0.00056)		0.1330% (0.0042)
0.50	0.0279% (0.00120)		0.1928% (0.0026)
0.60	0.0338% (0.00313)		0.2476% (0.0096)
0.70	0.0350% (0.00226)		0.2573% (0.0087)
0.80	0.0178% (0.00164)		0.1819% (0.0146)
0.90	0.0075% (0.00438)		0.1580% (0.0056)