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Supplement to "Evaluating the performance of pyrogenic and biogenic emission inventories against one decade of space-based formaldehyde columns"

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This supplement provides information about the chemical mechanism of the NMVOCs used in IMAGESv2 model. The NMVOC chemical species and the NMVOC chemical mechanism are presented in Tables 1 and 2. The photodissociations are summarized in Table 3.

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Table 1. IMAGESv2 NMVOC chemistry species

Formula	*Name*
C_2H_2	acetylene
C_2H_4	ethene
C_2H_6	ethane
C_3H_6	propene
C_3H_8	propane
C_5H_8	isoprene
CH_3COCH_3	acetone
CH_3CHO	acetaldehyde
CH_3OH	methanol
MEK ($CH_3COC_2H_5$)	methylethyl ketone
$(CH_3CO)_2$	2,3-butanedione
GLY (CHOCHO)	glyoxal
CH_3COOH	acetic acid
CH_3COOOH	peracetic acid
CH_3CO_3	acetylperoxy radical
PAN ($CH_3CO_3NO_2$)	peroxy acetyl nitrate
$C_2H_5O_2$	ethyl peroxy radical
C_2H_5OOH	ethyl hydroperoxide
C_2H_5OH	ethanol
$C_3H_7O_2$	propyl peroxy radical
C_3H_7OOH	propyl hydroperoxide
C_2H_5CHO	propanal
$C_2H_5CO_3$	peroxypropionyl radical
PPN ($C_2H_5CO_3NO_2$)	peroxypropionyl nitrate
RP (C_2H_5COOOH)	perproacid
RO_2 ($CH_3COCH_2O_2$)	peroxy radical from acetone
ROOH (CH_3COCH_2OOH)	hydroperoxide from acetone
MGLY (CH_3COCHO)	methylglyoxal
HYAC ($CH_2OHCOCH_3$)	hydroxyacetone
PO_2 ($C_3H_6OHO_2$)	peroxy radical from propylene
POOH (C_3H_6OHOOH)	hydroperoxide from propylene
QO_2 ($C_2H_4OHO_2$)	peroxy radical from ethene
QOOH (C_2H_4OHOOH)	hydroperoxide from ethene
GLYALD (CH_2OHCHO)	glycolaldehyde
$ISOPO_2$ ($C_5H_8OHO_2$)	peroxy radical from C_5H_8
ISOPOOH (C_5H_8OHOOH)	hydroperoxide from C_5H_8
ISON ($C_5H_8OHONO_2$)	nitrates from $ISOPO_2$+NO and C_5H_8+NO_3
MACR (CH_2CCH_3CHO)	methylacrolein
$MACRO_2$ ($CHOCH_3CO_2CH_2OH$)	peroxy radical from MACR+OH
MACROOH ($CH_3COCHOOHCH_2OH$)	hydroperoxide from MACR
MPAN ($CH_2CCH_3CO_3NO_2$)	peroxymethacrylic nitrate
GCO_3 ($HOCH_2CO_3$)	hydroxy peroxyacetyl radical
GP ($HOCH_2COOOH$)	hydroperoxide from GCO_3
GPAN ($HOCH_2COOONO_2$)	peroxyacyl nitrate from GCO_3
KO_2 ($CH_3COC_2H_5OHO_2$)	peroxy radical from MEK
C_4H_{10}	surrogate for the other NMVOCs

Table 2. IMAGESv2 NMVOC chemical mechanism

Reaction	*Rate* [*Reference*]
C_2H_2+OH→0.364HCOOH+0.364CO +0.364HO_2+0.636GLY+0.636OH	$k_0 = 5.5(-30)$ $k_\infty = 8.3(-13)(\frac{300}{T})^2$ [1]
C_2H_4+OH→QO_2	$k_0 = 1.0(-28)(\frac{300}{T})^{4.5}$ $k_\infty = 8.8(-12)(\frac{300}{T})^{0.85}$ [1]
C_2H_4+O_3→1.139HCHO+0.63CO+0.13HO_2 +0.13OH+0.231HCOOH+0.139H_2O_2	$1.2(-14)\exp(-2630/T)$ [1]
QO_2+CH_3CO_3→CH_3O_2+HO_2 +1.5HCHO+0.25GLYALD	$\frac{2.0(-12)\exp(500/T)}{(1+0.45(-6)\exp(3870/T))}$ [2]
QO_2+CH_3CO_3→CH_3COOH+GLYALD	$\frac{2.0(-12)\exp(500/T)}{(1+2.2(+6)\exp(-3870/T))}$ [2]
QO_2+NO→HCHO+HO_2+NO_2	$\frac{2.54(-12)\exp(360/T)}{(1+8.14(-29)\exp(5528/T)[M])}$ [3]
QO_2+NO→GLYALD+HO_2+NO_2	$\frac{2.54(-12)\exp(360/T)}{(1+1.23(+28)\exp(-5528/T)/[M])}$ [3]
QO_2+HO_2→QOOH	$2.0(-13)\exp(1250/T)$ [3]
QOOH+OH→QO_2	$1.9(-12)\exp(190/T)$ [3]
QOOH+OH→GLYALD+OH	$1.38(-11)$ [3]
C_2H_6+OH→$C_2H_5O_2$+H_2O	$8.7(-12)\exp(-1070/T)$ [1]
$C_2H_5O_2$+NO→CH_3CHO+HO_2+NO_2	$2.6(-12)\exp(365/T)$ [1]
$C_2H_5O_2$+NO_3→CH_3CHO+HO_2+NO_2	$2.5(-12)$ [3]
$C_2H_5O_2$+HO_2→C_2H_5OOH+O_2	$7.5(-13)\exp(700/T)$ [1]
$C_2H_5O_2$+CH_3O_2→0.7HCHO+0.8CH_3CHO +HO_2+0.3CH_3OH+0.2C_2H_5OH	$2.0(-13)$ [5]
C_2H_5OOH+OH→0.5$C_2H_5O_2$+0.5CH_3CHO+0.5OH	$3.8(-12)\exp(200/T)$ [4]
C_3H_6+OH→PO_2	$k_0 = 8.0(-27)(\frac{300}{T})^{3.5}$ $k_\infty = 3.0(-11), F_c = 0.5$ [3]
C_3H_6+O_3→0.54HCHO+0.19HO_2+0.33OH +0.08CH_4+0.56CO+0.5CH_3CHO+0.31CH_3O_2 +0.25CH_3COOH	$6.5(-15)\exp(-1900/T)$ [3]
PO_2+CH_3CO_3→CH_3O_2+CH_3CHO +HCHO+HO_2	$\frac{2.0(-12)\exp(500/T)}{(1+0.45(-6)\exp(3870/T))}$ [2]
PO_2+CH_3CO_3→CH_3COOH +0.35C_2H_5CHO+0.65HYAC	$\frac{2.0(-12)\exp(500/T)}{(1+2.2(+6)\exp(-3870/T))}$ [2]
PO_2+CH_3O_2→HO_2+0.5CH_3CHO +1.25HCHO+0.16HYAC +0.09C_2H_5CHO+0.25CH_3OH+0.25ROH	$5.92(-13)$ [6]
PO_2+NO→CH_3CHO+HCHO+HO_2+NO_2	$2.7(-12)\exp(350/T)$ [2]
PO_2+NO_3→CH_3CHO+HCHO+HO_2+NO_2	$2.5(-12)$ [3]
PO_2+HO_2→POOH+O_2	$7.5(-13)\exp(700/T)$ [5]
POOH+OH→PO_2	$1.9(-12)\exp(190/T)$ [3]
POOH+OH→HYAC+OH	$2.44(-11)$ [3]
C_3H_8+OH→$C_3H_7O_2$	$8.7(-12)\exp(-615/T)$ [1]
$C_3H_7O_2$+NO→NO_2+HO_2+CH_3COCH_3	$\frac{2.7(-12)\exp(350/T)}{(1+5.87\exp(-816/T)(300/T)^{0.64})}$ [2,10]
$C_3H_7O_2$+NO→NO_2+HO_2+C_2H_5CHO	$\frac{2.7(-12)\exp(350/T)}{(1+0.17\exp(816/T)(T/300)^{0.64})}$ [2,10]
$C_3H_7O_2$+HO_2→C_3H_7OOH	$1.513(-13)\exp(1300/T)$ [3]
$C_3H_7O_2$+CH_3CO_3→CH_3O_2+HO_2 +0.74CH_3COCH_3+0.26C_2H_5CHO	$\frac{2.0(-12)\exp(500/T)}{(1+0.45(-6)\exp(3870/T))}$ [2]
$C_3H_7O_2$+CH_3CO_3→CH3COOH +0.74CH_3COCH_3+0.26C_2H_5CHO	$\frac{2.0(-12)\exp(500/T)}{(1+2.2(+6)\exp(-3870/T))}$ [2]
C_3H_7OOH+OH→$C_3H_7O_2$	$1.9(-12)\exp(190/T)$ [3]

Table 2. IMAGESv2 NMVOC chemical mechanism (cont'd)

Reaction	*Rate* [*Reference*]
$C_3H_7OOH+OH \rightarrow 0.74CH_3COCH_3$ $+0.26C_2H_5CHO+OH$	$1.8(-11)$ [3,8]
$C_2H_5CHO+OH \rightarrow C_2H_5CO_3+H_2O$	$4.9(-12)\exp(405/T)$ [1]
$C_2H_5CHO+NO_3 \rightarrow HNO_3+C_2H_5CO_3$	$3.46(-12)\exp(-1862/T)$ [3]
$C_2H_5CO_3+CH_3O_2 \rightarrow HCHO+HO_2+C_2H_5O_2$	$1.68(-12)\exp(500/T)$ [6]
$C_2H_5CO_3+CH_3O_2 \rightarrow RCOOH+HCHO$	$1.87(-13)\exp(500/T)$ [6]
$C_2H_5CO_3+CH_3CO_3 \rightarrow CH_3O_2+C_2H_5O_2$	$2.50(-12)\exp(500/T)$ [2]
$C_2H_5CO_3+NO_2 \rightarrow PPN$	$k_0 = 9.0(-28)(300/T)^{8.9}$ $k_\infty = 7.7(-12)(300/T)^{0.2}$ [1]
$PPN \rightarrow C_2H_5CO_3+NO_2$	$K_{eq} = 9.0(-29)\exp(14000/T)$ [1]
$C_2H_5CO_3+NO \rightarrow NO_2+C_2H_5O_2$	$8.1(-12)\exp(270/T)$ [2]
$C_2H_5CO_3+HO_2 \rightarrow RP$	$\frac{4.3(-13)\exp(1040/T)}{(1+0.003\exp(1430/T))}$ [2]
$C_2H_5CO_3+HO_2 \rightarrow RCOOH+O_3$	$\frac{4.3(-13)\exp(1040/T)}{(1+330\exp(-1430/T))}$ [2]
$RP+OH \rightarrow C_2H_5CO_3$	$4.42(-12)$ [3]
$RCOOH+OH \rightarrow C_2H_5O_2+CO_2+H_2O$	$1.16(-12)$ [3]
$C_5H_8+OH \rightarrow ISOPO_2$	$2.54(-11)\exp(410/T)$ [7]
$C_5H_8+O_3 \rightarrow 0.65MACR+0.58HCHO+0.1MACRO_2$ $+0.1CH_3CO_3+0.08CH_3O_2+0.28HCOOH$ $+0.14CO+0.09H_2O_2+0.25HO_2+0.25OH$	$7.86(-15)\exp(-1913/T)$ [7]
$C_5H_8+NO_3 \rightarrow ISON$	$3.03(-12)\exp(-446/T)$ [7]
$ISOPO_2+NO \rightarrow NO_2+MACR+HCHO+HO_2$	$2.43(-12)\exp(360/T)$ [7]
$ISOPO_2+NO \rightarrow ISON$	$0.11(-12)\exp(360/T)$ [7]
$ISOPO_2+HO_2 \rightarrow ISOPOOH$	$2.05(-13)\exp(1300/T)$ [7]
$ISOPO_2+ISOPO_2 \rightarrow 2MACR+HCHO+HO_2$	$2.0(-12)$ [7]
$ISOPOOH+OH \rightarrow MACR+OH$	$1.0(-10)$ [7]
$ISON+OH \rightarrow MACR+0.5CO+0.5HO_2+HNO_3$	$1.5(-11)$ [3,8]
$MACR+OH \rightarrow MACRO_2$	$2.065(-12)\exp(452/T)+$ $0.93(-11)\exp(175/T)$ [7]
$MACR+O_3 \rightarrow 0.9MGLY+0.45HCOOH+0.32HO_2$ $+0.22CO+0.19OH+0.1CH_3CO_3$	$0.68(-15)\exp(-2112/T)+$ $3.755(-16)\exp(-1521/T)$ [7]
$MACRO_2+NO \rightarrow NO_2+0.2HYAC+0.21CO$ $+0.25CH_3CO_3+0.25MGLY+0.61HCHO$ $+0.75HO_2+0.5GLYALD+0.04GLY$	$2.54(-12)\exp(360/T)$ [7,8]
$MACRO_2+HO_2 \rightarrow MACROOH$	$1.82(-13)\exp(1300/T)$ [7]
$MACRO_2+MACRO_2 \rightarrow HYAC$ $+CH_3COCHO+0.5HCHO+0.5CO+HO_2$	$2.0(-12)$ [7]
$MACRO_2+NO_2 \rightarrow MPAN$	$k_0 = 1.2(-29)(\frac{300}{T})^{5.6}$ $k_\infty = 1.1(-12)(\frac{300}{T})^{1.5}$ [8]
$MPAN \rightarrow MACRO_2+NO_2$	$k_0 = 9.7(-29)(300/T)^{5.6}$ $k_\infty = 9.3(-12)(300/T)^{1.5}$ $K_{eq} = 9.0(-29)\exp(14000/T)$ [7]
$MPAN+OH \rightarrow 0.5HYAC+NO_2+0.5CO+GLYALD$	$3.6(-12)$ [7,8]
$MACROOH+OH \rightarrow MACRO_2$	$2.82(-11)$ [3]
$HYAC+OH \rightarrow CH_3COCHO+HO_2$	$2.15(-12)\exp(305/T)$ [9]
$MGLY+OH \rightarrow CH_3CO_3+CO+H_2O$	$8.4(-13)\exp(830/T)$ [5]
$MGLY+NO_3 \rightarrow HNO_3+CO+CH_3CO_3$	$3.46(-12)\exp(-1862/T)$ [3]
$CH_3COCH_3+OH \rightarrow RO_2+H_2O$	$1.33(-13) + 3.82(-11)\exp(-2000/T)$ [6]
$RO_2+NO \rightarrow NO_2+HCHO+CH_3CO_3$	$2.8(-12)\exp(300/T)$ [2]
$RO_2+HO_2 \rightarrow ROOH+O_2$	$8.6(-13)\exp(700/T)$ [2]
$RO_2+CH_3O_2 \rightarrow 0.3CH_3CO_3+0.5HCHO+0.2HO_2$ $+0.2HYAC+0.5MGLY+0.5CH_3OH$	$7.5(-13)\exp(500/T)$ [2,6]

Table 2. IMAGESv2 NMVOC chemical mechanism (cont'd)

Reaction	*Rate* [*Reference*]
ROOH+OH→RO_2+H_2O	$3.8(-12)\exp(200/T)$ [11,3]
ROOH+OH→MGLY+OH	$8.39(-12)$ [3]
CH_3CHO+OH→CH_3CO_3+H_2O	$4.4(-12)\exp(365/T)$ [10]
CH_3CHO+NO_3→CH_3CO_3+HNO_3	$1.4(-12)\exp(-1860/T)$ [10]
CH_3CO_3+HO_2→CH_3COOOH	$\frac{4.3(-13)\exp(1040/T)}{(1+0.003\exp(1430/T))}$ [2]
CH_3CO_3+HO_2→CH_3COOH+O_3	$\frac{4.3(-13)\exp(1040/T)}{(1+330\exp(-1430/T))}$ [2]
CH_3CO_3+NO→CH_3O_2+NO_2+CO_2	$8.1(-12)\exp(270/T)$ [2]
CH_3CO_3+NO_2→PAN	$k_0 = 9.7(-29)(\frac{300}{T})^{5.6}$
	$k_\infty = 9.3(-12)(\frac{300}{T})^{1.5}$ [1]
PAN→CH_3CO_3+NO_2	$K_{eq} = 9.0(-29)\exp(14000/T)$ [1]
PAN+OH→HCHO+NO_2	$4.0(-14)$ [7]
CH_3CO_3+CH_3O_2→HCHO+HO_2+CH_3O_2	$\frac{2.0(-12)\exp(500/T)}{(1+0.45(-6)\exp(3870/T))}$ [2]
CH_3CO_3+CH_3O_2→CH_3COOH+HCHO	$\frac{2.0(-12)\exp(500/T)}{(1+2.2(+6)\exp(-3870/T))}$ [2]
CH_3CO_3+CH_3CO_3→2CH_3O_2+2CO_2	$2.5(-12)\exp(500/T)$ [2]
CH_3CO_3+NO_3→CH_3O_2+NO_2	$4.0(-12)$ [3]
CH_3COOOH+OH→CH_3CO_3	$3.7(-12)$ [3]
CH_3COOH+OH→CH_3O_2	$4.2(-14)\exp(855/T)$ [10]
CH_3OH+OH→HO_2+HCHO	$2.9(-12)\exp(-345/T)$ [1]
MEK+OH→KO_2+H_2O	$1.3(-12)\exp(-25/T)$ [10]
MEK+NO_3→HNO_3+KO_2	$8.0(-16)$ [6]
KO_2+CH_3CO_3→CH_3O_2+CH_3CHO+CH_3CO_3	$\frac{2.0(-12)\exp(500/T)}{(1+0.45(-6)\exp(3870/T))}$ [2]
KO_2+CH_3CO_3→MEK+CH_3COOH	$\frac{2.0(-12)\exp(500/T)}{(1+2.2(+6)\exp(-3870/T))}$ [2]
KO_2+NO→NO_2+CH_3CHO+CH_3CO_3	$2.7(-12)\exp(350/T)$ [2]
KO_2+HO_2→CH_3O_2+CH_3COCHO	$7.4(-13)\exp(700/T)$ [2]
KO_2+CH_3O_2→0.5CH_3CHO+0.5CH_3CO_3 +0.25 MEK+0.75HCHO+0.25CH_3OH +0.25ROH+0.5HO_2	$8.37(-14)$ [6]
GLYALD+OH→0.8GCO_3+0.2GLY+0.2HO_2	$8.0(-12)$ [12]
GCO_3+CH3O_2→2HCHO+2HO_2	$1.68(-12)\exp(500/T)$ [6]
GCO_3+CH3O_2→RCOOH+HCHO	$1.87(-13)\exp(500/T)$ [6]
GCO_3+CH_3CO_3→CH_3O_2+HO_2+HCHO	$2.5(-12)\exp(500/T)$ [2]
GCO_3+HO_2→GP	$\frac{4.3(-13)\exp(1040/T)}{(1+0.003\exp(1430/T))}$ [2]
GCO_3+HO_2→RCOOH+O_3	$\frac{4.3(-13)\exp(1040/T)}{(1+330\exp(-1430/T))}$ [2]
GCO_3+NO→NO_2+HO_2+HCHO	$6.7(-12)\exp(340/T)$ [6]
GCO_3+NO_2→GPAN	$k_0 = 9.0(-28)(\frac{300}{T})^{8.9}$
	$k_\infty = 7.7(-12)(\frac{300}{T})^{0.2}$ [1]
GPAN→GCO_3+NO_2	$K_{eq} = 9.0(-29)\exp(14000/T)$ [1]
GP+OH→0.5OH+0.5GCO_3+0.5HCHO	$3.8(-12)\exp(200/T)$ [6]
GLY+OH→HO_2+1.6CO	$1.14(-11)$ [3]
GLY+NO_3→HNO_3+HO_2+1.6CO	$1.44(-12)\exp(-1862/T)$ [3,8]
C_4H_{10}+OH→0.8ISOPO$_2$	$6.0(-11)\exp(-540/T)$ [13]

Notes: Read $2.14(-11)$ as $2.14 \cdot 10^{-11}$; T: temperature (K); $[M]$: the air density (mol. cm^{-3}). Three-body reaction rates are calculated with $k = \frac{k_0[M]}{1+k_0[M]/k_\infty} F_c^{\{1+[\log_{10}(k_0[M]/k_\infty)]^2\}^{-1}}$, $F_c = 0.6$, unless otherwise stated. Units for first-, second-, and third-order reactions are sec^{-1}, cm^{3}mol.$^{-1}$sec^{-1} and cm^{6}mol.$^{-2}$sec^{-1}, respectively. Rates for equilibrium reactions calculated as $k = k_f/K_{eq}$, k_f being the rate of the formation reaction and K_{eq} the equilibrium constant. References: [1], Sander et al. (2006); [2], Tyndall et al. (2001); [3], Saunders et al. (2003); [4], Müller and Brasseur (1995); [5], Horowitz et al. (2003); [6], Evans et al. (2003); [7], Pöschl et al. (2000); [8], this work; [9], Dillon et al. (2006); [10], Atkinson et al. (2004), [11], Brasseur et al. (1998); [12], Karunanandan et al. (2006); [13], Müller and Stavrakou (2005). Formic acid (HCOOH), propanol (ROH) and propacid (RCOOH) are not treated.

Table 3. Photodissociations considered in the MNVOC chemistry meachanism of IMAGESv2

Reaction	*Cross section / Quantum yield / Products (Refs.)*
HCHO→CO+2HO_2	[5]/[5]/[1]
HCHO→CO+H_2	[5]/[5]/[1]
CH_3COOOH→CH_3O_2+OH+CO_2	[5]/[c]/[1]
CH_3OOH→HCHO+HO_2+OH	[5]/[c]/[1]
CH_3CHO→CH_3O_2+CO+HO_2	[5]/[5]/[1]
C_2H_5CHO→$C_2H_5O_2$+HO_2+CO	[5]/[5]/[1]
GLYALD→HCHO+CO+2HO_2	[5]/[5]/[1]
GLY→2CO+2HO_2	[5]/[5]/[1]
GLY→2CO+H_2	[5]/[5]/[1]
GLY→HCHO+CO	[5]/[5]/[1]
CH_3COCH_3→CH_3CO_3+CH_3O_2	[5]/[5]/[1]
HYAC→CH_3CO_3+HCHO+HO_2	[5]/[i]/[1]
MGLY→CH_3CO_3+CO+HO_2	[5]/[5]/[1]
MACR→CH_3CO_3+HCHO+CO+HO_2	[5]/[5,d]/[3]
MEK→CH_3CO_3+$C_2H_5O_2$	[6]/[6]/[1]
$(CH_3CO)_2$→2CH_3CO_3	[a]/[a]/[1]
ISON→MACR+HCHO+HO_2+NO_2	[4,b]/[4,c]/[3]
QOOH→0.17GLYALD+1.66HCHO +HO_2+OH	[e]/[e]/[1,2]
C_2H_5OOH→CH_3CHO+HO_2+OH	[e]/[e]/[1]
POOH→CH_3CHO+HCHO+HO_2+OH	[e]/[e]/[1]
C_3H_7OOH→0.74CH_3COCH_3 +0.26C_2H_5CHO+HO_2+OH	[e]/[e]/[1]
ISOPOOH→MACR+HCHO+HO_2+OH	[e]/[e]/[3]
MACROOH→OH+0.5HYAC+0.5CO +0.5MGLY+0.5HCHO+HO_2	[e]/[e]/[3]
ROOH→CH_3CO_3+HCHO+OH	[f]/[f]/[1]
PAN→CH_3CO_3+NO_2	[5]/[c]/[7]
PPN→$C_2H_5CO_3$+NO_2	[g]/[g]/[g]
MPAN→$MACRO_2$+NO_2	[g]/[g]/[g]
GPAN→GCO_3+NO_2	[g]/[g]/[g]
RP→$C_2H_5O_2$+OH	[h]/[h]/[1]
GP→HCHO+OH+HO_2	[h]/[h]/[1]

References: [1], Saunders et al. (2003); [2], this work; [3], Pöschl et al. (2000); [4], Atkinson et al. (2004); [5], Sander et al. (2006); [6], Capouet et al. (2004); [7], Müller and Stavrakou (2005). Notes: a) J=2·J(MGLY), based on MCM; b) Assumed to photolyse as n-$C_4H_9ONO_2$; c) Quantum yield is taken equal to 1; d) Quantum yield is equal to 0.005; e) J=J(CH_3OOH); f) J=J(CH_3OOH)+J(MEK); g) J=J(PAN); h) J=J(CH_3COOOH); i) Same as for acetone.