

Table S1. Measured and Predicted Aerosol Product Yields in the  $\alpha$ -Pinene/O<sub>3</sub> System

Product	$P_L^\circ$ (torr) <sup>a</sup>	$\alpha^b$	Aerosol yield $Y_i$ x 100 (%)						$R_i$		
			Exp. 6/9/98a		Exp. 6/9/98b		Exp. 6/17/98a		6/9/98a	6/9/98b	6/17/98a
			measured <sup>c</sup>	predicted	measured	predicted	measured	predicted			
Norpinonaldehyde	$1.74 \times 10^{-1}$	0.0208	0.2	0.0001	0.2	0.0001	0.2	0.00005	0.0004	0.0004	0.0002
Pinonaldehyde	$4.63 \times 10^{-2}$	0.1458	1.0	0.002	0.4	0.002	1.1	0.001	0.002	0.01	0.001
Hydroxy pinonaldehydes	$2.29 \times 10^{-4}$	0.0762	3.3	0.2	1.4	0.3	2.8	0.2	0.07	0.19	0.06
Norpinonic acid and isomers	$8.17 \times 10^{-6}$	0.1129	2.6	5.2	5.9	5.5	3.4	4.0	2.01	0.93	1.17
Norpinic acid	$7.50 \times 10^{-6}$	0.0012	0.1	0.1	0.1	0.1	0.06	0.05	0.61	0.64	0.79
Pinonic acid	$2.22 \times 10^{-6}$	0.0568	2.3	4.3	2.1	4.4	1.8	3.8	1.87	2.10	2.09
Pinic acid	$2.10 \times 10^{-6}$	0.0661	2.5	5.2	5.3	5.3	3.9	4.6	2.08	1.00	1.19
Hydroxy pinonic acid	$2.03 \times 10^{-6}$	0.0397	3.1	3.1	1.9	3.1	3.1	2.7	0.99	1.65	0.88
X (total unidentified mass) <sup>d</sup>	$1.00 \times 10^{-12}$	0.0167	2.6	2.6	1.2	1.2	1.2	1.2	1.00	1.00	1.00
Total Yield, $Y \times 100\%$			17.6	20.6	18.6	19.9	15.9	16.5	$R_T = 1.17$	1.07	1.04
$M_o$ ( $\mu\text{g m}^{-3}$ )			54.2	63.4	65.1	70.0	38.8	40.3			

<sup>a</sup> Predicted by UNIFAC vapor pressure method at 308 K.  
<sup>b</sup> Arithmetic average of measured  $\alpha$  values calculated for the three experiments.  
<sup>c</sup> Measured values are from Yu *et al.* [34].  
<sup>d</sup> Product X represents the total amount of unidentified aerosol mass, including two products identified only as  $A_{13}$  and  $A_{14}$  by Yu *et al.* [34]. Product X was assumed to consist of a compound with 2 CH<sub>3</sub>, 2 CH<sub>2</sub>, 2 CH, 1 C, 1 CH<sub>3</sub>CO, and 1 COOH UNIFAC functional groups,  $MW_X = 184 \text{ g mol}^{-1}$ . An alpha value for product X was calculated individually for each experiment. The vapor pressure of X is such that essentially all the available mass will partition into the aerosol phase.

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**Table S2.** Measured and Predicted Aerosol Product Yields in the  $\beta$ -Pinene/O<sub>3</sub> System

Product	$p_1^\circ$ (torr) <sup>a</sup>	$\alpha^b$	Aerosol yield $Y_i \times 100$ (%)				predicted/measured, $R_x$	
			measured <sup>c</sup>	predicted	measured	predicted	6/11/98b	6/17/98b
Hydroxy pina ketones	$1.09 \times 10^{-1}$	0.0923	0.74	0.0005	1.3	0.0001	0.001	0.00005
Norpinonic acid and isomers	$8.17 \times 10^{-6}$	0.1400	1.7	4.9	2.7	1.0	2.88	0.36
Norpinic acid	$7.50 \times 10^{-6}$	0.0039	0.17	0.15	0.12	0.03	0.89	0.26
Hydroxy norpinonic acid	$6.93 \times 10^{-6}$	0.0129	0.14	0.48	0.33	0.09	3.40	0.27
Pinonic acid	$2.22 \times 10^{-6}$	0.0085	0.14	0.56	0.25	0.18	4.00	0.72
Pinic acid	$2.10 \times 10^{-6}$	0.0431	1.2	3.0	1.6	1.0	2.49	0.65
Hydroxy pinonic acid	$2.03 \times 10^{-6}$	0.0054	0.25	0.37	0.2	0.1	1.47	0.59
X (total unidentified mass) <sup>d</sup>	$1.00 \times 10^{-12}$	0.0099	0.15	0.15	1.8	1.8	1.00	1.00
Total Yield, $Y \times 100\%$			4.5	9.6	8.3	4.3	$R_y =$ 2.13	0.52
$M_o$ ( $\mu\text{g m}^{-3}$ )			18.9	40.4	11.2	5.7		

<sup>a</sup> Predicted by UNIFAC vapor pressure method at 308 K.

<sup>b</sup> Arithmetic average of measured  $\alpha$  values calculated for the two experiments.

<sup>c</sup> Measured values are from Yu *et al.* [34].

<sup>d</sup> Product X represents the total amount of unidentified aerosol mass, including the product identified as 3-Oxo-pina-ketone by Yu *et al.* [34]. Product X was assumed to consist of a compound with 2 CH<sub>3</sub>, 2 CH<sub>2</sub>, 2 CH, 1 C, 1 CH<sub>3</sub>CO, and 1 COOH UNIFAC functional groups,  $MW_X = 184 \text{ g mol}^{-1}$ . An alpha value for product X was calculated individually for each experiment. The vapor pressure of X is such that essentially all the available mass will partition into the aerosol phase.

Table S3. Measured and Predicted Aerosol Product Yields in the Sabinene/O<sub>3</sub> System

Product	$p_{L,0}$ (torr) <sup>a</sup>	$\alpha^b$	Aerosol yield $Y_i$ x 100 (%)		$R_f =$	
			measured <sup>c</sup> 6/15/98a	predicted 6/15/98a		predicted/measured, $R_f$ 6/15/98a
2-(2-isopropyl)-2-formyl- cyclopropyl-methanoic acid	$1.75 \times 10^{-1}$	0.0030	0.13	0.000002	0.00002	
Hydroxy sabina ketones	$2.93 \times 10^{-2}$	0.4729	0.53	0.0005	0.0009	
Sabina ketone	$9.49 \times 10^{-3}$	0.0793	0.43	0.004	0.01	
Norsabironic acid and isomers	$8.17 \times 10^{-6}$	0.0588	1.4	0.8	0.55	
Norsabirnic acid	$7.50 \times 10^{-6}$	0.0032	0.09	0.04	0.49	
Sabirnic acid	$2.10 \times 10^{-6}$	0.0164	0.53	0.60	1.13	
Pinic acid	$2.10 \times 10^{-6}$	0.0191	0.39	0.70	1.79	
S <sub>10</sub> (exact structure unknown)	$2.03 \times 10^{-6}$	0.0021	0.03	0.08	2.73	
X (total unidentified mass) <sup>d</sup>	$1.00 \times 10^{-12}$	0.0001	0.01	0.01	1.00	
Total Yield, $Y \times 100\%$			3.5	2.2	$R_f =$	0.63
$M_o$ ( $\mu\text{g m}^{-3}$ )			17.6	11.1		

<sup>a</sup> Predicted by UNIFAC vapor pressure method at 308 K.

<sup>b</sup> Measured  $\alpha$  values for the single experiment.

<sup>c</sup> Measured values are from Yu et. al. [34].

<sup>d</sup> Product X represents the total amount of unidentified aerosol mass, including the product identified as 3-Oxo-sabina-ketone by Yu et. al. [34]. Product X was assumed to consist of a compound with 2 CH<sub>3</sub>, 2 CH<sub>2</sub>, 2 CH, 1 C, 1 CH<sub>3</sub>CO, and 1 COOH UNIFAC functional groups,  $MW_X = 184 \text{ g mol}^{-1}$ . The vapor pressure of X is such that essentially all the available mass will partition into the aerosol phase.

**Table S4.** Measured and Predicted Aerosol Product Yields in the  $\Delta^3$ -Carene/ $O_3$  System

Product	$p_{L^o}$ (torr) <sup>a</sup>	$\alpha^b$	Aerosol yield $Y_i$ x 100 (%)		$R_f$
			Exp. 6/15/98b measured <sup>c</sup>	predicted 6/15/98b	
$C_5$ (exact structure unknown)	>10	0.0261	0.25	0.000000	0.000000
Caronaldehyde	$2.97 \times 10^1$	0.1050	0.83	0.000001	0.000002
Hydroxy caronaldehydes	$5.38 \times 10^2$	0.0433	0.25	0.0004	0.002
Nor-3-caronic acid and isomers	$5.55 \times 10^3$	0.0288	0.68	0.002	0.004
$C_4$ (exact structure unknown)	$4.77 \times 10^3$	0.0061	0.54	0.0001	0.0003
3-Caronic acid	$1.46 \times 10^3$	0.0568	2.1	0.02	0.01
3-Caric acid	$2.10 \times 10^6$	0.026	1.8	1.8	1.01
Pinic acid	$2.10 \times 10^6$	0.0164	0.46	1.15	2.51
Hydroxy 3-caronic acid	$2.03 \times 10^6$	0.0162	1.0	1.1	1.11
X (total unidentified mass) <sup>d</sup>	$1.00 \times 10^{12}$	0.0514	5.1	5.1	1.00
Total Yield, $Y \times 100\%$			13.0	9.3	$R_f = 0.72$
$M_o$ ( $\mu\text{g m}^{-3}$ )			63.3	44.9	

<sup>a</sup> Predicted by UNIFAC vapor pressure method at 308 K.

<sup>b</sup> Measured  $\alpha$  values for the single experiment.

<sup>c</sup> Measured values are from Yu *et. al.* [34].

<sup>d</sup> Product X represents the total amount of unidentified aerosol mass. Product X was assumed to consist of a compound with 3 CH<sub>3</sub>, 1 CH<sub>2</sub>, 2 CH, 1 C, 1 CH<sub>2</sub>CO, and 1 COOH UNIFAC functional groups,  $MW_X = 184 \text{ g mol}^{-1}$ . The vapor pressure of X is such that essentially all the available mass will partition into the aerosol phase.

Table S5a. Measured and Predicted Aerosol Product Yields in the Cyclohexene/O<sub>3</sub> System

Product	$p_L^o$ (torr) <sup>a</sup>	$\alpha^b$	Aerosol yield $Y_i$ x 100 (%)				predicted/measured, $R_{Y_i}$	
			measured <sup>c</sup>	predicted	measured	predicted	5/13/99a	5/13/99b
2-hydroxy-pentanoic acid	$1.52 \times 10^{-3}$	0.0158	0.1	0.01	0.1	0.01	0.04	0.08
4-hydroxy-butyraldehyde	$1.24 \times 10^{-3}$	0.0303	0.3	0.01	0.2	0.01	0.04	0.07
oxalic acid	$2.03 \times 10^{-4}$	0.0703	1.3	0.1	1.3	0.1	0.11	0.11
malonic acid	$1.59 \times 10^{-4}$	0.0969	0.6	0.32	0.64	0.34	0.55	0.54
1,4-butanediol	$1.54 \times 10^{-4}$	0.0061	0.1	0.02	0.03	0.02	0.33	0.55
4-oxo-butanoic acid	$1.45 \times 10^{-4}$	0.0963	0.4	0.4	0.3	0.4	0.86	1.15
succinic acid	$9.64 \times 10^{-5}$	0.0096	0.2	0.1	0.2	0.1	0.35	0.34
glutaraldehyde	$7.82 \times 10^{-5}$	0.0060	0.03	0.03	0.01	0.03	1.04	2.05
5-oxo-pentanoic acid	$7.49 \times 10^{-5}$	0.0688	0.49	0.5	0.56	0.5	0.97	0.89
glutaric acid	$5.09 \times 10^{-5}$	0.1064	0.7	1.1	0.2	1.1	1.61	5.60
adipaldehyde	$3.62 \times 10^{-5}$	0.0262	0.02	0.2	0.01	0.2	11.83	41.18
6-oxo-hexanoic acid	$3.53 \times 10^{-5}$	0.0714	0.56	0.86	0.48	0.90	1.53	1.88
adipic acid	$2.47 \times 10^{-5}$	0.0406	0.8	0.7	0.1	0.7	0.84	5.12
2-hydroxy-glutaric acid	$1.40 \times 10^{-7}$	0.0331	2.0	3.2	1.2	3.2	1.65	2.69
2-hydroxy-adipic acid	$7.76 \times 10^{-8}$	0.0187	2.1	1.8	1.7	1.8	0.87	1.07
X (total unidentified mass) <sup>d</sup>	$1.00 \times 10^{-12}$	0.0505	0.3	0.3	5.7	5.7	1.00	1.00
Total Yield, $Y \times 100\%$			9.9	9.7	12.8	15.3	$R_Y =$ 0.97	1.19
$M_o$ ( $\mu\text{g m}^{-3}$ )			43.4	42.1	36.4	43.6		

<sup>a</sup> Predicted by UNIFAC vapor pressure method at 298 K.

<sup>b</sup> Arithmetic average of measured  $\alpha$  values calculated for five of six experiments. Experiment 5/17/99b was neglected in computing the average. Four of six experiments were used in calculating the average  $\alpha$  value for product X (see below)<sup>d</sup>.

<sup>c</sup> Measured values are from Kalberer *et al.* [35].

<sup>d</sup> Product X represents the total amount of unidentified aerosol mass. Product X was assumed to consist of a compound with 2 CH<sub>2</sub> and 2 COOH UNIFAC functional groups,  $MW_X = 118 \text{ g mol}^{-1}$ . An alpha value for product X was calculated individually for each experiment. The vapor pressure of X was set such that essentially all the available mass would partition into the aerosol phase.

**Table S5b.** Measured and Predicted Aerosol Product Yields in the Cyclohexene/O<sub>3</sub> System

Product	$p_{L^0}$ (torr) <sup>a</sup>	$\alpha^b$	Aerosol yield $Y_i$ , x 100 (%)				predicted/measured, $R_y$ ,	
			Exp. 5/17/99a measured <sup>c</sup>	predicted	Exp. 5/17/99b measured	predicted	5/17/99a	5/17/99b
2-hydroxy-pentanoic acid	$1.52 \times 10^{-3}$	0.0158	0.2	0.02	0.03	0.01	0.09	0.37
4-hydroxy-butyraldehyde	$1.24 \times 10^{-3}$	0.0303	0.5	0.1	0.4	0.03	0.11	0.06
oxalic acid	$2.03 \times 10^{-4}$	0.0703	0.8	0.5	0.9	0.2	0.62	0.27
malonic acid	$1.59 \times 10^{-4}$	0.0969	0.8	1.1	0.3	0.6	1.36	2.24
1,4-butanediol	$1.54 \times 10^{-4}$	0.0061	0.1	0.1	0.01	0.03	0.68	3.06
4-oxo-butanoic acid	$1.45 \times 10^{-4}$	0.0963	0.8	1.3	0.2	0.7	1.79	4.30
succinic acid	$9.64 \times 10^{-5}$	0.0096	0.2	0.2	0.1	0.1	1.08	1.06
glutaraldehyde	$7.82 \times 10^{-5}$	0.0060	0.1	0.1	0.01	0.05	1.94	3.74
5-oxo-pentanoic acid	$7.49 \times 10^{-5}$	0.0688	0.2	1.6	0.2	0.8	6.42	4.52
glutaric acid	$5.09 \times 10^{-5}$	0.1064	2.8	3.3	0.2	1.9	1.18	10.54
adipaldehyde	$3.62 \times 10^{-5}$	0.0262	0.1	0.7	0.003	0.4	11.67	140.88
6-oxo-hexanoic acid	$3.53 \times 10^{-5}$	0.0714	0.7	2.6	0.2	1.5	3.73	9.36
adipic acid	$2.47 \times 10^{-5}$	0.0406	3.6	1.9	0.2	1.2	0.53	7.45
2-hydroxy-glutaric acid	$1.40 \times 10^{-7}$	0.0331	2.0	3.3	0.4	3.3	1.63	8.46
2-hydroxy-adipic acid	$7.76 \times 10^{-8}$	0.0187	0.4	1.9	1.3	1.9	4.87	1.44
X (total unidentified mass) <sup>d</sup>	$1.00 \times 10^{-12}$	0.0505	7.3	7.3	6.8	6.8	1.00	1.00
Total Yield, $Y$ x 100%			20.5	26.0	11.1	19.4	$R_y =$ 1.27	1.75
$M_o$ ( $\mu\text{g m}^{-3}$ )			126	159	43.4	76.3		

<sup>a</sup> Predicted by UNIFAC vapor pressure method at 298 K.

<sup>b</sup> Arithmetic average of measured  $\alpha$  values calculated for five of six experiments. Experiment 5/17/99b was neglected in computing the average. Four of six experiments were used in calculating the average  $\alpha$  value for product X (see below)<sup>d</sup>.

<sup>c</sup> Measured values are from Kalberer *et al.* [35].

<sup>d</sup> Product X represents the total amount of unidentified aerosol mass. Product X was assumed to consist of a compound with 2 CH<sub>2</sub> and 2 COOH UNIFAC functional groups,  $MW_x = 118 \text{ g mol}^{-1}$ . An alpha value for product X was calculated individually for each experiment. The vapor pressure of X was set such that essentially all the available mass would partition into the aerosol phase.

**Table S5c.** Measured and Predicted Aerosol Product Yields in the Cyclohexene/O<sub>3</sub> System

Product	$p_L^o$ (torr) <sup>a</sup>	$\alpha^b$	Aerosol yield $Y_i$ , x 100 (%)				predicted/measured, $R_y$	
			Exp. 5/19/99a measured <sup>c</sup>	predicted	Exp. 5/19/99b measured	predicted	5/19/99a	5/19/99b
2-hydroxy-pentanoic acid	$1.52 \times 10^{-3}$	0.0158	0.1	0.001	0.4	0.01	0.02	0.01
4-hydroxy-butylaldehyde	$1.24 \times 10^{-3}$	0.0303	1.7	0.002	0.5	0.01	0.001	0.03
oxalic acid	$2.03 \times 10^{-4}$	0.0703	2.2	0.03	0.5	0.1	0.01	0.26
malonic acid	$1.59 \times 10^{-4}$	0.0969	1.1	0.1	0.3	0.3	0.06	0.97
1,4-butanediol	$1.54 \times 10^{-4}$	0.0061	0.1	0.003	0.1	0.02	0.05	0.18
4-oxo-butanoic acid	$1.45 \times 10^{-4}$	0.0963	0.4	0.1	0.2	0.4	0.18	1.74
succinic acid	$9.64 \times 10^{-5}$	0.0096	0.2	0.01	0.1	0.1	0.05	0.63
glutaraldehyde	$7.82 \times 10^{-5}$	0.0060	0.2	0.01	0.03	0.03	0.03	1.08
5-oxo-pentanoic acid	$7.49 \times 10^{-5}$	0.0688	0.3	0.1	0.5	0.5	0.31	0.96
glutaric acid	$5.09 \times 10^{-5}$	0.1064	0.2	0.2	0.6	1.1	0.94	1.88
6-oxo-hexanoic acid	$3.62 \times 10^{-5}$	0.0714	0.03	0.04	0.03	0.2	1.20	7.00
adipaldehyde	$3.53 \times 10^{-5}$	0.0262	0.22	0.16	0.42	0.9	0.72	2.11
adipic acid	$2.47 \times 10^{-5}$	0.0406	0.2	0.1	0.6	0.7	0.67	1.19
2-hydroxy-glutaric acid	$1.40 \times 10^{-7}$	0.0331	0.9	2.9	7.0	3.2	3.18	0.46
2-hydroxy-adipic acid	$7.76 \times 10^{-8}$	0.0187	1.4	1.7	1.3	1.8	1.20	1.45
X (total unidentified mass) <sup>d</sup>	$1.00 \times 10^{-12}$	0.0505	0	0	0	0	1.00	1.00
Total Yield, $Y$ x 100%			6.6	5.5	7.9	9.5	$R_y =$ 0.83	1.19
$M_o$ ( $\mu\text{g m}^{-3}$ )			9.8	8.1	36.4	43.3		

<sup>a</sup> Predicted by UNIFAC vapor pressure method at 298 K.<sup>b</sup> Arithmetic average of measured  $\alpha$  values calculated for five of six experiments. Experiment 5/17/99b was neglected in computing the average.<sup>c</sup> Four of six experiments were used in calculating the average  $\alpha$  value for product X (see below)<sup>d</sup>.<sup>d</sup> Measured values are from Kalberer *et al.* [35].<sup>e</sup> Product X represents the total amount of unidentified aerosol mass. Product X was assumed to consist of a compound with 2 CH<sub>2</sub> and 2 COOH UNIFAC functional groups, MW<sub>X</sub> = 118 g mol<sup>-1</sup>. An alpha value for product X was calculated individually for each experiment; alpha = 0 for the 5/19/99 experiments in which all of the aerosol mass was identified. The vapor pressure of X was set that essentially all the available mass would partition into the aerosol phase.