Supplementary Material (ESI) for PCCP

Electronic Supplementary Information

Kinetics of the Heterogeneous Conversion of 1,4-Hydroxycarbonyls to Cyclic Hemiacetals and Dihydrofurans on Organic Aerosol Particles

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* * Generated by FACSIMILE Reaction Wizard -
27 March 2008 ;
*========================================================= ;
* C14 1hr Dry                                             ;
*========================================================= ;

EXECUTE OPEN 8 "C:\CHA model\C14_sample.out";

PARAMETER
 K1f K2f K3f K4f K5f 0.001  K6f 0.04  K7f K8f K9f K10f 1.7e-3;

VARIABLE
Alk       CHAp      DHFg      DHFp      HCg       Palk      Pdhf
Phc;

COMPILE INSTANT;
Alk = 1 ;
**;

COMPILE GENERAL;
K1f = 0.5*16.8e-12*3.15e8*(TIME+0.1)@-0.36275 ;
K2f = 0.5*16.8e-12*3.15e8*(TIME+0.1)@-0.36275 ;
K3f = 24.6e-12*3.15e8*(TIME+0.1)@-0.36275 ;
K4f = 0.5*4.13e3*1e-6*(500-436*exp(-TIME/910)) ;
K7f = 186*(0.129+0.179*exp(-TIME/420)) ;
K8f = 4.35e3*1e-6*(500-436*exp(-TIME/910)) ;
K9f = 2.18e-10*3.15e8*(TIME+0.1)@-0.36275 ;
**;

COMPILE EQUATIONS ;
% K1f  : Alk = Palk;
% K2f  : Alk = HCg;
% K3f  : HCg = Phc;
% K4f  : HCg = CHAp;
% K5f  : CHAp = DHFp;
% K6f  : DHFp = CHAp;
% K7f  : DHFp = DHFg;
% K8f  : DHFg = DHFp;
% K9f  : DHFg = Pdhf;
% K10f  : HCg = DHFg;
**;

SETPSTREAM 1 8 ;
TIME ;
Alk       CHAp      DHFg      DHFp      HCg       Palk      Pdhf       ;
Phc        ;
**;

COMPILE OUT ;
PSTREAM 1 ;
**;

WHENEVER
TIME= 67 * (+54.686) 0  %
CALL OUT;
**;

BEGIN;
STOP;
```

Table S1. Rate constants for reactions of alkanes and 1, 4-HC with OH radicals, calculated using a structure-reactivity method.

compound carbon number	k_{Alk-OH}[1] (10^{-12} cm^3 $molecule^{-1}$ s^{-1})	k_{OH-HC}[1,2] (10^{-12} cm^3 $molecule^{-1}$ s^{-1})
11	12.5	20.4
12	13.9	21.8
13	15.3	23.2
14	16.8	24.6
15	18.2	26.0
16	19.6	27.4
17	21.0	28.9

[1]E. S. C. Kwok and R. Atkinson, *Atmos. Environ*. 1995, **29**, 1685-1695.

[2]H. L. Bethel, R. Atkinson and J. Arey, *Int. J. Chem. Kinet*. 2001, **33**, 310-316.

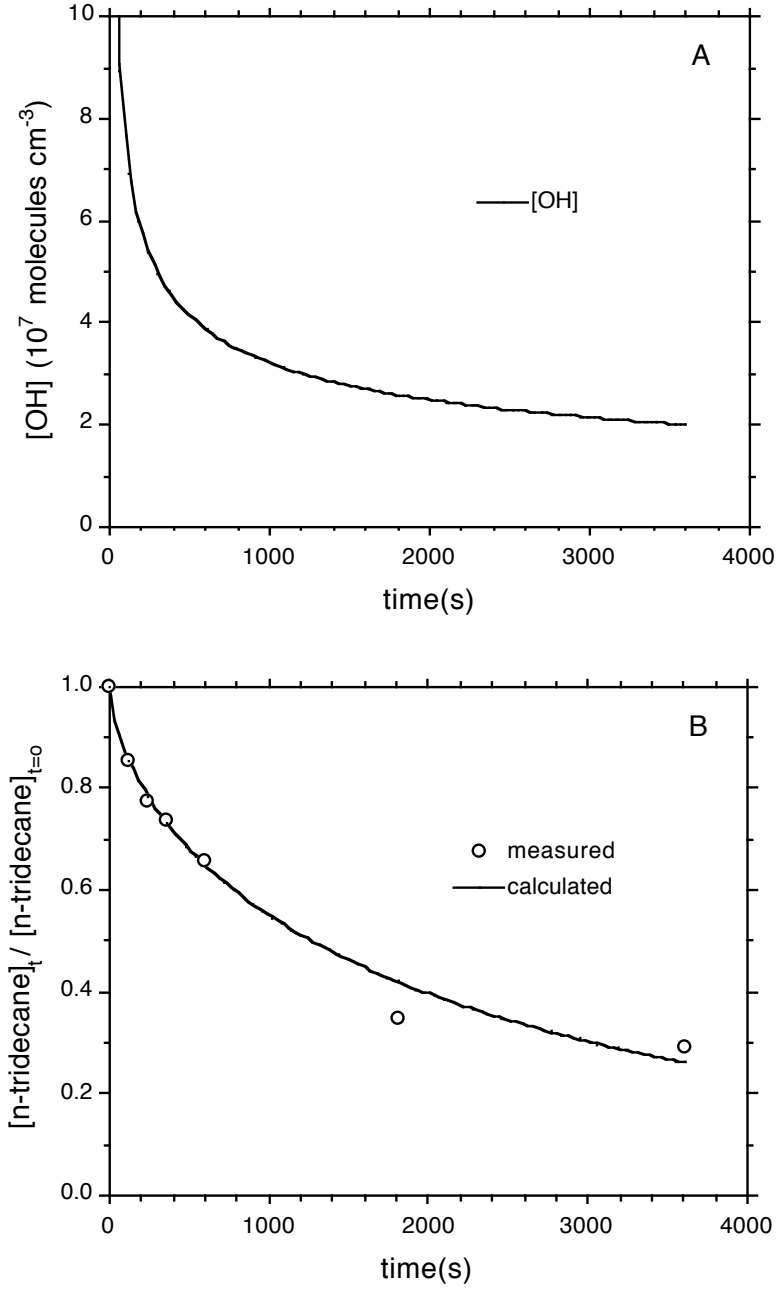

Fig. S1. Plots of (A) [OH_g] time profile determined from concentrations of *n*-tridecane measured during the environmental chamber reaction with OH radicals and (B) measured concentrations *n*-tridecane profile and curve calculated using the equation for [OH_g], $k_{Alk\text{-}OH}$, and eqn (1) in the text.

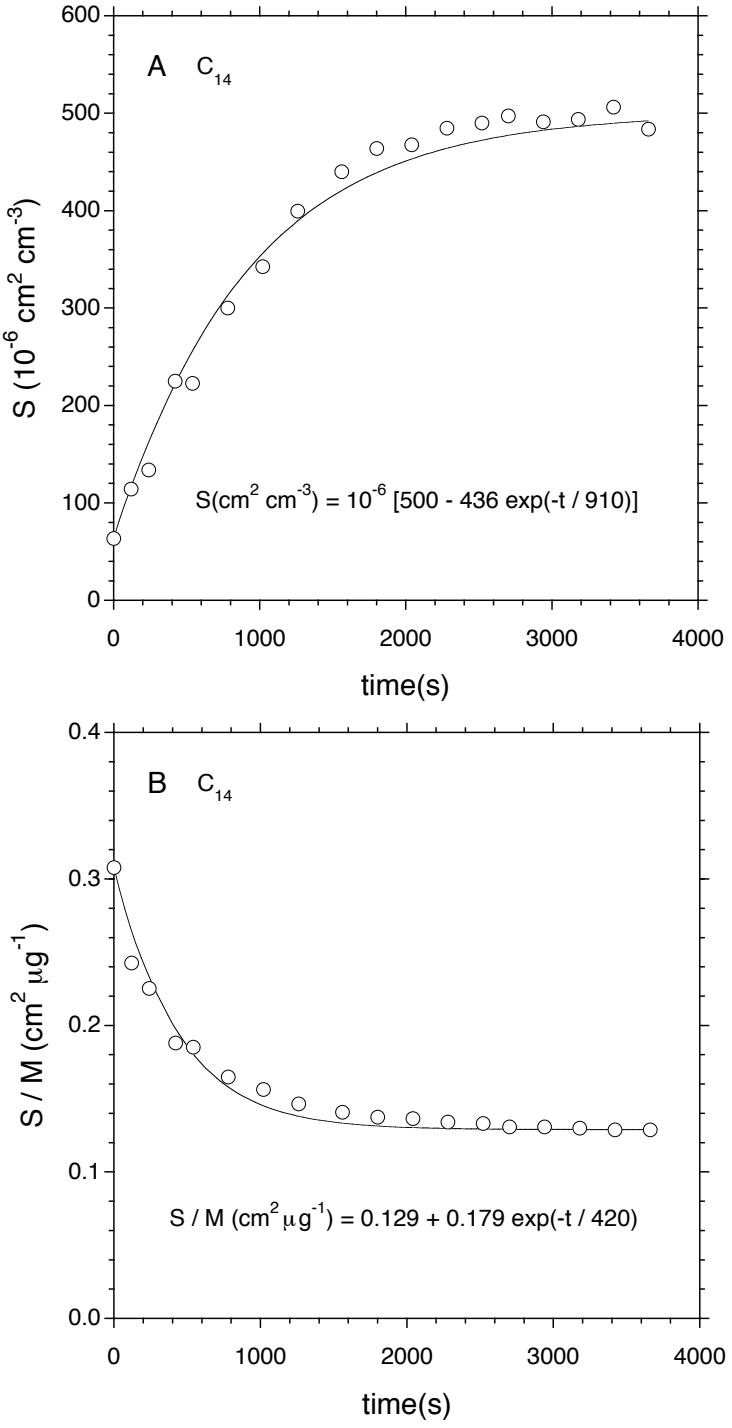

Fig. S2. (A) Surface area and (B) surface area/mass concentrations measured for the reaction of the C_{14} alkane in the presence NO_x in air at <1% RH and curves fit to the data.