

# Pressure dependence of the deuterium isotope effect in the photolysis of formaldehyde by ultraviolet light

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## Supplementary information

Information concerning the Kintecus box model used for simulating photoreactor chemistry and estimating loss of formaldehyde through OH and HO<sub>2</sub> reactions (Ianni, 2009):

### Initial conditions:

293 K

O<sub>2</sub>, 0.765E19 per cm<sup>3</sup>

N<sub>2</sub>, 1.785E19 per cm<sup>3</sup>

H<sub>2</sub>O, 1.0E10 per cm<sup>3</sup>

HCHO, 1.96E13 per cm<sup>3</sup>

H<sub>2</sub>, 6.36E12 per cm<sup>3</sup>

### List of reactions:

#A	n	E/R	Reaction	Source
4.0E-6	0.0	0.0	H2O2==>OH+OH	
8.5E-7	0.0	0.0	HCHO==>H+HCO	
3.0E-6	0.0	0.0	HCHO==>H2+CO	
5.5E-12	0.0	-125	OH+HCHO==>H2O+HCO	JPL
2.14E-12	1.62	1090	HCHO+H==>HCO+H2	NIST
5.2E-12	0.0	0.0	HCO+O2==>CO+HO2	JPL
5.96E-11	0.50	11500	CO+HO2==>CO2+OH	NIST
2.8E-12	0.0	1800	OH+H2==>H+H2O	JPL
4.4E-32	1.3	0	H+O2+M==>HO2+M	JPL
5.9E-33	1.4	0	OH+CO+M==>HOCO+M	JPL
1.25E-13	0.0	0.0	OH+CO==>H+CO2	JPL
2.0E-12	0.0	0.0	O2+HOCO==>HO2+CO2	JPL
1.8E-12	0.0	0.0	OH+H2O2==>H2O+HO2	JPL
4.8E-11	0.0	-250	OH+HO2==>H2O+O2	JPL
3.5E-13	0.0	-430	HO2+HO2==>H2O2+O2	JPL
1.7E-33	0.0	1000	HO2+HO2+M==>H2O2+O2+M	JPL
1.8E-12	0.0	0	OH+OH==>H2O+O	JPL
6.9E-31	1.0	0	OH+OH+M==>H2O2+M	JPL
6.7E-15	0.0	-600	HO2+HCHO==>HOCH2O2	JPL
4.0E-13	0.0	0	2OH+HCOOH==>CO2+2H2O	JPL
151	0.0	0	HOCH2O2==>HO2+HCHO	NIST
5.7E-14	0.0	750	HOCH2O2+HOCH2O2==>HCOOH+CH2OHOH+O2	NIST
5.5E-12	0.0	0	HOCH2O2+HOCH2O2==>HOCH2O+HOCH2O+O2	IUPAC
6.0E-12	0.0	0.0	HOCH2O2+HO2==>HOCH2OOH+O2	Nilsson
3.6E-12	0.0	0.0	HOCH2O2+HO2==>HCOOH+H2O+O2	Nilsson
2.4E-12	0.0	0.0	HOCH2O2+HO2==>HOCH2O+OH+O2	Nilsson
3.5E-14	0.0	0	HOCH2O+O2==>HCOOH+HO2	Nilsson
END				

### References:

Ianni, J. C.: Kintecus V3.962 for windows, [www.kintecus.com](http://www.kintecus.com), 2009.

IUPAC: Atkinson, R. et al., Evaluated kinetic and photochemical data for atmospheric chemistry: Volume II - reactions of organic species, *Atmospheric Chemistry and Physics Discussions*, 5, 6295-7168, 2005.

JPL: Sander, S. P., et al. (2006), *Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies*.

Evaluation Number 15, National Aeronautics and Space Administration, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California.

Nilsson, E., Johnson, M. S., Taketani, F., Matsumi, Y., Hurley, M. D., and Wallington, T. J.: Atmospheric deuterium fractionation: HCHO and HCDO yields in the CH<sub>2</sub>DO + O<sub>2</sub> reaction, *Atmospheric Chemistry and Physics*, 7, 5873-5881, 2007.