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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Evaluated kinetic and photochemical data for atmospheric chemistry: Volume II – reactions of organic species" *by* R. Atkinson et al.

Anonymous Referee #1

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General Comments:

This manuscript provides the latest recommendations from the IUPAC panel on rate coefficients for reactions of organic compounds under atmospheric conditions. As is the norm for this panel, the present work represents a thorough, accurate and trusted database for gas-phase organic reaction rates. Publication of these data in an easily accessible forum like ACP provides an extremely valuable service to the atmospheric sciences community, and publication is recommended without hesitation.

Specific Comments:

As stated above, the review is remarkably complete and thorough. A few minor thoughts/suggestions and perhaps some missing references that the panel may wish to take into consideration in this or future publications are given below:

p. 6424, Vakhtin et al., JPC A v. 107, p. 10055 (2003) provides studies of the OH reaction with ethene, propene, and 1-butene vs. temperature.

p. 6476, Some newer studies of OH + methacrolein (and MVK) are available from Chuong and Stevens, JPC A, v. 107, 2185, 2003 and IJCK 36, 12, 2004.

p. 6487, Orlando and Tyndall (IJCK, v. 33, 149, 2001) have looked at the temperature dependence of the HCOCO chemistry.

p. 6507 and 6513, There are new data on the temperature-dependent rate coefficient for reaction of OH with methanol and ethanol from Jimenez et al. (J. Photochem. Photobiol. A: Chemistry, 157, 237, 2003). As an aside, it seems to me that the recommended Arrhenius expression for OH + ethanol is unduly influenced below RT by extrapolation to lower temperatures of the three-parameter fit to the Hess and Tully data. A firmer low-temperature parameterization can ultimately be obtained by inclusion of the Jimenez et al. data (which agrees perfectly with the current recommendation), and perhaps the Wallington and Kurylo data, as well?.

p. 6513, Wu et al. (IJCK, v. 35, p. 81, 2003) have looked at OH and Cl rate coefficients with numerous alcohols.

p. 6546, Chowdhury, Chem. Phys. Letters, v. 351, p. 201, 2002 have also measured the OH + hydroxyacetone rate coefficient.

p. 6556, Butkovskaya et al. JPC A, v.108, p. 7021, 2004 have new data for OH + acetic acid. Also, there are new product data from De Smedt et al., JPC A, v. 109, 2401, 2005.

p. 6783, The decomposition of 2-butoxy has also been studied by Libuda et al., PCCP 4, 2579, 2002 and by Meunier et al., PCCP 5, 4834, 2003.

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p. 6818, There are new data on methyl peroxy + NO from Bacak et al., JPC A v. 108, p. 10681 (2004).

p. 6832, table, There are new data on the isopropyl nitrate yield from Chow et al., JPC A 107, 3040, 2003. These authors also give a rate coefficient for propyl peroxy radicals with NO.

p. 6870, There are other data available from Sehested et al., IJCK, 30, 475, 1998.

p. 6963, Stutz et al., JPC A 102, 8510 (1998) have data for Cl + propene as well.

p. 6966, Sarzynski and Sztuba have looked at total and site-specific rate coefficients for reaction of Cl with propane, n-butane, and isobutane (IJCK, v. 34, 651, 2002).

p. 6984, Christensen et al. JPC A 104, 345, 2000 have a measurement of the Cl + acetone rate coefficient.

p. 6989, Albaladejo et al. Atmos. Environ. 37, 455 (2003) have data on the Cl + MEK reaction.

p. 7009, Crawford et al. JPC A v. 103, 365, have a measurement of the Cl + acetic acid rate coefficient.

p. 7014, There is considerable evidence to support a lower k(Cl+C2H5Cl) value than 1.1 x 10-11 cm3 molecule-1 s-1 (see Bryukov et al., JPC A 107, 6565, 2003 for example). Downward revision of this reference rate would lower the ethyl, n-propyl, and isopropyl nitrate measurements of Wallington et al. 1990a, and provide better agreement with Nielsen et al. (1991) on the first two of these rates.

p. 7074, There are other measurements of the glyoxal UV spectrum (Horowitz et al., J. Photochem. Photobiol. A: Chem., 146, 19, 2001; Orlando et al., IJCK 33, 149, 2001).

p. 7094, If at all possible, the new data of Blitz et al. (GRL, 31, L06111, 10.1029/2003GL018793, 2004) should be included regarding acetone photolysis.

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p. 7162. There are newer data on PAN photolysis quantum yields from Harwood et al., JPC A 107, 1148 (2003), and Mazely et al., JPC A 101, 7090 (1997).

Technical Comments:

Minor comments, typos, etc. are indicated below:

p. 6299, r4, a recommendation for k-infinity is given here, but not in the appendix?

p. 6302, r56, The appendix discusses the possibility of an OH channel. Thus, rate coefficients given here for individual channels no longer apply?

p. 6307, r137, a “C” is missing in CH3O2 reactant.

p. 6308, r143, product of second channel should be C2H5O not C2H5OH.

p. 6321, line 13, delete “given”

p. 6332, Rate coefficient of Seakins and Leone is 9.4x10-11.

p. 6334, line 18, change “in” to “is”

p. 6341, line 27, should be “Bergamaschi, P.”

p. 6344, middle of table, change “Richard” to “Rickard”

p. 6345, second radical from Z-2-pentene should be CH3CH2CHOO

p. 6366, line 12, missing bracket

p. 6367, line 15, missing arrow in equation

p. 6375, line 4, missing bracket

p. 6384, line 20, “El Hag” instead of “El Haag”? Also, p. 6387, line 22.

p. 6385, top, formula for MVK incorrect in top line

p. 6398, middle of table, “Finlayson-Pitts” spelled incorrectly.

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p. 6398, Gierczak et al. rate coefficient should be Tˆ(+2.82)

p. 6406, in some cases a value for k(OH + cyclohexane) of about 7.2e-12 is used, in others 7.0e-12 is used?

p. 6408, line 1, coefficient is spelled incorrectly.

p. 6409, should be “Pitts Jr., J. N.: J. Chem. Phys. ...”

p. 6414, line 13, should be k-infinity;

p. 6418, should be Clarke et al.?

p. 6432, table, “KS” not defined.

p. 6435, line 14, should be “exp(-87/T)”

p. 6438, comma missing after “Barone, S.”

p. 6447, table, should be “Chuong” not “Choung”. Also, p. 6449, line 10 and p. 6451, line 6.

p. 6453, Overend and Paraskevopoulos, 1977, should be FP-RA (b,f)?

p. 6454, table, all entries should be 10ˆ(+19).

p. 6455, line 14, insert “10ˆ(19)” after “4.2 x”

p. 6458, line 2/3, should be v. 105, p. 983, 1996?

p. 6460, bottom, should be “(8.40 ...” ?

p. 6472, line 9, should be “Atkinson, R.”

p. 6497, line 17, Horowitz spelled incorrectly. Also, should be “J. Phys. Chem. A ...”

p. 6521, should be “Yarwood, G.”

p. 6532, table, for Rudich et al., 1995 should be “PLP-LIF(a)”

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p. 6536, line 12, should be dihydroxynitrates, not dinitrates?

p. 6541, line 14, Mellouki spelled incorrectly.

p. 6550, table, Vaghjiani spelled incorrectly.

p. 6566, line 11, should be “ethyl nitrate.”

p. 6573, line 10, change “were” to “was”

p. 6586, line 12, change “IPUAC” to “IUPAC”.

p. 6594, line 11, should be “(Atkinson, 1989).”

p. 6607, table, should the “FP-AS(c)” entry appear next to Fenter et al.?

p. 6614, line 10, missing bracket

p. 6615, line 1, should be “photolysis of Cl2...”

p. 6615, line 3, remove hard carriage return.

p. 6617, line 10-16, awkward sentence.

p. 6619, line 7, should be “HOCH2CH2I”?

p. 6619, line 16, should be “C2H4-O2-H2O-SF6”?

p. 6637, line 9, should be “k(NO3 + C2H2)/k(NO3 + C2H4)...”

p. 6653, comment (a), should be “NO3 radicals were...”

p. 6656, line 24 (equation), first product should be O2NOCH2C(CH3)CH=CH2. Also, first line of p. 6657.

p. 6658, line 6, should be “decomposition of N2O5...”

p. 6666, line 3, should be “NO3 + NO2...”

p. 6668, line 5, should be “Nielsen, C. J.,” p. 6669, table, Papagni et al. published in

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2000? Also, p. 6671, line 9, table on p. 6674, p. 6677, line 9.

p. 6670, line 1, “method” spelled incorrectly.

p. 6679, line 15, should be “2-methylpropanal and propene”.

p. 6680, line 7, absolute value of Ullerstam et al. is actually lower than the relative rate measurements?

p. 6680, line 10, insert “of” after “suppression”.

p. 6682, table, Chew et al. published in 1998 ?

p. 6715, table, subscripts missing on “N2”

p. 6718, table, Keiffer et al. should be “PLP-AS”.

p. 6721, line 8, should be “Paltenghi”?

p. 6721, line 17, should be “from the CH3 + O3 reaction...”

p. 6729, line 4, should be “C2H5 radicals were...”

p. 6729, line 11, should be “C2H5Cl + Cl...”

p. 6730, line 5, there appears to be a phrase missing after “the combination...”?

p. 6732, line 8, should be C6F5C4H9, I think.

p. 6742, table, Stief et al. entry is missing a superscript.

p. 6747, line 10, remove hard carriage return.

p. 6755, line 15, should be “involving Cl attack on C2H5OH...”

p. 6762, line 7, should be “C2H5ONO”.

p. 6789, line 8, should be “McCaulley et al.”

p. 6792, line 17, remove extra period after “Zellner, R.”

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p. 6805, table, should be “Wollenhaupt and Crowley”.

p. 6808, table, should be “Wollenhaupt and Crowley, 2000”.

p. 6821, line 22, should be “formation of CH3ONO2...”

p. 6824, line 4/5, decomposition of n-propyl nitrite, I think.

p. 6824, line 17, should be Ranschaert et al. (2000).

p. 6828, references, Ferronato spelled incorrectly.

p. 6829, line 6, pyrolysis of n-butyl nitrite, I think.

p. 6833, thermal decomposition of isobutyl nitrite, I think.

p. 6837, top, product of reaction should be CH3C(O)O.

p. 6860, line 2-4, should be comments (a),(b),(c), not (b),(c),(d).

p. 6866, line 20, should be “J. Phys. Chem. A ...”

p. 6868, line 5, Kirchner spelled incorrectly.

p. 6874, table, should be “k1/k $>$ 0.9”?

p. 6915, line 17, should be volume 29?

p. 6931, line 27, delete space between “CH3” and “(CH2)”.

p. 6931, line 28, Delete “I” after “H2O.”

p. 6950, line 16, should be “HCCHCl adduct”?

p. 6951, line 7, should be “C2H4” not “C2H6”.

p. 6967, line 11, remove extra period.

p. 6972, line 15, “infra red” one word?

p. 6978, line 15, tunable is spelled incorrectly?

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p. 6980, line 9, journal should be “Phys. Chem. Chem. Phys.”

p. 6982, line 12, Tyndall et al. is from 1997, I think. Also, p. 6983, line 7.

p. 6991, line 9, Aschmann spelled incorrectly.

p. 6991, line 14, should be “(C2H6 and C2H4)...”

p. 6992, line 9 and 23, Jodkowski is spelled incorrectly.

p. 6998, table, the paper by Cheema et al. is from 2002, I think. Also, p. 7000, line 14.

p. 7011, line 15, should be “Nelsen, W., ...”

p. 7018, title, should be “Cl + n-C4H9ONO2”.

p. 7018, line 9, insert “of” after “by use”

p. 7031, line 2, change “C2H2” to “C2H4”.

p. 7033, line 14, should be “Becker, K. H., Overath, R., and Tong, Z.: ...”

p. 7054, line 21, should be “Warneck, P.: J. Chem. ...”

p. 7058, line 7, product of reaction should be CH3CHO?

p. 7070, quantum yield data table, Kamens spelled incorrectly.

p. 7079, lines 11 and 19, Klotz et al. is from 2001, I think.

p. 7092, line 10, remove hard carriage return.

p. 7097, there are four lines in the table that can be removed (duplication).

p. 7104, table, there appears to be two rows missing at the bottom of the table.

p. 7106, quantum yield table, should be 308 nm, not 208?

p. 7115, Gierczak spelled incorrectly throughout the comments section.

p. 7117, line 9, should be “(275-380 nm)...”?

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p. 7117, line 11, should be “CO and C2H4...”

p. 7124, line 13, should be “J. Geophys. ...”

p. 7126, table, value at 255 nm doesn’t look right, 2.88?

p. 7142, line 4, should be “Nunnermacker, L. J.:”

p. 7146, line 10, insert “above” after “at wavelengths”?

p. 7153, first line of table can be removed (duplication).

p. 7154, line 8, Dickerson is spelled incorrectly.

p. 7156, four lines in table are duplicated (210, 215, 230 and 235 nm).

p. 7162, line 16, Schmoltner spelled incorrectly.

p. 7165, co-product of CH4 is CO2?

Interactive comment on Atmos. Chem. Phys. Discuss., 5, 6295, 2005.