

The Jülich Photolysis Frequency Browser

Version 2016 zu VDI-Richtlinie 3783 Blatt 18 30.5.2016

List of Absorption Cross Sections and Quantum Yields

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A. Calculation of the spectral actinic photon flux densities

The calculations of the spectral actinic photon flux densities were carried out by the state-of-the-art radiative transport model 'libRadtran' (Mayer and Kylling, 2005) at the Meteorological Institute of the Ludwig Maximilian University (LMU). As the photolysis frequencies listed below shall reflect the main meteorological conditions in Central Europe, the following variations were chosen for the calculation of the photon flux densities:

- The ozone column density was varied between 220 and 450 Dobson Units with a step width of 30 Dobson Units. The O₃ profile of Anderson et al. (1986) was kept constant and multiplied by an altitudinally independent factor to achieve the required column density.
- The lower boundary of the aerosol profile was a homogeneous layer of 1 km thickness with different characteristics. The following aerosol types were chosen, each with the appropriate number density and optical properties of the aerosol particles: **cc** (continental clean), **ca** (continental average), and **cp** (continental polluted). Above the boundary layer up to 12 km height, the aerosol was always modelled with the type 'free troposphere' and an altitudinal dependence proportional to $\exp(z/8 \text{ km})$. The aerosol amount in the boundary layer was adjusted to the respective type (Hess et al., 1998), using the following aerosol optical depths (AOD) at 550 nm: 0.05 for cc, 0.2 for ca, and 0.4 for cp.

- The calculations were carried out either for clear sky conditions or for an overcast sky with a cloud of 0.5 km thickness between 2 and 2.5 km. The cloud optical depth (COD) was varied between 10 and 40. In the clouds, the droplet's mean diameter and the water concentration was adapted to the COD (according to Hu and Stamnes, 1993).
- The ground level was fixed at 200 m above sea level to meet average conditions in Central Europe. The photolysis frequencies are listed for ground level and 1000 m above ground.
- As the sun's radiation reaching the earth surface is strongly dependent on the solar zenith angle (SZA), this parameter was varied between $\cos(\text{SZA})=0.95$ and $\cos(\text{SZA})=0.05$ with a step width of 0.10.
- The extra-terrestrial spectrum of the sun's radiation according to Bernhard et al. (2004) was kept constant, valid for the mean distance sun-earth (solar constant). The surface albedo was set to spectral values of pasture land (Feister and Grewe, 1995).

For every meteorological condition, the global irradiance was calculated together with the photon flux density to obtain a functional dependency.

B. Selection of the absorption cross sections and their temperature dependences

The absorption cross sections used were recommended by JPL and IUPAC. They are available in digitized form from the MPI – Mainz UV-Vis Spectral Atlas of Gaseous Molecules (Keller-Rudek and Moortgat, 2015).

The photon flux densities were calculated with a resolution of 0.1 nm in the UV-B region to meet the strong decay towards shorter wavelengths caused by the ozone absorption. The recommended values of IUPAC and JPL, on the other hand, are given with a resolution of 1 nm, so we fall back on the original literature of the recommended data, which often have a higher resolution.

Sometimes, it is necessary to combine two original spectra to cover the whole spectral region from 280 to 650 nm. The transitions from one spectrum to the other are not smoothed out. This is implemented in the integration in the course of the calculations of the photolysis frequencies.

The spectrally resolved absorption cross sections are mostly listed for a reference temperature of 298 K. By multiplication of the listed spectra with a temperature dependent factor, absorption cross sections for other temperatures than 298 K can be obtained. These temperature factors were determined separately, ideally from measurements of the respective original publication. The absorption cross sections are wavelength dependent, the temperature factors are likewise. They are presented as temperature dependent functions.

In Table 1a the references of the applied absorption cross sections are listed, and Table 1b shows the corresponding functions of the temperature factors.

C. Determination of the quantum yield functions

In contrast to the absorption cross sections, the quantum yields of photolysis reactions are often measured with an insufficient spectral resolution. Moreover, measurements are difficult and possess a larger uncertainty than the cross sections. Due to these facts, we use the quantum yields in terms of combinations of energy-dependent functions of the type

$$\frac{A}{1 + \exp\left(-\left(\frac{1}{\lambda} - \frac{1}{\lambda_0}\right)/b\right)}$$

The choice of energy-dependent ($\sim 1/\lambda$) instead of wavelength-dependent functions has the advantage that the parameters have a physical meaning. E.g. the parameter $1/\lambda_0$ corresponds to the energy threshold of the photolysis reaction and b defines the spectral range of change of the quantum yield. Consequently, the individual terms of the combination of functions describe different transitions between the energy levels of the molecule. Due to the physical meaning of the parameters, it is possible to estimate their values from thermodynamic quantities, if the quantum yield itself has not been measured.

To determine the parameters, we use a fit through all original measurements without an obvious bias, e.g. the measurements should show the same form as the recommendations by IUPAC and JPL. If there are enough data, the parameters are determined by assuming a linear temperature dependence. To obtain the fit parameters and their errors, a simplex algorithm (Nelder and Mead, 1965) is used in combination with a bootstrapping method with 2000 arbitrary removals of 20 % of the data.

The references of the included quantum yield measurements are listed in Table 2a, the results of the fit procedures are given in Table 2b.

D. Calculation of the photolysis frequencies

The photolysis frequencies are determined by the integral

$$j = \int_{280}^{650nm} \phi(\lambda) \sigma(\lambda) F_{\lambda}(\lambda) d\lambda$$

The actinic flux densities F_{λ} and the absorption cross sections σ are described above, as well as the quantum yields Φ . At the moment, there are 2400 meteorological situations for 25 photolysis reactions available. The wavelength range 280 nm to 650 nm was chosen due to the fact that a) no sun's radiation below 280 nm reaches the lower part of the troposphere and b) the photon energy for wavelengths above 650 nm is generally not sufficient for photolytic processes.

The photolysis frequencies depend on the solar zenith angle χ given by the function

$$j = a \cdot e^{b(1-1/\cos(c\chi))}$$

The parameters of these functions for the different photolysis reactions were also determined by a simplex technique (Nelder and Mead, 1965) and are made available.

As the global irradiance and the photolysis frequencies depend in a similar way on the solar radiation, 100 functions of the dependence of the photolysis frequencies on the global irradiance are additionally on display. The respective parameters of these functions are determined by least-square-fit calculations based on the simulated data.

Due to this similarity, the functions are independent on the aerosol burden and type, on the cloud optical depth or on the solar zenith angle. Only the dependence on the ozone column density remains for those reactions, which absorb in the UV-B range (280 – 320 nm) of the solar spectrum.

References

- Anderson, G.P., Chetwynd, J.H., Clough, S.A., Shettle, E.P. and Kneizys, F.X. : AFGL Atmospheric Constituent Profiles (0 – 120 km), Air Force Geophysics Laboratory AFGL-TR-86-0110, 1986
- Bernhard, G. Booth, C.R. and Ebrahimian, J.C. : Version 2 data of the National Science Foundation's ultraviolet radiation monitoring network : South Pole, J. Geophys. Res. 109, doi:10.1029/2004JD004937, 2004
- Feister, U. and Grewe, R. : Spectral albedo measurements in the UV and visible region over different types of surfaces, Photochem. Photobiol. 62, 736 – 744, 1995
- Hess, M., Koepke and P., Schult, I. : Optical Properties of Aerosols and Clouds. The Software Package OPAC, Bull. Am. Meteorol. Soc. 79, 831-844, 1998
- Hu, Y.X. and Stamnes, K. : An accurate parametrization of the radiative properties of water clouds suitable for use in climate models, J. Climate 16, 728 – 742, 1993
- IUPAC : IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet P1, available at : <http://iupac.pole-ether.fr>, last access July 2015
- JPL : Sander, S.P., Friedl, R.R., Abatt, J.P.D., Barker, J.R., Burkholder, J.B., Golden, D.M., Kolb, C.E., Kurylo, M.J., Moortgat, G.K., Wine, P.H., Huie, R.E. and Orkin, V.L. : Chemical kinetics and photochemical data for use in atmospheric studies. Evaluation 17, JPL-Publ. 10-6, Pasadena, 2011
- Keller-Rudek, H. and Moortgat, G.K. : MPI-Mainz UV-VIS Spectral Atlas of Gaseous Molecules, www.atmosphere.mpg.de/enid/2295, last access July 2015
- Mayer, B. and Kylling, A. : Technical Note: The libRadtran Software Package for radiative transfer calculations: Description and examples, Atm. Chem. Phys. 5, 18855 – 18877, 2005
- Nelder, J.A. and Mead, R. : A simplex method for function minimization, Comput. J. 7, 308 -313, 1965

Table 1a: References of the absorption spectra used

substance	references	wavelength range
O ₃	Malicet et al., J. Atmos. Chem. 21 (1995) 263 - 273 Brion et al., J. Atmos. Chem. 30 (1998) 291 - 299	195 - 360 nm 345 – 770 nm
H ₂ O ₂	Madronich & Röth, priv. comm. (2006)	200 – 400 nm
NO ₂	Merienne et al., J. Atmos. Chem. 20 (1995) 281 - 297	200 – 500 nm
NO ₃	Sander, J. Phys. Chem. 90 (1986) 4135 - 4142	400 – 690 nm
N ₂ O ₅	Harwood et al., J. Phys. Chem. A 102 (1998) 1309 - 1317	208 – 398 nm
HONO	Stutz et al., J Geophys. Res. 105 (2000) 14585 - 14592	292 – 403.5 nm
HNO ₃	Burkholder et al., J. Geophys. Res. 98 (1993) 22937 - 22948	200 – 350 nm
HNO ₄	Knight et al., Phys. Chem. Chem. Phys. 4 (2002) 1432-1437	280 – 350 nm
CH ₂ O	Meller & Moortgat, J. Geophys. Res. 105 (2000) 7089 -7101	225 – 375 nm
CH ₃ O ₂	Maricq & Wallington, J. Phys. Chem. 96 (1992) 986 - 992	200 – 330 nm
CH ₃ OOH	Vaghjiani & Ravishankara, J. Geophys. Res. 94 (1989) 3487 - 3492 Matthews et al., Proc. Nat. Acad. Sci. USA 102 (2005) 7449-7452	210 – 365 nm 365 – 405 nm
C ₂ H ₅ O ₂	Maricq & Wallington, J. Phys. Chem. 96 (1992) 986 - 992	190 – 341 nm
CH ₃ CHO	Schneider & Moortgat, MPI Mainz (1989) priv. comm.	197 – 362 nm
CH ₃ COCH ₃	Martinez et al., Atm. Environm. A 26 (1992) 785 - 792 Gierczak et al., Chem. Phys. 231 (1998) 229 - 244	202 – 355 nm 215 – 349 nm

Table 1b: Temperature factors for the absorption spectra

substance	function $(\Delta=T_m-T)$	c1	c2	c3	c4	c5	c6	T _m
O ₃	$1 - (c1\Delta + c2\Delta^2) \exp\{c3 + c4*T\}[\lambda - (c5 + c6*T)]^2\}$.0116	0	-5(-4)	0	436	-.27	298
H ₂ O ₂	c1	1.0						
NO ₂	$1 - c1*\Delta \exp\{c3(\lambda - c5)\} + c2*\Delta \exp\{c4*(\lambda - c6)\}$.0023	.004	-.005	-3(-4)	272	600	298
NO ₃	1	1.0						
N ₂ O ₅	$1 - (c1\Delta + c2*\Delta^2) \exp\{c3 + c4*T\}[\lambda - (c5 + c6*T)]^2\}$.02295	-1.08(-4)	-1.5(-4)	0	390	0	277
HONO	c1	1.0						
HNO ₃	$\frac{(c1 + c2*\Delta)}{\{1 + \exp\{(c3 + c4*\Delta)[\lambda - (c5 + c6*\Delta)]\}\}}$	1.0	-.001	.07	0	236	.4	298
HNO ₄	c1	1.0						
CH ₂ O	$1 - (c1*\Delta + c2*\Delta^2) \exp\{c3 + c4*T\}[\lambda - (c5 + c6*T)]^2\}$.014	0	-.383	.001	347.5	0	293
CH ₃ O ₂	c1	1.0						
CH ₃ OOH	c1	1.0						
C ₂ H ₅ O ₂	c1	1.0						
CH ₃ CHO	c1	1.0						
CH ₃ COCH ₃	c1	1.0						

Table 2a : References of the quantum yield literature used

substance	references
O ₃	Brock & Watson, Chem. Phys. 46 (1980) 477 - 484 Trolier & Wiesenfeld, J. Geophys. Res. 93 (1988) 7119 - 7124 Cooper et al., J. Geophys. Res. 98 (1993) 12795 - 12800 Armerding et al., J. Phys. Chem. 99 (1995) 3137 - 3143 Ball & Hancock, Geophys. Res. Lett. 22 (1995) 1213 - 1216 Takahashi et al., J. Phys. Chem. 100 (1996) 4084 - 4089 Ball et al., Chem. Phys. Lett. 264 (1997) 531 - 538 Silvente et al., Chem. Phys. Lett. 264 (1997) 309 - 315 Takahashi et al., J. Chem. Phys. 108 (1998) 7161 - 7172 Talukdar et al., Geophys. Res. Lett. 25 (1998) 144 - 146 Taniguchi et al., J. Phys. Chem. 104 A (2000) 8936 - 8944 Bauer et al., Phys. Chem. Chem. Phys. 2 (2000) 1421 - 1424 Smith et al., J. Phys. Chem. 104 A (2000) 8916 - 8921 Matsumi et al., J. Geophys. Res. 107 (2002) 10.1029/2001JD000510
H ₂ O ₂	Gerlach-Meyer et al., Chem. Phys. Lett. 133 (1987) 113 - 115 Vaghijani & Ravishankara, J. Chem. Phys. 92 (1990) 996 - 1003 Vaghijani et al., J. Chem. Phys. 96 (1992) 5878 - 5886 Schiffman et al., J. Chem. Phys. 98 (1993) 6935 - 6940
NO ₂	Jones & Bayes, J. Chem. Phys. 59 (1973) 4836 - 4844 Gaedtke & Troe, Ber. Bunsenges. Phys. Chem. 79 (1975) 184 - 192 Harker et al., Chem. Phys. Lett. 50 (1977) 394 - 397 Davenport, FAA-EQ-78-05 (1978) Gardner et al., J. Geophys. Res. 92 (1987) 6642 - 6652 Roehl et al., J. Phys. Chem. 98 (1994) 7837 - 7843 Troe, Z. Phys. Chem. 14 (2000) 573 - 581

NO ₃	<p>Graham & Johnston, J. Phys. Chem. 82 (1978) 254 - 268 Magnotta & Johnston, Geophys. Res. Lett. 17 (1980) 769 - 772 Wayne et al., Atm. Environm. 25 A (1991) 1 - 203 Orlando et al., J. Phys. Chem. 97 (1993) 10996 - 11000 Johnston et al., J. Phys. Chem. 100 (1996) 4713 - 4723</p>
N ₂ O ₅	<p>Swanson et al., J. Phys. Chem. 88 (1984) 3115 - 3118 Barker et al., Int. J. Chem. Kin. 17 (1985) 991 - 1006 Ravishankara et al., J. Geophys. Res. 91 (1986) 5355 - 5360 Oh et al., J. Chem. Phys. 85 (1986) 7146 - 7158 Harwood et al., J. Phys. Chem. 101 (1998) 1309 - 1317</p>
HONO	<p>Cox & Derwent, J. Photochem. 6 (1976) 23 - 34 Kenner et al., J. Phys. Chem. 90 (1986) 2635-2639 Wollenhaupt et al., J. Phys. Chem. 104 A (2000) 2695 - 2705 Amanal et al., J. Phys. Chem. 105 A (2001) 1465 - 1475 Wall et al., J. Atm. Chem. 55 (2006) 31 - 54</p>
HNO ₃	<p>Johnston et al., J. Phys. Chem. 78 (1974) 1 - 7 Margitan & Watson, J. Phys. Chem. 86 (1982) 3819 - 3824 Jolly et al., J. Chem. Phys. 84 (1986) 6662 - 6667 Turnipseed et al., J. Chem. Phys. 96 (1992) 5887 - 5895 Felder et al., Chem. Phys. Lett. 215 (1993) 221 - 227 Schiffman et al., J. Chem. Phys. 98 (1993) 6935 - 6946 Myers et al., J. Chem. Phys. 107 (1997) 5361 - 5373</p>
HNO ₄	<p>MacLeod et al., J. Geophys. Res. 93 (1988) 3813 - 3823 Roehl et al., J. Phys. Chem. 105 A (2001) 1592 - 1598 Jimenez et al., Phys. Chem. Chem. Phys. 7 (2005) 342 - 348</p>

CH ₂ O	<p>Calvert et al., Science 175 (1972) 751 - 752 Turco, Geophys. Surveys 2 (1975) 153 - 192 Lewis et al., J. Chem. Phys. 65 (1976) 2910 - 2911 Clark et al., J. Chem. Phys. 68 (1978) 1264 - 1271 Horowitz & Calvert, Int. J. Chem. Kin. 10 (1978) 805 - 819 Moortgat & Warneck, WMO (1978) 295 - 296 Moortgat et al., Chem. Phys. Lett. 54 (1978) 444 - 447 Warneck et al., Ber. Bunsenges. Phys. Chem. 82 (1978) 1136 - 1142 Moortgat & Warneck, J. Chem. Phys. 70 (1979) 3639 - 3651 Tang et al., J. Phys. Chem. 83 (1979) 569 - 573 Moortgat et al., J. Chem. Phys. 78 (1983) 1185 - 1190 Smith et al., J. Phys. Chem. 106 A (2002) 1233 - 1240 Pope et al., Faraday Disc. 130 (2005) 59 - 72 Trope, J. Phys. Chem. 111 A (2007) 3868 - 3874 Gorrotxategi et al., J. Phys. Chem. 112 A (2008) 12437 - 12448 Tatum Ernest et al., J. Phys. Chem. 116 A (2012) 6983 - 6995 Röth & Ehhalt, Atm. Chem. Phys. 15 (2015) 7195 - 7202</p>
CH ₃ O ₂	Sander et al., JPL-Publ. 10-6 (2011)
CH ₃ OOH	<p>Vaghijani & Ravishankara, J. Chem. Phys. 92 (1990) 996 - 1003 Thelen et al., Chem. Phys. Lett. 213 (1993) 275 - 281</p>
C ₂ H ₅ O ₂	Sander et al., JPL-Publ. 10-6 (2011)
CH ₃ CHO	<p>Calver & Pitts, 'Photochemistry' (1966) 371 Weaver et al., J. Photochem. 6 (1976) 111 - 126 Meyrahn et al., J. Photochem. 17 (1981) 138 Horowitz & Calvert, J. Phys. Chem. 86 (1982) 3105 - 3114 Calvert et al., 'Mechanisms of Atmosph. Oxidations of Alkenes' (2000) 384</p>

CH_3COCH_3	Gardner et al., J. Phys. Chem. 88 (1984) 5069 - 5076 Meyrahn et al., J. Atm. Chem. 4 (1986) 277 - 291 Horowitz, J. Phys. Chem, 95 (1991) 10816 - 10823 Cierczak et al., Chem. Phys. 231 (1998) 229 - 244 Emrich & Warneck, J. Phys. Chem. 104 A (2000) 9436 - 9442 Aloisio & Francisco, Chem. Phys. Lett. 329 (2000) 179 - 184 Warneck, Atm. Environm. 35 (2001) 5773 - 5777 Blitz et al., Geophys. Res. Lett. 31 (2004) 10.1029/2003GL018793 Blitz et al., J. Phys. Chem. 110 A (2006) 6742 - 6756 Nadasdi et al., Chem. Phys. Lett. 440 (2007) 31 - 55 Rajakumar et al., J. Photochem. Photobiol. 199 A (2008) 336 - 344 Khamaganov et al., Phys. Chem. Chem. Phys. 9 (2007) 4098 - 4113 Khamaganov et al., Phys. Chem. Chem. Phys. 11 (2009) 6173 - 6181 Somnitz et al., Phys. Chem. Chem. Phys. 11 (2009) 8522 - 8531
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Table 2b : Quantum yield functions

no	reaction	function	c1	c2	c3	c4	c5	c6	c7	c8
1	O ₃ → O(¹ D)	$\frac{c1+c2*e^{c3*T}}{1+\exp(\frac{1/\lambda-1/c5}{c4})}$ $- \frac{c2*e^{c3*T}}{1+\exp(\frac{1/\lambda-1/c7}{c6})} + c8$	0.84	-7.6(-5)	+0.0253	-1.0(-5)	309.8	-1.6(-5)	320.0	0.08 ^a 0.0 ^b
2	O ₃ → O(³ P)	1-QY(O ₃ →O(¹ D))								
3	H ₂ O ₂ → OH+OH	c1	1.0							
4	NO ₂ → NO+O	$\frac{c1 + c2 * T}{1 + \exp(\frac{1/\lambda - 1/(c5 + c6 * T)}{c3 + c4 * T})}$	1.0	0	-2.1(-5)	0	397.8	0.02		
5	NO ₃ → Prod	$\frac{c1 + c2 * T}{1 + \exp(\frac{1/\lambda - 1/(c5 + c6 * T)}{c3 + c4 * T})}$	1.0	0	+4.0(-6)	-8.0(-8)	594.0	0.065		
6	NO ₃ → NO ₂ + O	$\frac{c1 + c2 * T}{1 + \exp(\frac{1/\lambda - 1/(c5 + c6 * T)}{c3 + c4 * T})}$	1.0	0	-2.1(-6)	-8.0(-8)	586.0	0.065		
7	NO ₃ → NO + O ₂	QY(NO ₃ →Prod)-QY(NO ₃ →NO ₂ +O)								
8	N ₂ O ₅ → NO ₃ +NO ₂	c1	1.0							
9	HONO → NO+OH	c1	1.0							

10	HNO ₃ → NO ₂ +OH	$\frac{c1 + c2 * T}{1 + \exp\left(\frac{1/\lambda - 1/(c5 + c6 * T)}{c3 + c4 * T}\right)}$	1.0	0	+2.5(-4)	0	205.0	0		
11	HNO ₃ → HONO+O	1-QY(HNO ₃ →NO ₂ +OH)								
12	HNO ₄ → HO ₂ +NO ₂	$\frac{c1 + c2 * T}{1 + \exp\left(\frac{1/\lambda - 1/(c5 + c6 * T)}{c3 + c4 * T}\right)}$	1.0	0	+6.4(-4)	0	183.8	0		
13	HNO ₄ → OH+NO ₃	1-QY(HNO ₄ →HO ₂ +NO ₂)								
14	CH ₂ O → CHO+H	$\frac{c1}{1 + \exp\left(\frac{1/\lambda - 1/(c4 + c5 * T)}{c2 + c3 * T}\right)} + \frac{c6}{1 + \exp\left(\frac{1/\lambda - 1/c8}{c7}\right)}$	0.74	-5.4(-5)	0	327.4	0	-0.40	-5.2(-5)	279.0
15	CH ₂ O → products	$\frac{c1}{1 + \exp\left(\frac{1/\lambda - 1/(c4 + c5 * T)}{c2 + c3 * T}\right)} \frac{M}{M_0} + \frac{c6}{1 + \exp\left(\frac{1/\lambda - 1/c8}{c7}\right)}$	1.0	-5.4(-5)	0	346.9	0	-0.22	-5.2(-5)	279.0
16	CH ₂ O → H ₂ +CO	QY(CH ₂ O→prod) - QY(CH ₂ O→CHO+H)								
17	CH ₃ O ₂ → CH ₃ O+O	c1	1.0							

18	CH ₃ OOH → CH ₃ O+OH	c1	1.0							
19	C ₂ H ₅ O ₂ → C ₂ H ₅ O+O	c1	1.0							
20	CH ₃ CHO → CH ₄ +CO	$\frac{c1 + c2 * T}{1 + \exp\left(\frac{1/\lambda - 1/(c5 + c6 * T)}{c3 + c4 * T}\right)}$	0.65	0	-7.0(-5)	0	268.0	0		
21	CH ₃ CHO → products	$\frac{c1}{1 + \exp\left(\frac{1/\lambda - 1/(c4 + c5 * T)}{c2 + c3 * T}\right)} + \frac{c6}{1 + \exp\left(\frac{1/\lambda - 1/c8}{c7}\right)}$	1.0	-1.2(-4)	0	297.0	0	-0.20	-5.0(-5)	295.0
22	CH ₃ CHO → CH ₃ +CHO	QY(CH ₃ CHO→prod)-QY(→CH ₄ +CO)								
23	CH ₃ COCH ₃ → CH ₃ +CO+CH ₃	$\frac{1}{1 + \exp\left(\frac{1/\lambda - 1/(c3 + c4 * T)}{c1 + c2 * T}\right)} * \frac{1}{1 + \exp\left(\frac{1/\lambda - 1/(c7 + c8 * T)}{c5 + c6 * T}\right)} * M/M_0$	+2.2(-4)	-1.6(-6)	214.5	+0.116	+1.5(-3)	0	257.0	0

24	CH ₃ COCH ₃ → products	$\frac{1}{1 + \exp\left(\frac{1/\lambda - 1/(c3 + c4 * T)}{c1 + c2 * T}\right)}$ $* \frac{1}{1 + \exp\left(\frac{1/\lambda - 1/(c7 + c8 * T)}{c5 + c6 * T}\right)} * M/M_0$	-8.5(-5)	+7.1(-8)	268.5	+0.136	-1.5(-4)	0	290.0	0
25	CH ₃ COCH ₃ → CH ₃ CO+CH ₃	QY(→prod)-QY(→CH ₃ +CO+CH ₃)								

a) below 400 nm b) above 400 nm