SUPPLEMENTARY INFORMATION FOR:

UVC based advanced oxidation processes for simultaneous removal of microcontaminants and pathogens from simulated municipal wastewater at pilot plant scale

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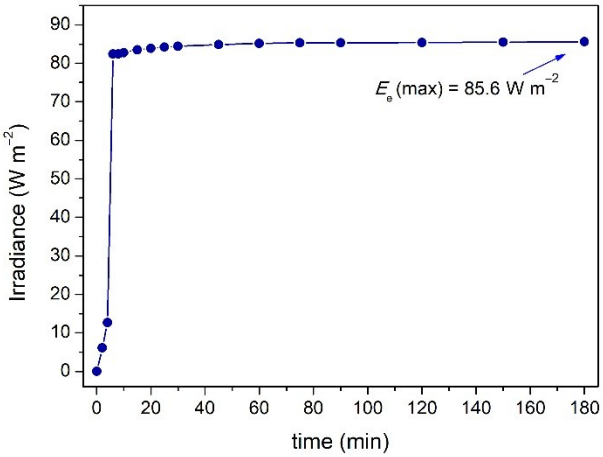
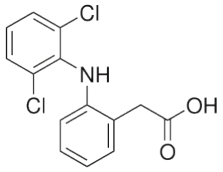
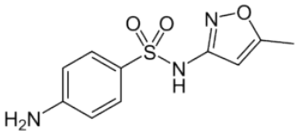
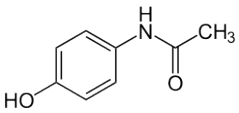
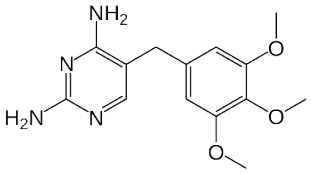
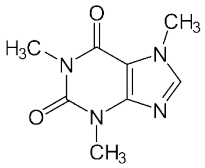
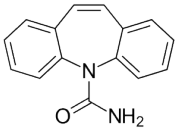


Fig. S1 – Irradiance profile of the UV-C lamp measured during 180 min in distilled water (maximum value 85.6 W m^{-2}).

Table S1 – Chromatographic parameters: retention time, wavelength of maximum absorbance and area of each microcontaminant peak at 100 µg L^{-1}.

Microcontaminant	**Retention time (min)**	**λ (nm)**	**Area - 100 µg L^{-1} (a. u.)**
Acetaminophen (ACT)	2.48	245	18.2
Caffeine (CAF)	3.60	270	14.0
Carbamazepine (CBZ)	3.94	270	5.5
Trimethoprim (TMP)	5.01	267	20.0
Sulfamethoxazole (SMX)	7.2	2.67	8.7
Diclofenac (DCF)	10.6	2.80	9.7

Table S2 – Photochemical properties of the microcontaminants and experimental degradation percentages under UVC irradiation

Microcontaminant	Chemical structure	* $A_{254\ nm}$ (a. u.)	$\varepsilon_{254\ nm}$ [1] ($10^3\ M^{-1}\ cm^{-1}$)	[1] $\Phi_{254\ nm}$ (10^{-2} mol Es^{-1})	*Deg. (%)
DCF		0.023	6.1	22.2	~100% (200 min)
SMX		0.064	16.5	5.8	~100% (30 min)
ACT		0.056	6.6	4.6	75% (180 min)
TMP		0.017	2.9	0.6	40% (180 min)
CAF		0.022	4.2	0.3	30% (180 min)
CBZ		0.026	5.5	0.2	20% (180 min)

$\varepsilon_{254\ nm}$ ($M^{-1}\ cm^{-1}$) = molar absorptivity coefficient

$\Phi_{254\ nm}$ (mol Es^{-1}) = quantum efficiency

*Experimental values obtained in this work

[1] H. W. Yu, M. Park, S. Wu, I.J. Lopez, W. Ji, J. Scheideler, S. A. Snyder, Strategies for selecting indicator compounds to assess attenuation of emerging contaminants during UV advanced oxidation processes. Water Research, 2019. 166: p. 115030. doi: 10.1016/j.watres.2019.115030.

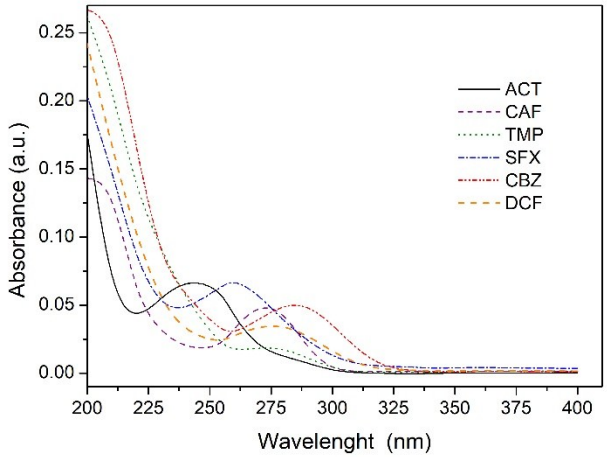


Fig. S2 – UV absorption spectrum of each microcontaminant. This measurement was carried out using 1 mg L^{-1} of each compound dissolved in distilled water between 200-400 nm. The obtained absorbance at 254 nm can be seen in Table S2 above.

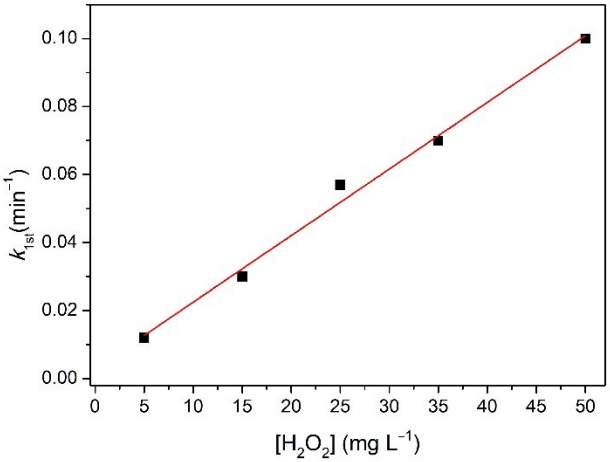


Fig. S3 – Pseudo first order kinetic constant (k_{1st}) as a function of H_2O_2 concentration ([H_2O_2]) for UVC/H_2O_2 process. The obtained slope and R^2 for the linear regression were 0.00196 L (mg min)$^{-1}$ and 0.990, respectively.

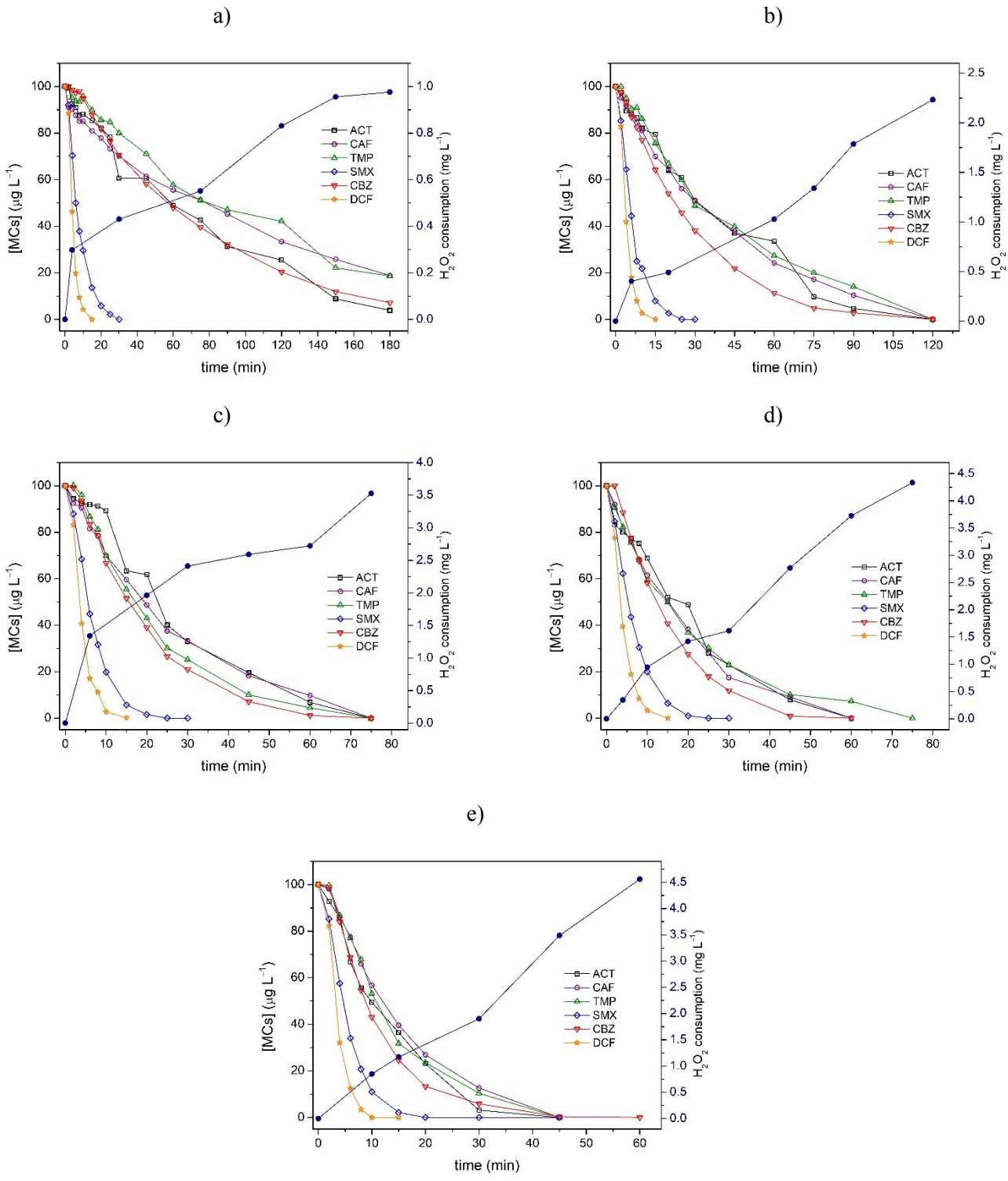


Fig. S4 – Degradation profile of each MCs and H_2O_2 consumption for the UVC/H_2O_2 process: a) 5 mg L^{-1}, b) 15 mg L^{-1}, c) 25 mg L^{-1}, d) 35 mg L^{-1}, and e) 50 mg L^{-1}.

Table S3 – Pseudo first-order kinetic constants (k_{1st}) for the UVC/H_2O_2 process during degradation of MCs. The values in parentheses correspond to the coefficient of determination (R^2).

	k_{1st} (10^{-2} min^{-1})					
UV-C/H_2O_2 (mg L^{-1})	ACT	CAF	TMP	SFX	CBZ	DCF
5	1.7 (0.97)	0.9 (0.99)	1.0 (0.99)	15.5 (0.99)	1.45 (0.97)	32.1 (0.94)
15	3.3 (0.97)	2.4 (0.99)	2.2 (0.99)	18.5 (0.99)	4.0 (0.99)	37.2 (0.97)
25	4.4 (0.97)	4.0 (0.99)	5.4 (0.99)	21.5 (0.98)	7.1 (0.97)	44.4 (0.96)
35	5.5 (0.98)	5.4 (0.99)	4.6 (0.99)	22.5 (0.97)	9.9 (0.94)	35.0 (0.98)
50	11 (0.93)	7.1 (0.99)	8.0 (0.99)	26.4 (0.97)	12.3 (0.98)	43.4 (0.95)

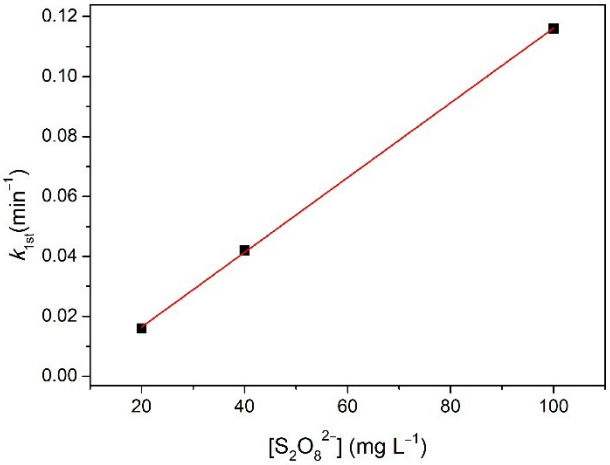


Fig. S5 – Pseudo first order kinetic constant (k_{1st}) as a function of $S_2O_8^{2-}$ concentration ([$S_2O_8^{2-}$]) for UVC/$S_2O_8^{2-}$ process. The obtained slope and R^2 for the linear regression were 0.00125 L (mg min)$^{-1}$ and 0.999, respectively.

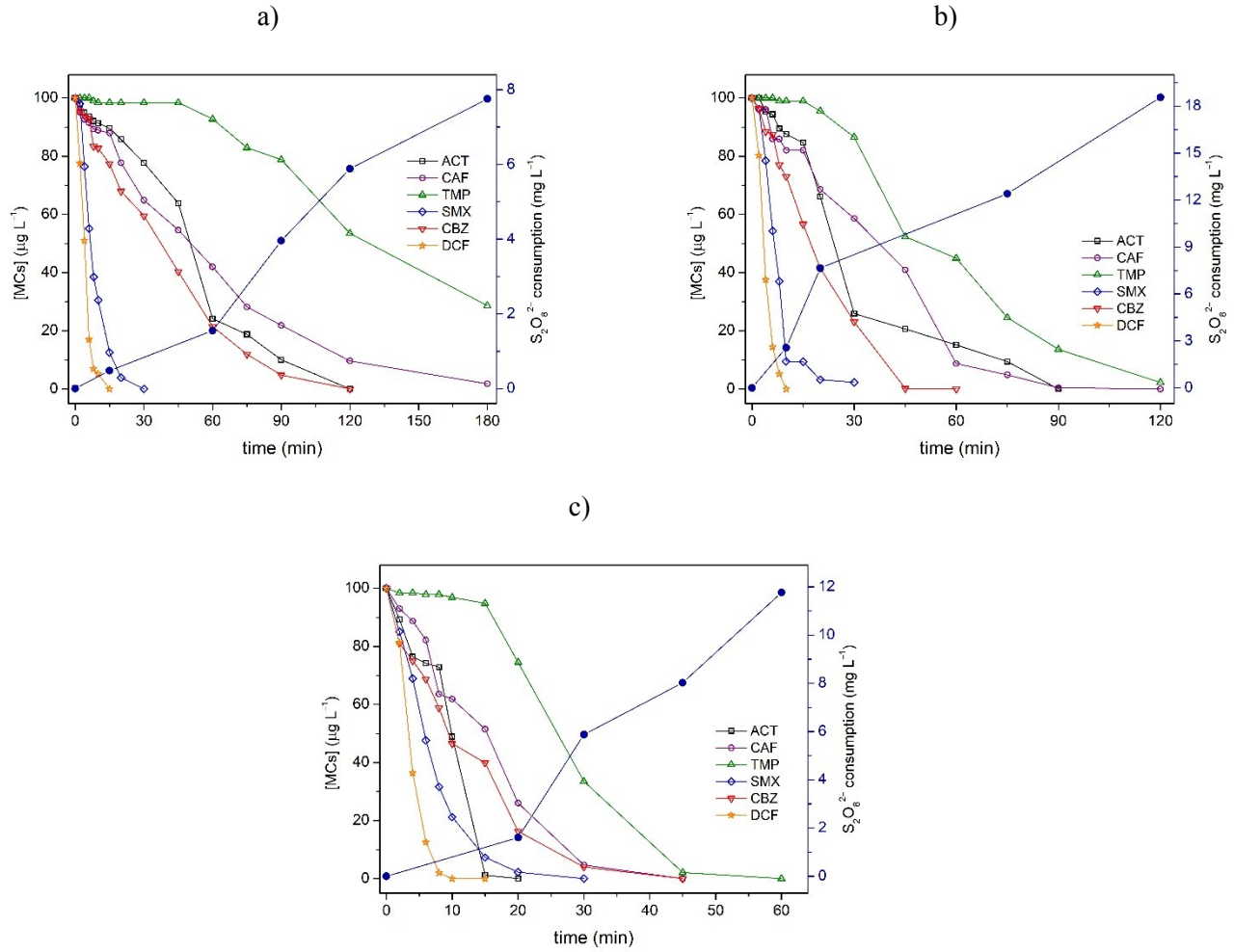


Fig. S6 – Degradation profile of each MCs and H_2O_2 consumption for the UVC/$S_2O_8^{2-}$ process: a) 20 mg L^{-1}, b) 40 mg L^{-1}, and c) 100 mg L^{-1}.

Table S4 – Pseudo first-order kinetic constants (k_{1st}) for the UVC/$S_2O_8^{2-}$ process during degradation of MCs. The values in parentheses correspond to the coefficient of determination (R^2).

	k_{1st} (10^{-2} min^{-1})					
UV-C/$S_2O_8^{2-}$ (mg L^{-1})	ACT	CAF	TMP	SFX	CBZ	DCF
20	2.5 (0.96)	2.1 (0.99)	0.9 (0.98)	16.5 (0.97)	3.1 (0.96)	33.1 (0.96)
40	3.4 (0.97)	3.8 (0.91)	3.6 (0.94)	14.6 (0.95)	4.9 (0.98)	38.1 (0.96)
100	6.0 (0.85)	9.6 (0.91)	8.1 (0.81)	19.5 (0.98)	10.3 (0.95)	48.4 (0.98)

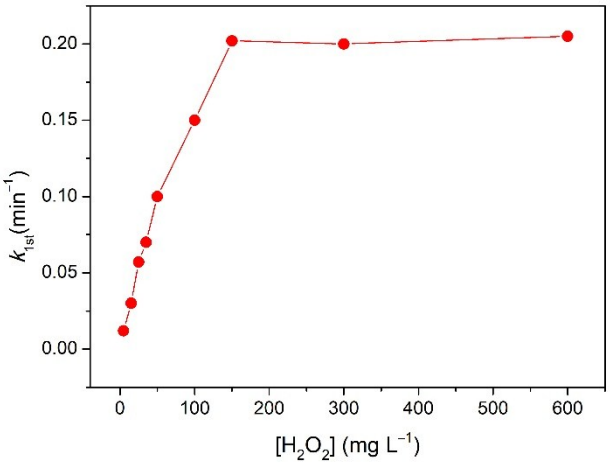


Fig. S7 – Pseudo first order kinetic constant (k_{1st}) as a function of H_2O_2 concentration ([H_2O_2]) for UVC/H_2O_2 process.

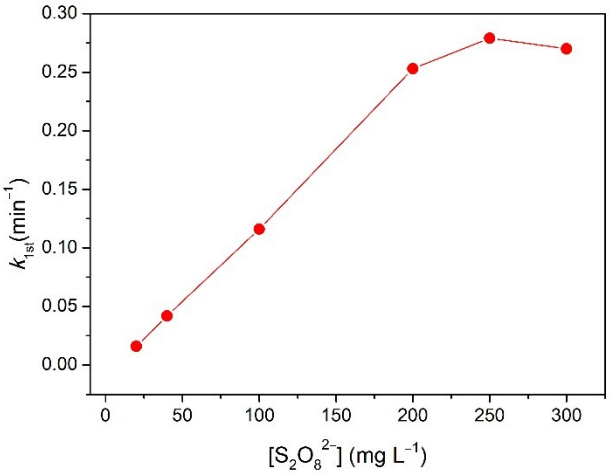


Fig. S8 – Pseudo first order kinetic constant (k_{1st}) as a function of $S_2O_8^{2-}$ concentration ([$S_2O_8^{2-}$]) for UVC/$S_2O_8^{2-}$ process.

Table S5 – Radical self-scavenging reactions involved in UVC/H_2O_2 and UVC/$S_2O_8^{2-}$ processes.

Reactions	Rate constants	Reference
$2OH^{\bullet} \rightarrow H_2O_2$	k = 5.5 x 10^9 M^{-1} s^{-1}	[2]
$H_2O_2 + OH^{\bullet} \rightarrow H_2O + HO_2^{\bullet} \leftrightarrow O_2^{\bullet-} + H^+$	k = 2.7 x 10^7 M^{-1} s^{-1}	[3]
$HO^{\bullet} + O_2^{\bullet-} \rightarrow HO^- + O_2$	k = 8.0 x 10^9 M^{-1} s^{-1}	[4]
$HO^{\bullet} + HO_2^{\bullet} \rightarrow H_2O + O_2$	k = 7.1 x 10^9 M^{-1} s^{-1}	[5]
$SO_4^{\bullet-} + S_2O_8^{2-} \rightarrow HO^{\bullet} + SO_4^{2-} + S_2O_8^{\bullet-}$	k = 6.1 x 10^5 M^{-1} s^{-1}	[6]
$SO_4^{\bullet-} + SO_4^{\bullet-} \rightarrow S_2O_8^{2-}$	k = 4.0 x 10^8 M^{-1} s^{-1}	[7]
$SO_4^{\bullet-} + H_2O \rightarrow OH^{\bullet} + SO_4^{2-} + H^+$	k < 3 x 10^8 s^{-1}	[7]

[2] G. V. Buxton, C.L. Greenstock, W.P. Helman, A.B. Ross, Critical review of rate constants for reactions of hydrated electrons, hydrogen atoms and hydroxyl radicals (·OH/·O^-) in aqueous solution, J. Phys. Chem. Ref. Data 17 (1988) 513–886. doi:10.1063/1.555805.

[3] G. Beck, Elektrische nachweis geladener zwischenprodukte pulsradiolyse, Int. J. Radiat. Phys. Chem. 1 (1969) 361–371. doi:10.1016/0020-7055(69)90033-3.

[4] K. Sehested, O.L. Rasmussen, H. Fricke, Rate constants of OH with HO_2, O_2^-, and $H_2O_2^+$ from hydrogen peroxide formation in pulse-irradiated oxygenated water, J. Phys. Chem. 72 (1968) 626–631. doi:10.1021/j100848a040.

[5] G. V. Buxton, M. Bydder, G. Arthur Salmon, The reactivity of chlorine atoms in aqueous solution Part II. The equilibrium $SO_4^{\bullet-}$ + Cl^- ⇌ $Cl^{\bullet}$ + SO_4^{2-}, Phys. Chem. Chem. Phys. 1 (1999) 269–273. doi:10.1039/a807808d.

[6] R.E. Huie, C.L. Clifton, Rate constants for hydrogen abstraction reactions of the sulfate radical, SO_4^-. Alkanes and ethers, Int. J. Chem. Kinet. 21 (1989) 611–619. doi:10.1002/kin.550210802.

[7] E. Hayon, A. Treinin, J. Wilf, Electronic spectra, photochemistry, and autoxidation mechanism of the sulfite-bisulfite-pyrosulfite systems. SO_2^-, SO_3^-, SO_4^-, and SO_5^- radicals, J. Am. Chem. Soc. 94 (1972) 47–57. doi:10.1021/ja00756a009.