Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information

Temperature Dependent Absorption Cross-Sections of O_2-O_2 collision pairs between 340 and 630 nm

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Table S1: Description of light sources, cavity mirrors, optical filters and spectrometer settings

Cavity	O_4 Bands	Mirror Center λ	Reflectivity (Peak)	Range (nm)	Filters	Resolution FWHM (nm)	Grating (g/mm)	Light Source
UV	344[a], 360[a,b], 380[a]	355 (ATF)	0.99983	335-387	Pyrex plate, 325 LPF (CVI), UG11 (Schott)	0.32	1200	Xe-arc
Blue	446[a] 477[b]	455 (ATF)	0.99997	420-495	GG435(Schott), 500SWP (Thorlabs), 450 BPF (Thorlabs)	0.36	1200	LED LZ1-10B205
Green	532[a]	532 (ATF)	0.99998	510-555	OG515 (Schott), 550SWP (Newport)	0.38	1200	Green LED LZ1-10G105
Amber	577[b]	580 (crd-optics)	0.999978	550-596	550 LWP (Thorlabs), 600SWP (Thorlabs)	0.38	1200	Warm White LED LZ1-10WW00
Red	630[b]	630 (Los-Gatos)	0.99993	550-680	600 LWP (Thorlabs)	0.4 and 0.68	600	Red LED LZ1-10R205

[a] Measurement/Reference gas: O_2/Ar; [b] Measurement/Reference gas: Air/N_2;

Table S2: Comparison of Literature Data

Study	Year	[a] Temp (K)	Wavelength (nm)	Peak ($x10^{-46}$ cm^5 $molecule^{-2}$)	Integral ($x10^{-43}$ cm^4 $molecule^{-2}$)	Width (nm/cm^{-1})
Salow and Steiner [b]	1936	-	343.6	0.99	-	-
			360.7	3.6		
			380.3	2.1		
			446.4	0.3		
			477.0	5.3		
			532.3	0.4		
			577.3	7.7		
			629.9	5.3		
Hermans [b]	1939	-	477.3	8.0	-	-
			577.2	13		
			630.0	6.2		
Dianov-Klokov [b]	1964	-	360.5	4.4	-	-
			380.2	2.2		
			446.7	0.70		
			477.3	5.5		
			532.2	1.5		
			577.2	9.8		
			630.0	6.9		
			1065.2	12		
Blickensderfer and Ewing (1σ)	1969	78	477	-	2.5(4)	-
			577		6.1(4)	
			630		5.4(6)*	
		300	477		2.4(4)	
			577		3.5(4)	
			630		1.5(6)*	
Tabniz et al.	1969	577	-	-	4.63(7)	-
		630			3.47(7)	
McKellar et al.*	1972	90	477	17.4	2.47	-
			577	29.2	6.48	
			630	22	5.03	
		113	477	11.3	2.03	
			577	20.4	5.52	
			630	14.1	4.18	
		295	477	6.1	2.18	
			577	10.8	4.56	
			630	6.6	3.52	
Long and Ewing*	1973	87	577	35.8		7.3/220

Perner and Platt	1980	279	343.9	0.70(24)	-	1.6/
			360.5	5.4(1.5)		4.9/
			380.2	<1.4		~6/
			444.0	1.0(12)		7.4/
			476.9	5.9(1.8)		5.8/
			575.0	16(6)		9.5/
Greenblatt et al. (3σ)	1990	296	343.4	1.2(1)	-	4.2/
			360.5	4.1(4)		4.8/
			380.2	2.4(2)		4.4/
			446.7	0.57(6)		5.6/
			477.3	6.3(6)		6.2/
			532.2	1.0(1)		10.2/
			577.2	11(1)		11.6/
			630.0	7.2(7)		13.8/
		196	360.8	5.7(6)		4.2/
			380.2	3.7(4)		3.7/
			477.3	7.6(13)		4.7/
Volkamer (3σ)	1996	296	342.7	1.18(9)	-	5.8(5)/
			360.8	5.42(7)		4.3(1)/
			380.2	2.4(2)		3.6(2)/
			477.1	6.1(3)		5.2(8)/
			531.7	1.3(3)		13(8)/
			576.9	10.3(3)		11.2(1)/
			630.6	5.5-6.9(6)		14.(1)/
Newnham and Ballard (3σ)	1998	223	477	6.99(35)	1.629(21)	339(15)/
			532	1.31(20)	0.404(11)	369(6)/
			577	12.61(11)	4.3585(76)	
			630	8.8(13)	2.766(72)	
			630*	8.34(83)	2.9227(76)	
		283	477	1.23(38)	2.483(48)	
			532	11.75(20)	0.431(17)	
			577	7.9(15)	4.625(14)	
			630		2.769(99)	
			630*		3.025(17)	
Osterkamp et al. (data extracted from Table 4 of Wagner 2002)	1998	204	477	7.9(3)		
			532	1.4(2)		
			577	12.2(4)		
		256	477	7.0(3)		
			532	1.2(2)		
			577	13.6(4)		
Hermans et al. [c]	1998	RT	343.96	0.983	0.307	3.65/309.5
			360.89	4.291	1.578	4.15/319.6
			380.25	2.467	0.771	4.06/280.6
			446.39	0.502	0.124	3.97/199.1
			477.10	6.553	1.99	5.36/235.3
			532.36	0.907	0.29	8.25/292.2

			577.5	11.01	4.23	11.0/331.8
			630.3	7.076	2.87	13.77/347.4
Naus and Ubachs	1999	294	577	11.41(15)	4.66(9)	/340(3)
(1σ)			630	7.55(15)	3.19(9)	/367(3
Tiedje et al. (1σ)	2001	-	577	12.07(30)	4.93(20)	/337(3)
			630	7.71(20)	3.26(14)	/360(3)
Wagner et al.	2002	241	360.5	5.70(50)		
			380.2	2.44(40)		
			477.3	7.80(20)		
			532.2	1.74(50)		
			577.2	13.50(40)		
			630.0	9.61(30)		
Morville et al. (1σ)	2002	296	576.3	11.22(25)	-	/345(2)
			629.3	7.2(3)	-	/323(15)
		192.5	577.3	12.8(4)	-	/292(2)
			629.3	8.7(3)	-	/281(15)
		132	575.3	17.5(16)	-	/276(2)
			629.3	11.6(1)	-	/173(15)
Sneeps et al.	2006	294	477.79(6)	6.60(6)	2.34(6)	5.64(16)/247.1(68)
(294K 577 data from			577.17	11.5(1)	4.70(6)	11.5(1)/346.5(30)
Naus and Ubachs, /		268	577.3(1)	11.1(3)	4.47(13)	11.3(2)/342.3(71)
1σ)		230	477.47(26)	5.78(23)	1.90(22)	5.2(6)/228(26)
		190	577.6(2)	12.6(5)	4.06(24)	9.6(3)/290(10)
		184	477.25(14)	7.33(20)	2.07(16)	4.5(3)/239(14)
Chen and Venables	2009	296	360.1	4.0	-	-

[a] Temperatures are assumed to be room temperature unless reported
[b]Data reproduced from the MPI Mainz database (http://www.atmosphere.mpg.de/enid/5db486bc26e00f61354f2fbe841be944,0/Spectra/Introduction_1rr.html)
*Data retrieved from digitized versions of the graphs published in these respective works.
[c] http://spectrolab.aeronomie.be/o2.htm

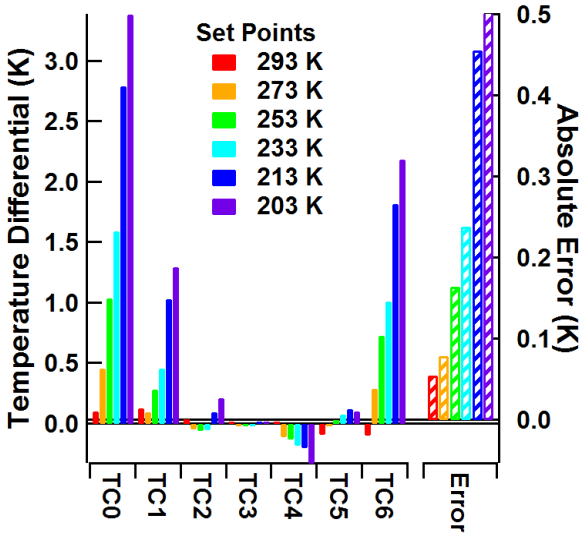

Figure S1: Temperature variation across the cavity. The ‘error’ denotes the integral temperature variation over length, and is given as the average error over the full cavity length in units of Kelvin. TC0 to TC6 refer to Figure 1.

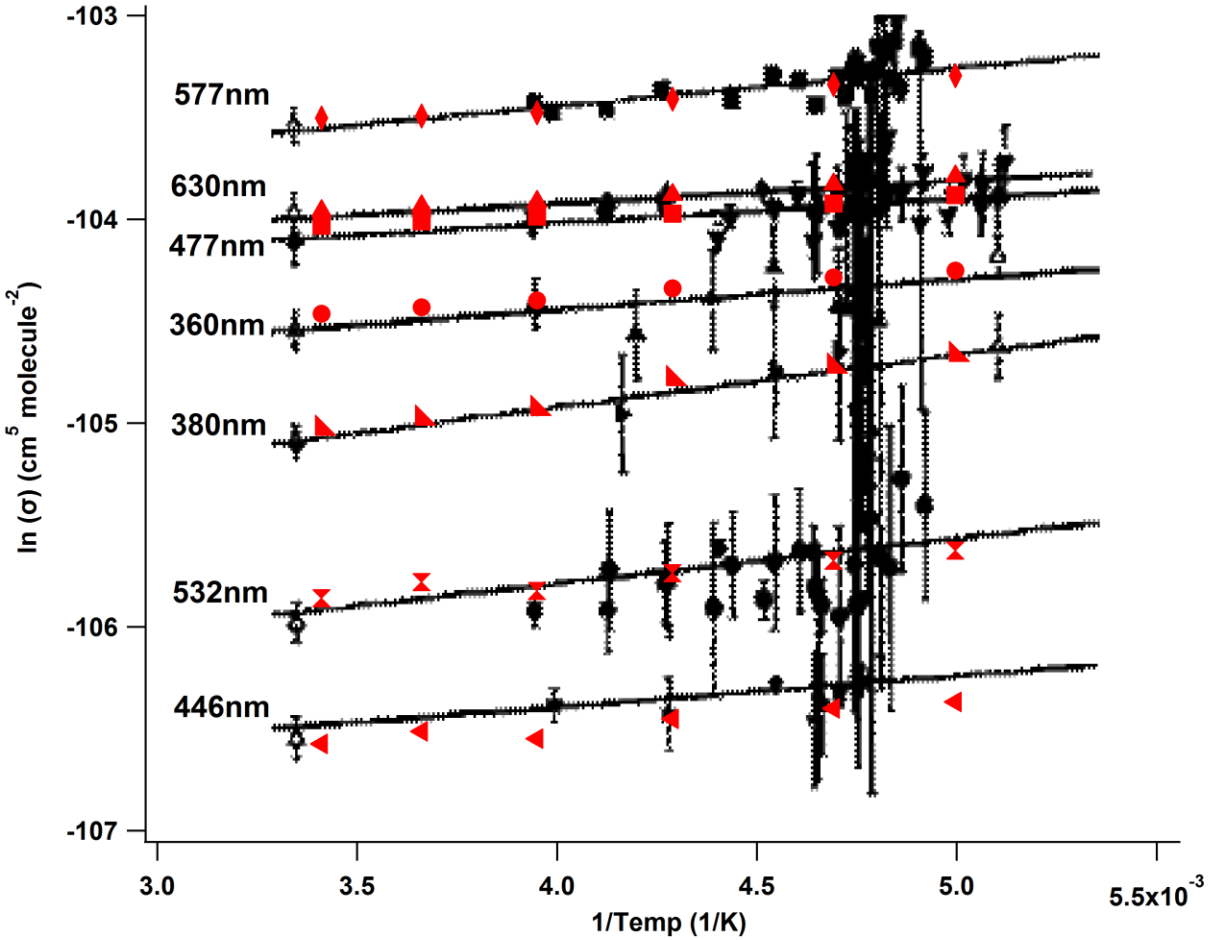

Figure S2: Comparison of Peak $\sigma_{O4\text{-}CIA}$ of this work to Figure 3 of Pfeilsticker et al. 2001. The red triangles represent our data, while the black circles are measurements from a balloon-borne DOAS instrument, combined with the room temperature cross-section of Greenblatt et al. (black diamonds).