Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Photolysis of O_2 dispersed in solid neon with far-ultraviolet radiation

Sheng-Lung Chou,[1] Jen-Iu Lo,[1] Yu-Chain Peng,[1] Hsiao-Chi Lu,[1] Bing-Ming Cheng,[1]*and J. F. Ogilvie[2,3]*

[1]*National Synchrotron Radiation Research Center, 101 Hsin-Ann Road, Hsinchu Science Park, Hsinchu 30076, Taiwan*
[2]*Department of Mathematics, Simon Fraser University, 8888 University Drive, Burnaby, British Columbia V5A1S6 Canada*
[3]*Escuela de Quimica, Universidad de Costa Rica, Ciudad Universitaria Rodrigo Facio, San Pedro de Montes de Oca, San Jose 11501-2060, Costa Rica*

*To whom correspondence should be addressed; electronic mail: bmcheng@nsrrc.org.tw (B.-M. Cheng); ogilvie@cecm.sfu.ca (J. F. Ogilvie)

Table S1. Sequence of emission lines of CO in system a $^3\Pi_r \rightarrow X\ ^1\Sigma^+$ recorded after irradiation of samples of $^{16}O_2$ in Ne at 143 nm but not 173 nm

CO in Ne				gaseous CO		
λ/nm [a]	ν/cm^{-1} [b]	Δν/cm^{-1} [c]	v',v'' [d]	ν/cm^{-1} [e]	Δν/cm^{-1} [c]	Δν/cm^{-1} [f]
205.9	48564		0,0	48473.2		91
215.4	46411	2153	0,1	46330.0	2143.2	81
225.8	44271	2140	0,2	44213.2	2116.8	58
237.0	42174	2097	0,3	42122.8	2090.4	52
249.2	40121	2053	0,4	40058.8	2064.0	62
262.6	38072	2049	0,5	38021.0	2037.8	51

[a] Wave length λ/nm is measured in air.
[b] Wavenumber ν/cm^{-1} pertains to vacuum.
[c] Wavenumber difference Δν/cm^{-1} is the progressive difference from the preceding row.
[d] v',v'' denotes the vibrational numbering for transitions between vibrational ground state v'=0 of the excited electronic state and vibrational state $v'' \geq 0$ in ground electronic state.
[e] ν/cm^{-1} are calculated wavenumbers for the transitions in the preceding column.
[f] Wavenumber difference Δν/cm^{-1} is the difference between neon and gaseous values..

Table S2. Lines of OH in system A $^2\Sigma^+ \rightarrow$ X $^2\Pi_i$ emitted during photolysis of $^{16}O_2$

OH in Ne			gaseous OH			
λ/nm [a]	ν/cm^{-1} [b]	Δν/cm^{-1} [c]	*v*',*v*"Ω [d]	ν/cm^{-1} [e]	Δν/cm^{-1} [c]	Δν/cm^{-1} [f]
307.8	32479		0,0 1/2	32402.4		77
309.0	32353	126	0,0 3/2	32276.1	126.2	77
313.5	31889		1,1 1/2	31821.0		68
314.9	31747	142	1,1 3/2	31694.8	126.2	52

[a-f] As footnotes [a-f] in Table S1.

Table S3. Lines of $^{12}C^{18}O$ in system a $^3\Pi_r \rightarrow X\ ^1\Sigma^+$

	$^{12}C^{18}O$ in Ne		gaseous $^{12}C^{18}O$			
λ/nm [a]	ν/cm^{-1} [b]	Δν/cm^{-1} [c]	*v*',*v*'' [d]	ν/cm^{-1} [e]	Δν/cm^{-1} [c]	Δν/cm^{-1} [f]
			0,0	48473		
			0,1	46381	2091.8	
225.1	44411		0,2	44264	2066.0	147
236.2	42324	2087	0,3	42173	2040.2	151
247.9	40327	1997	0,4	40108	2014.5	219
260.8	38332	1995	0,5	38070	1988.9	262

[a-f] As footnotes [a-f] in Table S1.

Table S4. Broad lines in emission present after irradiation of $^{18}O_2$ (in Ne at 4 K) at 143 nm but not at 173 nm [a]

λ/nm [b]	ν/cm^{-1} [c]
488.1	20482
490.0	20402
539.9	18537*
542.0	18438*
594.8	16808*
598.0	16712*
646.0	15475*
653.3	15303
657.5	15205
720.3	13880*
726.1	13767*
734.0	13620
736.3	13575*
739.4	13521
742.5	13472*
782.8	12773*
789.9	12670*
822.1	12159*
827.7	12077*
835.0	11973
841.2	11886*

[a] Lines marked * have the same wavenumber in both $^{16}O_2$ and $^{18}O_2$ experiments.
[b] Wave length λ/nm is measured in air.
[c] Wavenumber ν/cm^{-1} pertains to vacuum.

Table S5. Unidentified emission lines present during irradiation of $^{18}O_2$ (in Ne at 4 K) at 143 nm but not at 173 nm [a]

λ/nm [b]	ν/cm^{-1} [c]
361.9	27626*
379.4	26346*
398.7	25075
506.4	19742*
531.3	18817
563.7	17735
570.2	17533
582.6	17160*
584.4	17107*
586.3	17051*
603.1	16576*
689.9	14491
864.9	11559

[a-c] As footnotes [a-c] in Table S4.

Figure S1. Emission spectra of $^{12}C^{16}O$ and $^{12}C^{18}O$ recorded during irradiation of $^{18}O_2$ dispersed in solid neon excited at 143 nm during periods (a) 7 - 17 min, (b) 47 - 76 min.