APPENDIX B

Tables

B.1. STANDARD ATMOSPHERIC VARIABLES VERSUS ALTITUDE

Table B.1. Variation of Geopotential Height (Z), Air Pressure, Air Temperature, and Air Density with Altitude in a Standard Atmosphere

Alt. (km)	Geopot. Height (km)	Press. (mb)	Temp. (K)	Density (kg m^{-3})	Alt. (km)	Geopot. Height (km)	Press. (mb)	Temp. (K)	Density (kg m^{-3})
0	0	1013.25	288.15	1.225	22	21.924	40.5	218.57	0.0645
0.1	0.1	1001.20	287.50	1.213	23	22.917	34.7	219.57	0.0550
0.2	0.2	989.45	286.85	1.202	24	23.910	29.7	220.56	0.0469
0.3	0.3	977.72	286.20	1.190	25	24.902	25.5	221.55	0.0401
0.4	0.4	966.11	285.55	1.179	26	25.894	21.9	222.54	0.0343
0.5	0.5	954.61	284.90	1.167	27	26.886	18.8	223.54	0.0293
0.6	0.6	943.22	284.25	1.156	28	27.877	16.2	224.53	0.0251
0.7	0.7	931.94	283.60	1.145	29	28.868	13.9	225.52	0.0215
0.8	0.8	920.77	282.95	1.134	30	29.859	12.0	226.51	0.0184
0.9	0.9	909.71	282.30	1.123	31	30.850	10.3	227.50	0.0158
1	1.0	898.80	281.65	1.112	32	31.840	8.89	228.49	0.0136
1.5	1.5	845.59	278.40	1.058	33	32.830	7.67	230.97	0.0116
2	1.999	795.0	275.15	1.007	34	33.819	6.63	233.74	0.00989
2.5	2.499	746.9	271.91	0.957	35	34.808	5.75	236.51	0.00846
3	2.999	701.2	268.66	0.909	36	35.797	4.99	239.28	0.00726
3.5	3.498	657.8	265.41	0.863	37	36.786	4.33	242.05	0.00624
4	3.997	616.6	262.17	0.819	38	37.774	3.77	244.82	0.00537
4.5	4.497	577.5	258.92	0.777	39	38.762	3.29	247.58	0.00463
5	4.996	540.5	255.68	0.736	40	39.750	2.87	250.35	0.00400
5.5	5.495	505.4	252.43	0.697	41	40.737	2.51	253.11	0.00346
6	5.994	472.2	249.19	0.660	42	41.724	2.20	255.88	0.00299
6.5	6.493	440.7	245.94	0.624	43	42.711	1.93	258.64	0.00260
7	6.992	411.1	242.70	0.590	44	43.698	1.69	261.40	0.00226
7.5	7.491	383.0	239.46	0.557	45	44.684	1.49	264.16	0.00197
8	7.990	356.5	236.22	0.526	46	45.669	1.31	266.93	0.00171
8.5	8.489	331.5	232.97	0.496	47	46.655	1.16	269.68	0.0015
9	8.987	308.0	229.73	0.467	48	47.640	1.02	270.65	0.00132
9.5	9.486	285.8	226.49	0.440	49	48.625	0.903	270.65	0.00116
10	9.984	265.0	223.25	0.414	50	49.610	0.798	270.65	0.00103
11	10.981	227.0	216.78	0.365	55	54.528	0.425	260.77	5.7×10^{-4}
12	11.977	194.0	216.65	0.312	60	59.439	0.220	247.02	3.1×10^{-4}
13	12.973	165.8	216.65	0.267	65	64.342	0.109	233.29	1.6×10^{-4}
14	13.969	141.7	216.65	0.228	70	69.238	0.0522	219.59	8.3×10^{-5}

(cont.)

Table B.1. (cont.)

Alt. (km)	Geopot. Height (km)	Press. (mb)	Temp. (K)	Density (kg m^{-3})	Alt. (km)	Geopot. Height (km)	Press. (mb)	Temp. (K)	Density (kg m^{-3})
15	14.965	121.1	216.65	0.195	75	74.125	0.0239	208.40	4.0×10^{-5}
16	15.960	103.5	216.65	0.166	80	79.006	0.0105	198.64	1.8×10^{-5}
17	16.955	88.5	216.65	0.142	85	83.878	0.0045	188.89	8.2×10^{-6}
18	17.949	75.7	216.65	0.122	90	88.744	0.0018	186.87	3.4×10^{-6}
19	18.943	64.7	216.65	0.104	95	93.601	0.00076	188.42	7.5×10^{-7}
20	19.937	55.3	216.65	0.0889	100	98.451	0.00032	195.08	5.6×10^{-7}
21	20.931	47.3	217.58	0.0757					

Source: NOAA (1976).

B.2. SOLAR IRRADIANCE AT THE TOP OF THE ATMOSPHERE

Table B.2. Extraterrestrial Solar Irradiance at the Top of the Earth's Atmosphere versus Wavelength

λ (μm)	$\bar{F}_{s,\lambda}$ (W m^{-2} μm^{-1})	λ (μm)	$\bar{F}_{s,\lambda}$ (W m^{-2} μm^{-1})	λ (μm)	$\bar{F}_{s,\lambda}$ (W m^{-2} μm^{-1})	λ (μm)	$\bar{F}_{s,\lambda}$ (W m^{-2} μm^{-1})	λ (μm)	$\bar{F}_{s,\lambda}$ (W m^{-2} μm^{-1})
0.105	0.055	0.355	1125	0.605	1773	0.855	909	3.1	26
0.110	0.050	0.360	1077	0.610	1722	0.860	953	3.2	22.6
0.115	0.039	0.365	1274	0.615	1671	0.865	896	3.3	19.2
0.120	1.168	0.370	1359	0.620	1721	0.870	933	3.4	16.6
0.125	0.371	0.375	1219	0.625	1665	0.875	928	3.5	14.6
0.130	0.060	0.380	1340	0.630	1658	0.880	907	3.6	13.5
0.135	0.080	0.385	1113	0.635	1639	0.885	904	3.7	12.3
0.140	0.061	0.390	1345	0.640	1632	0.890	894	3.8	11.1
0.145	0.063	0.395	1096	0.645	1601	0.895	892	3.9	10.3
0.150	0.096	0.400	1796	0.650	1557	0.9	891	4	9.5
0.155	0.194	0.405	1643	0.655	1502	0.91	880	4.1	8.7
0.160	0.206	0.410	1768	0.660	1562	0.92	869	4.2	7.8
0.165	0.372	0.415	1810	0.665	1570	0.93	858	4.3	7.1
0.170	0.607	0.420	1760	0.670	1539	0.94	847	4.4	6.5
0.175	0.885	0.425	1719	0.675	1556	0.95	837	4.5	5.92
0.180	1.90	0.430	1615	0.680	1526	0.96	820	4.6	5.35
0.185	2.53	0.435	1798	0.685	1481	0.97	803	4.7	4.86
0.190	3.88	0.440	1829	0.690	1460	0.98	785	4.8	4.47
0.195	5.35	0.445	1951	0.695	1491	0.99	767	4.9	4.11
0.200	7.45	0.450	2048	0.700	1453	1.0	748	5	3.79
0.205	10.7	0.455	2043	0.705	1420	1.05	668	6	1.82
0.210	23.4	0.460	2054	0.710	1407	1.1	593	7	.99
0.215	36.3	0.465	2012	0.715	1376	1.15	535	8	.585
0.220	44.7	0.470	2007	0.720	1351	1.2	485	9	.367
0.225	55.0	0.475	2042	0.725	1358	1.25	438	10	.241
0.230	50.5	0.480	2061	0.730	1331	1.3	397	11	.165
0.235	49.5	0.485	1867	0.735	1322	1.35	358	12	.117
0.240	47.0	0.490	1943	0.740	1282	1.4	337	13	.0851
0.245	62.2	0.495	1993	0.745	1276	1.45	312	14	.0634

(cont.)

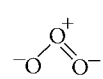
Table B.2. (cont.)

λ (μm)	$\bar{F}_{s,\lambda}$ (W m^{-2} μm^{-1})	λ (μm)	$\bar{F}_{s,\lambda}$ (W m^{-2} μm^{-1})	λ (μm)	$\bar{F}_{s,\lambda}$ (W m^{-2} μm^{-1})	λ (μm)	$\bar{F}_{s,\lambda}$ (W m^{-2} μm^{-1})	λ (μm)	$\bar{F}_{s,\lambda}$ (W m^{-2} μm^{-1})
0.250	55.2	0.500	1892	0.750	1272	1.5	288	15	.0481
0.255	69.5	0.505	1941	0.755	1262	1.55	267	16	.0371
0.260	111	0.510	1937	0.760	1241	1.6	245	17	.0291
0.265	212	0.515	1805	0.765	1220	1.65	223	18	.0231
0.270	255	0.520	1811	0.770	1195	1.7	202	19	.0186
0.275	197	0.525	1850	0.775	1179	1.75	180	20	.0152
0.280	186	0.530	1907	0.780	1189	1.8	159	25	.00617
0.285	317	0.535	1894	0.785	1183	1.85	142	30	.00297
0.290	546	0.540	1840	0.790	1151	1.9	126	35	.0016
0.295	573	0.545	1866	0.795	1142	1.95	114	40	.000942
0.300	493	0.550	1845	0.800	1126	2	103	50	.000391
0.305	669	0.555	1854	0.805	1112	2.1	90	60	.00019
0.310	711	0.560	1801	0.810	1080	2.2	79	80	.0000416
0.315	765	0.565	1828	0.815	1073	2.3	69	100	.0000257
0.320	777	0.570	1824	0.820	1049	2.4	62	120	.0000126
0.325	935	0.575	1851	0.825	1050	2.5	55	150	.00000523
0.330	1041	0.580	1833	0.830	1027	2.6	48	200	.00000169
0.335	950	0.585	1838	0.835	1012	2.7	43	250	.0000007
0.340	1035	0.590	1760	0.840	1006	2.8	39	300	.00000023
0.345	980	0.595	1791	0.845	983	2.9	35	400	.00000011
0.350	1019	0.600	1752	0.850	951	3	31	1000	0

λ is the midpoint of a wavelength interval, and the irradiance at each λ is integrated from the lower to the upper edge of the interval. For example, the irradiance in the interval from $\lambda = 0.1475$ to 0.1575 μm, centered at $\lambda = 0.15$ μm is $\bar{F}_{s,\lambda}$, $\Delta\lambda = 0.096$ W m^{-2} μm^{-1} × 0.005 mm = 0.00048 W m^{-2}. The sum of irradiance over all bins is the solar constant. The data were derived from Woods et al. (1996) for $\lambda < 0.275$ μm, Nicolet (1989) for $0.275 < \lambda < 0.9$ μm, and Thekaekara (1974) for $\lambda > 0.9$ μm.

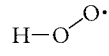
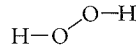
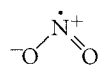
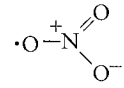
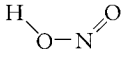
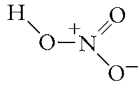
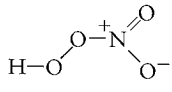
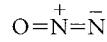
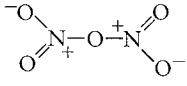
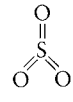
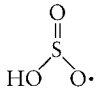
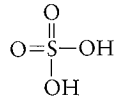
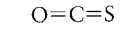
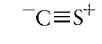
B.3. GAS-PHASE SPECIES

Table B.3. Inorganic and Organic Gases and Their Possible Chemical Structures

Chemical Name Molecular Formula Chemical Structure			
Inorganic			
Hydrogen and Oxygen Species			
Atomic hydrogen H	Atomic oxygen (triplet) O	Molecular oxygen O_2	Ozone O_3
H·	:Ö·	O=O	

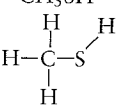
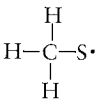
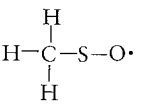
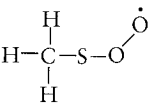
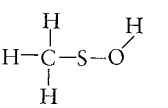
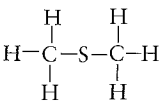
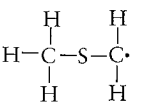
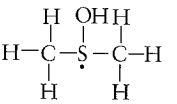
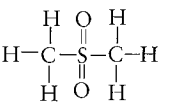
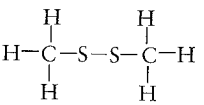
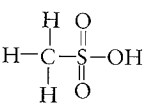
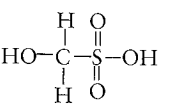
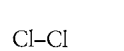
(cont.)

Table B.3. (cont.)

Chemical Name Molecular Formula Chemical Structure			
Inorganic			
Hydroxyl radical OH	Hydroperoxy radical HO_2	Hydrogen peroxide H_2O_2	Water vapor H_2O
			
Nitrogen Species			
Molecular nitrogen N_2	Nitric oxide NO	Nitrogen dioxide NO_2	Nitrate radical NO_3
			
Nitrous acid HONO	Nitric acid HNO_3	Peroxynitric acid HO_2NO_2	Nitrous oxide N_2O
			
Dinitrogen pentoxide N_2O_5			
			
Sulfur Species			
Atomic sulfur S	Sulfur monoxide (sulfonyl or thionyl radical) SO	Sulfur dioxide SO_2	Sulfur trioxide SO_3
			
Bisulfite HSO_3	Sulfuric acid H_2SO_4	Carbonyl sulfide OCS	Carbon monosulfide CS
			

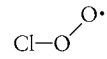
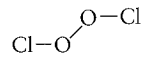
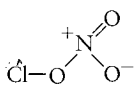
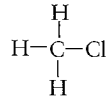
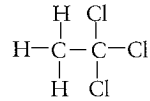
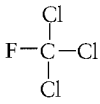
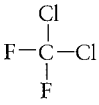
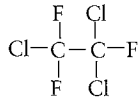
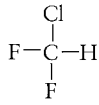
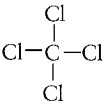
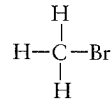
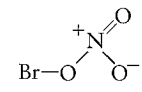
(cont.)

Table B.3. (cont.)

Chemical Name Molecular Formula Chemical Structure			
Inorganic			
Carbon disulfide CS_2	Hydrogen sulfide radical HS	Hydrogen sulfide H_2S	Methanethiol (Methyl sulfide) MeSH CH_3SH
			
Methanethiolate radical CH_3S	Methanethiolate oxy radical CH_3SO	Methanethiolate peroxy radical CH_3SO_2	Methanesulfenic acid CH_3SOH
			
Dimethyl sulfide DMS CH_3SCH_3	Dimethyl sulfide radical CH_3SCH_2	Dimethyl sulfide–OH adduct $CH_3S(OH)CH_3$	Dimethyl sulfone $DMSO_2$ $CH_3S(O)_2CH_3$
			
Dimethyl disulfide DMDS CH_3SSCH_3	Methanesulfonic acid MSA $CH_3S(O)_2OH$	Hydroxymethane-sulfonic acid HMSA $HOCH_2S(O)_2OH$	
			
Chlorine Species			
Atomic chlorine Cl	Molecular chlorine Cl_2	Hydrochloric acid HCl	Chlorine monoxide ClO
			

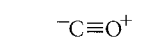
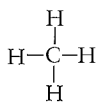
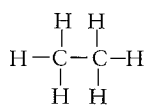
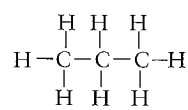
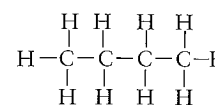
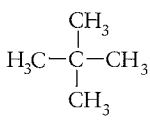
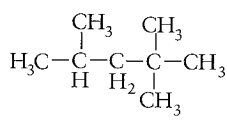
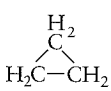
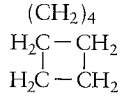
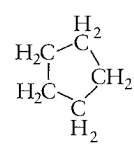
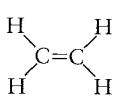
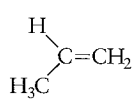
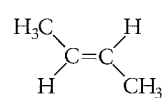
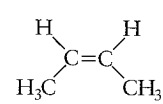
(cont.)

Table B.3. (cont.)

Chemical Name Molecular Formula Chemical Structure			
Inorganic			
Hypochlorous acid HOCl	Chlorine peroxy radical OClO	Chlorine peroxy radical ClOO	Dichlorine dioxide Cl_2O_2
			
Chlorine nitrate $ClONO_2$	Chlorine nitrite $ClNO_2$	Methyl chloride CH_3Cl	Methyl chloroform CH_3CCl_3
			
Trichlorofluoromethane (CFC-11) $CFCl_3$	Dichlorodifluoromethane (CFC-12) CF_2Cl_2	1-Fluorodichloro, 2-difluorochloroethane (CFC-113) $CFCl_2CF_2Cl$	Chlorodifluoromethane (HCFC-22) CF_2ClH
			
Carbon tetrachloride CCl_4			
			
Bromine Species			
Atomic bromine	Molecular bromine	Hydrobromic acid	Bromine chloride
Br	Br_2	HBr	BrCl
	Br–Br	H–Br	Br–Cl
Hypobromous acid HOBr	Bromine monoxide BrO	Methyl bromide CH_3Br	Bromine nitrate $BrONO_2$
			

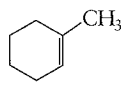
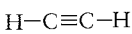
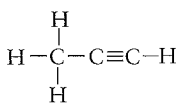
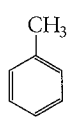
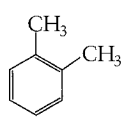
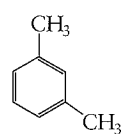
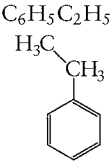
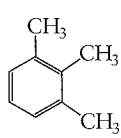
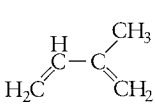
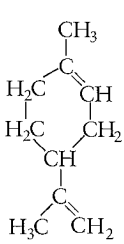
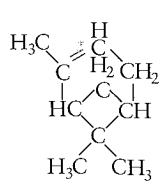
(cont.)

Table B.3. (cont.)

Chemical Name Molecular Formula Chemical Structure			
Inorganic			
Inorganic Carbon Species			
Carbon monoxide CO 	Carbon dioxide CO_2 		
Organic			
Alkanes			
Methane CH_4 	Ethane C_2H_6 	Propane C_3H_8 	Butane C_4H_{10} 
2,2-Dimethylpropane (neopentane) $C(CH_3)_4$ 	2,2,4-Trimethylpentane (isooctane) $(CH_3)_2CHCH_2C(CH_3)_3$ 		
Cycloalkanes			
Cyclopropane $(CH_2)_3$ 	Cyclobutane $(CH_2)_4$ 	Cyclopentane $(CH_2)_5$ 	
Alkenes			
Ethene (ethylene) C_2H_4 	Propene (propylene) C_3H_6 	*trans*-2-Butene C_4H_8 	*cis*-2-Butene C_4H_8 

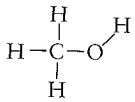
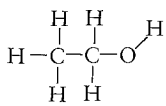
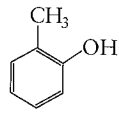
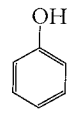
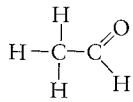
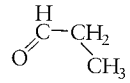
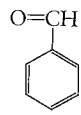
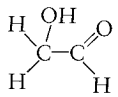
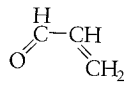
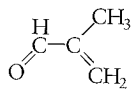
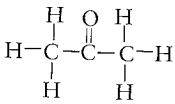
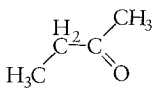
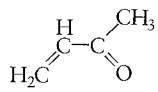
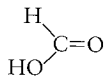
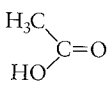
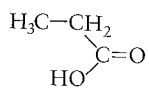
(cont.)

Table B.3. (cont.)

Chemical Name Molecular Formula Chemical Structure			
Organic			
Cycloalkenes			
Cyclopentene C_5H_8	Cyclohexene C_6H_{10}	1-Methylcyclohexene C_7H_{12}	
			
Alkynes			
Ethyne (acetylene) C_2H_2	Propyne C_3H_4		
			
Aromatics			
Benzene C_6H_6	Toluene (methylbenzene) **TOL**	*o*-Xylene (1,2-dimethylbenzene) **XYL**	*m*-Xylene (1,3-dimethylbenzene) **XYL**
	$C_6H_5CH_3$ 	$1,2\text{-}(CH_3)_2C_6H_4$ 	$1,3\text{-}(CH_3)_2C_6H_4$ 
Ethylbenzene $C_6H_5C_2H_5$	1,2,3-Trimethylbenzene $1,2,3\text{-}(CH_3)_3C_6H_3$		
			
Terpenes			
Isoprene (2-methyl-1,3-butadiene) **ISOP** C_5H_8	*d*-Limonene $C_{10}H_{16}$	α-Pinene $C_{10}H_{16}$	
			

(cont.)

Table B.3. (cont.)

Chemical Name Molecular Formula Chemical Structure			
Organic			
Alcohols			
Methanol (methyl alcohol) CH_3OH	Ethanol (ethyl alcohol) C_2H_5OH	*o*-Cresol **CRES** $2\text{-}CH_3C_6H_4OH$	Phenol (hydroxybenzene) C_6H_5OH
			
Aldehydes			
Formaldehyde (methanal) HCHO	Acetaldehyde (ethanal) CH_3CHO	Propionaldehyde (propanal) CH_3CH_2CHO	Benzaldehyde **BZA** C_6H_5CHO
			
Glycol aldehyde $HOCH_2CHO$	Acrolein (propenal) $CH_2CH{=}CHO$	Methacrolein (2-methyl-2propenal) **MACR** $CH_2{=}C(CH_3)CHO$	
			
Ketones			
Acetone (2-propanone) CH_3COCH_3	Methylethylketone (2-butanone) $CH_3CH_2COCH_3$	Methylvinylketone (3-buten-2-one) **MVK** $CH_2{=}CHCOCH_3$	
			
Carboxylic Acids			
Formic acid (methanoic acid) HCOOH	Acetic acid (ethanoic acid) CH_3COOH	Propionic acid (propanoic acid) CH_3CH_2COOH	
			

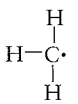
(cont.)

Table B.3. (cont.)

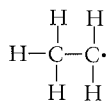
Chemical Name Molecular Formula Chemical Structure
Organic

Alkyl Radicals

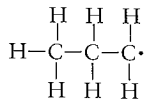
Methyl radical
CH_3



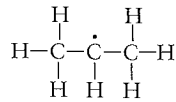
Ethyl radical
C_2H_5



n-Propyl radical
C_3H_7

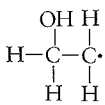


Isopropyl radical
C_3H_7



Hydroxyalkyl Radicals

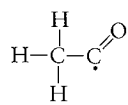
Hydroxyethyl radical
(ethanyl radical)
$HOCH_2CH_2$



Acyl (Alkanoyl) Radicals

Formyl radical
(methanoyl radical)
HCO

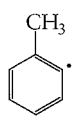
Acetyl radical
(ethanoyl radical)
CH_3CO



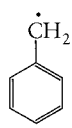
Aryl Radicals

Phenyl radical
C_6H_5

Methylphenyl radical
$C_6H_4(CH_3)$

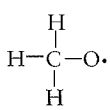


Benzyl radical
$C_6H_5CH_2$

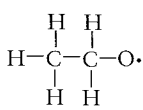


Alkoxy Radicals

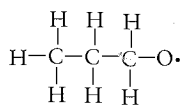
Methoxy radical
CH_3O



Ethoxy radical
C_2H_5O

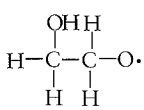


n-Propoxy radical
C_3H_7O



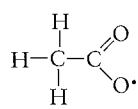
Hydroxyalkoxy Radicals

Hydroxyethyloxy radical
(ethanoloxy radical)
$HOCH_2CH_2O$



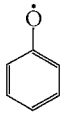
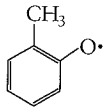
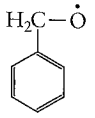
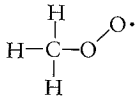
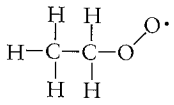
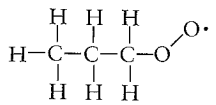
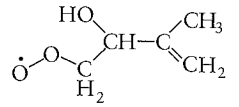
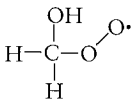
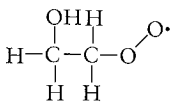
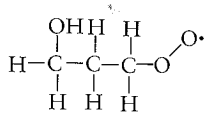
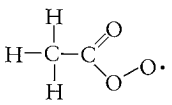
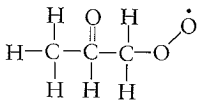
Acyloxy (Alkanoyloxy) Radicals

Acetyloxy radical
$CH_3C(O)O$



(cont.)

Table B.3. (cont.)

Chemical Name Molecular Formula Chemical Structure
Organic
Aryloxy Radicals
Phenoxy radical **PHO** C_6H_5O

Methylphenoxy radical **CRO** $2\text{-}OC_6H_4CH_3$

Benzoxy radical $C_6H_5CH_2O$

Alkylperoxy Radicals
Methylperoxy radical CH_3O_2

Ethylperoxy radical $C_2H_5O_2$

n-Propylperoxy radical $C_3H_7O_2$

Alkylperoxy radical from OH addition to isoprene **ISOH**

Hydroxyalkylperoxy Radicals
Hydroxymethylperoxy radical (methanolperoxy radical) $HOCH_2O_2$

Hydroxyethylperoxy radical (ethanolperoxy radical) $HOC_2H_4O_2$

Hydroxypropylperoxy radical (propanolperoxy radical) $HOC_3H_6O_2$

Acylperoxy (Alkanoylperoxy) Radicals
Peroxyacetyl radical $CH_3C(O)OO$

Acetylmethylperoxy radical CH_3COCH_2OO


(cont.)

Table B.3. (cont.)

Chemical Name Molecular Formula Chemical Structure			
Organic			
Arylperoxy Radicals			
Phenylperoxy radical **PHO_2** C_6H_5OO	Methylphenylperoxy radical **CRO_2** $2\text{-}O_2C_6H_4CH_3$	Benzylperoxy radical **BO_2** $C_6H_5CH_2OO$	Methylbenzylperoxy radical **XLO_2** $2\text{-}CH_2OOC_6H_5CH_3$
Other Peroxy Radicals			
Peroxybenzoyl radical **BZO_2** C_6H_5OCOO	MVK+O_3 product $OOCCH_3CHCH_2$	2-Methylperoxy propenoyl radical $CH_2CCH_3C(O)OO$	MACR+O_3 product CH_2CCH_3CHOO
Peroxy radical of methylglyoxal **MGPX** $CH_3COC(O)OO$	MACR+OH product $CH_2CCH_3C(O)OO$	Nitrated organic peroxy radical **PNO_2**	
OH-Adducts			
Methylvinylketone-OH adduct **MV1** $OOCH_2CH(OH)C(CH_3)O$	Methylvinylketone-OH adduct **MV2** $HOCH_2CH(OO)C(CH_3)O$	Methacrolein-OH adduct **MAC1** $OCHC(O_2)(CH_3)CH_2OH$	Methacrolein-OH adduct **MAC2** $OCHC(OH)(CH_3)CH_2OO$

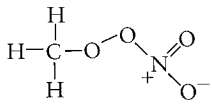
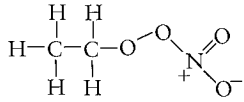
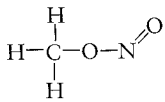
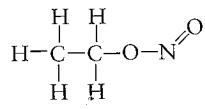
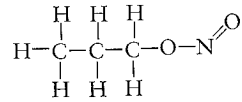
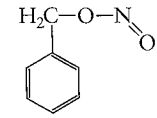
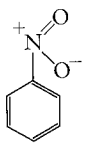
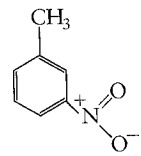
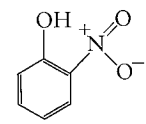
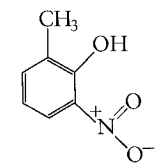
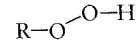
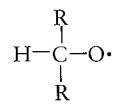
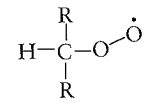
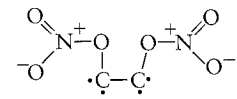
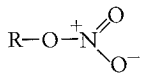
(cont)

Table B.3. (cont.)

Chemical Name Molecular Formula Chemical Structure
Organic
Toluene–OH adduct **TO_2** $2\text{-}OHC_6H_5(O_2)CH_3$
o-Xylene–OH adduct **XINT** $4\text{-}OH\text{-}3\text{-}O_2\text{-}2\text{-}CH_3C_6H_4CH_3$
Molozonides
Ethene molozonide **OZD** $CH_2O_3CH_2$
Propene molozonide **OZD** $CH_3CHO_3CH_2$
Biradicals
Criegee biradical H_2COO
Methyl criegee biradical CH_3HCOO
Dicarbonyls
Glyoxal (ethanedial) $(CHO)_2$
Methylglyoxal **MGLY** CH_3COCHO
Organic Peroxides
Methyl hydroperoxide CH_3OOH
Nitrates
Methyl nitrate CH_3ONO_2
Ethyl nitrate $C_2H_5ONO_2$
Propyl nitrate $C_3H_7ONO_2$
Benzyl nitrate $C_6H_5CH_2ONO_2$
Peroxyacetyl nitrate **PAN** $CH_3C(O)OONO_2$
2-Methylperoxy propenoylnitrate **MPAN** $CH_2CCH_3C(O)OONO_2$
Peroxybenzoyl nitrate **PBZN** $C_6H_5C(O)OONO_2$
Isoprene-NO_3 adduct **ISNT** $C_5H_8ONO_2$

(cont.)

Table B.3. *(cont).*

Chemical Name Molecular Formula Chemical Structure
Organic
Nitric Acids
Methylperoxy nitric acid $CH_3O_2NO_2$ 
Ethylperoxy nitric acid $C_2H_5O_2NO_2$ 
Nitrites
Methyl nitrite CH_3ONO 
Ethyl nitrite C_2H_5ONO 
Propyl nitrite C_3H_7ONO 
Benzyl nitrite $C_6H_5CH_2ONO$ 
Nitro Group
Nitrobenzene $C_6H_5NO_2$ 
m-Nitrotoluene $3\text{-}NO_2C_6H_4CH_3$ 
o-Nitrophenol **NPHN** $2\text{-}NO_2C_6H_4OH$ 
m-Nitrocresol **NCRE** $3\text{-}NO_2\text{-}2\text{-}OHC_6H_3CH_3$ 
Carbon-Bond Groups
Paraffin carbon bond **PAR** 
Olefin carbon bond **OLE** 
Ketone carbonyl group **KET** 
Organic peroxide **ROOH** 
Primary organic peroxy radical **RO_2** 
Secondary organic oxy radical **ROR** 
Secondary organic peroxy radical **RO_2R** 
C_2 dinitrate group **DNIT** 
Organic nitrate **NTR** 

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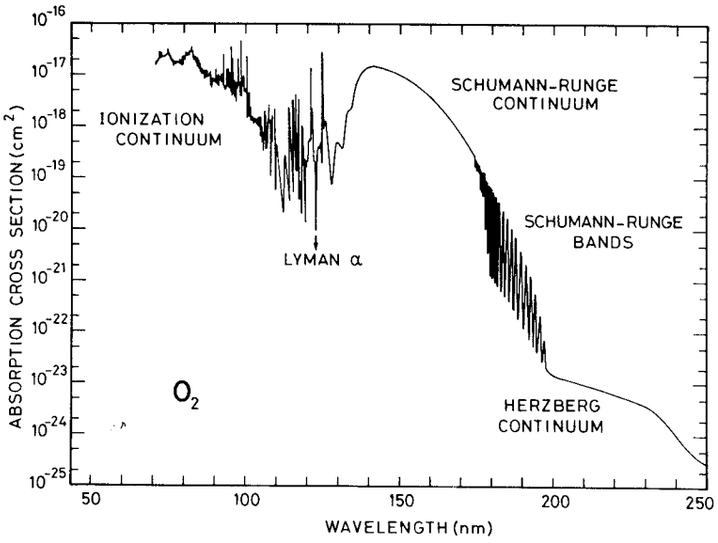

Fig. 4.26. Spectral distribution of the absorption cross section of molecular oxygen.

($\lambda < 137$nm) some diffuse bands occur, but these are interspersed with a series of windows, which allow some wavelengths to penetrate relatively deep into the atmosphere. One of these windows coincides by chance with the solar Lyman α line, which plays an important role in atmospheric chemistry. Figure 4.26 shows the general shape of the spectral distribution of the absorption cross section. At wavelengths less than 102.8 nm, photoionization can occur.

The absorption coefficient of molecular oxygen has been the subject of numerous laboratory investigations. In the Herzberg continuum, the measurements of Ditchburn and Young (1962), Blake et al. (1966), Ogawa (1971), Hasson and Nicholls (1971) and Shardanand and Prasad-Rao (1977) indicate an absorption cross section less than 1.5×10^{-23} cm^{-2}, but exhibit some discrepancies in the absolute value, especially at long wavelengths (see Fig. 4.27). Part of the difficulty associated with measuring this cross section in the laboratory arises from the formation of the Van Der Waal's molecule, O_4, for which observational evidence has even been found in the atmosphere (Perner and Platt, 1980). Balloon observations of the solar irradiance in the stratosphere have led to inferences of the O_2 absorption cross section in-situ (Frederick and Mentall, 1982; Herman and Mentall, 1982), and these have resulted in values somewhat lower than the laboratory investigations. The inferred cross section depends sensitively on the accuracy of a simultaneous measurement of the ozone amount and on the adopted value for the ozone cross sections used in the analysis. Rayleigh scattering, which contributes at least 10% to the total