

## Water (H<sub>2</sub>O)

$$Z = 10$$

$$\text{Molecular Mass : } M_A = 18.01528$$

$$\sigma_a(\text{Mb}) = 109.76097 \frac{df}{dE} (\text{eV}^{-1})$$

$$\mu_m = \sigma_a \cdot N_A \cdot M_A^{-1}$$

Table I. Integrated oscillator strength,  $f$ , for transitions below the IP.

Energy (eV)	$f$	$\lambda$ (Å)
7.4 band	0.0460	—
9.7 band	0.0732	—
9.994	0.0052	1240.6
10.168 – 10.171	0.0140	1219.4 – 1219.0
10.332 – 10.338	0.0107	1200.0 – 1199.3
10.559 – 10.575	0.0092	1174.2 – 1172.4
10.765 – 10.780	0.0069	1151.7 – 1150.1
10.990 – 11.057	0.0218	1128.2 – 1121.3
11.122	0.0223	1114.8
11.200 – 12.617	0.1240	1107.0 – 982.68

Table II. Oscillator-strength density,  $df/dE$ , photoabsorption cross section,  $\sigma_a$ , and mass absorption coefficient,  $\mu_m$ .

Energy (eV)	$f_n$ (eV <sup>-1</sup> )	$\sigma_a$ (Mb)	$\mu_m$ (cm <sup>2</sup> g <sup>-1</sup> )	$\lambda$ (Å)
1.2617E+01	1.1797E-01	1.2949E+01	4.3286E+05	9.8264E+02
1.2629E+01	1.2077E-01	1.3256E+01	4.4312E+05	9.8171E+02
1.2641E+01	1.4832E-01	1.6280E+01	5.4421E+05	9.8080E+02
1.2677E+01	1.3411E-01	1.4720E+01	4.9207E+05	9.7800E+02
1.2688E+01	1.3411E-01	1.4720E+01	4.9207E+05	9.7720E+02
1.2735E+01	1.3322E-01	1.4623E+01	4.8881E+05	9.7360E+02
1.2749E+01	1.3411E-01	1.4720E+01	4.9207E+05	9.7250E+02
1.2782E+01	1.2257E-01	1.3453E+01	4.4970E+05	9.7000E+02
1.2803E+01	1.5720E-01	1.7255E+01	5.7679E+05	9.6840E+02
1.2818E+01	1.5632E-01	1.7157E+01	5.7354E+05	9.6730E+02
1.2843E+01	1.4832E-01	1.6280E+01	5.4421E+05	9.6540E+02
1.2871E+01	1.5809E-01	1.7352E+01	5.8005E+05	9.6330E+02
1.2904E+01	1.5720E-01	1.7255E+01	5.7679E+05	9.6080E+02
1.2918E+01	1.7230E-01	1.8912E+01	6.3219E+05	9.5980E+02

Table II. Oscillator-strength density,  $df/dE$ , photoabsorption cross section,  $\sigma_a$ , and mass absorption coefficient,  $\mu_m$ . (Continued)

Energy (eV)	$f_n$ (eV <sup>-1</sup> )	$\sigma_a$ (Mb)	$\mu_m$ (cm <sup>2</sup> g <sup>-1</sup> )	$\lambda$ (Å)
1.2939E+01	1.6520E-01	1.8132E+01	6.0612E+05	9.5820E+02
1.3022E+01	1.7941E-01	1.9692E+01	6.5826E+05	9.5210E+02
1.3036E+01	1.7941E-01	1.9692E+01	6.5826E+05	9.5110E+02
1.3059E+01	1.8296E-01	2.0082E+01	6.7130E+05	9.4940E+02
1.3079E+01	1.7763E-01	1.9497E+01	6.5175E+05	9.4800E+02
1.3116E+01	1.8296E-01	2.0082E+01	6.7130E+05	9.4530E+02
1.3142E+01	1.9362E-01	2.1252E+01	7.1040E+05	9.4340E+02
1.3153E+01	2.1405E-01	2.3494E+01	7.8535E+05	9.4260E+02
1.3173E+01	2.0339E-01	2.2324E+01	7.4625E+05	9.4120E+02
1.3242E+01	1.9539E-01	2.1447E+01	7.1692E+05	9.3630E+02
1.3263E+01	2.0872E-01	2.2909E+01	7.6580E+05	9.3480E+02
1.3277E+01	2.1582E-01	2.3689E+01	7.9187E+05	9.3380E+02
1.3297E+01	2.1316E-01	2.3396E+01	7.8209E+05	9.3240E+02
1.3332E+01	1.7141E-01	1.8815E+01	6.2893E+05	9.3000E+02
1.3369E+01	2.0783E-01	2.2811E+01	7.6254E+05	9.2740E+02
1.3386E+01	2.2559E-01	2.4761E+01	8.2772E+05	9.2620E+02
1.3399E+01	2.1049E-01	2.3104E+01	7.7232E+05	9.2530E+02
1.3421E+01	1.9984E-01	2.1934E+01	7.3321E+05	9.2380E+02
1.3497E+01	2.0339E-01	2.2324E+01	7.4625E+05	9.1860E+02
1.3513E+01	2.1405E-01	2.3494E+01	7.8535E+05	9.1750E+02
1.3525E+01	2.2826E-01	2.5054E+01	8.3749E+05	9.1670E+02
1.3543E+01	1.9984E-01	2.1934E+01	7.3321E+05	9.1550E+02
1.3602E+01	1.8740E-01	2.0569E+01	6.8759E+05	9.1150E+02
1.3625E+01	2.0605E-01	2.2617E+01	7.5602E+05	9.1000E+02
1.3640E+01	2.1493E-01	2.3591E+01	7.8861E+05	9.0900E+02
1.3653E+01	2.1316E-01	2.3396E+01	7.8209E+05	9.0810E+02
1.3700E+01	1.6964E-01	1.8620E+01	6.2242E+05	9.0500E+02
1.3730E+01	1.9273E-01	2.1154E+01	7.0714E+05	9.0300E+02
1.3771E+01	2.1493E-01	2.3591E+01	7.8861E+05	9.0030E+02
1.3862E+01	2.0250E-01	2.2227E+01	7.4299E+05	8.9440E+02
1.3884E+01	2.1049E-01	2.3104E+01	7.7232E+05	8.9300E+02
1.3909E+01	1.9184E-01	2.1057E+01	7.0388E+05	8.9140E+02
1.3972E+01	1.8474E-01	2.0277E+01	6.7782E+05	8.8740E+02
1.3997E+01	2.0072E-01	2.2032E+01	7.3647E+05	8.8580E+02
1.4036E+01	1.8207E-01	1.9984E+01	6.6804E+05	8.8330E+02
1.4105E+01	1.9273E-01	2.1154E+01	7.0714E+05	8.7900E+02

Table II. Oscillator-strength density,  $df/dE$ , photoabsorption cross section,  $\sigma_a$ , and mass absorption coefficient,  $\mu_m$ . (Continued)

Energy (eV)	$f_n$ (eV <sup>-1</sup> )	$\sigma_a$ (Mb)	$\mu_m$ (cm <sup>2</sup> g <sup>-1</sup> )	$\lambda$ (Å)
1.4126E+01	1.8207E-01	1.9984E+01	6.6804E+05	8.7770E+02
1.4184E+01	1.8207E-01	1.9984E+01	6.6804E+05	8.7410E+02
1.4212E+01	1.8296E-01	2.0082E+01	6.7130E+05	8.7240E+02
1.4248E+01	1.8207E-01	1.9984E+01	6.6804E+05	8.7020E+02
1.4286E+01	1.7674E-01	1.9400E+01	6.4849E+05	8.6790E+02
1.4304E+01	1.7586E-01	1.9302E+01	6.4523E+05	8.6680E+02
1.4333E+01	1.7497E-01	1.9205E+01	6.4197E+05	8.6500E+02
1.4375E+01	1.6964E-01	1.8620E+01	6.2242E+05	8.6250E+02
1.4400E+01	1.5809E-01	1.7352E+01	5.8005E+05	8.6100E+02
1.4430E+01	1.7497E-01	1.9205E+01	6.4197E+05	8.5920E+02
1.4459E+01	1.7586E-01	1.9302E+01	6.4523E+05	8.5750E+02
1.4498E+01	1.6697E-01	1.8327E+01	6.1264E+05	8.5520E+02
1.4542E+01	1.6520E-01	1.8132E+01	6.0612E+05	8.5260E+02
1.4568E+01	1.7586E-01	1.9302E+01	6.4523E+05	8.5110E+02
1.4607E+01	1.6253E-01	1.7840E+01	5.9635E+05	8.4880E+02
1.4687E+01	1.6697E-01	1.8327E+01	6.1264E+05	8.4420E+02
1.4822E+01	1.6520E-01	1.8132E+01	6.0612E+05	8.3650E+02
1.4872E+01	1.5632E-01	1.7157E+01	5.7354E+05	8.3370E+02
1.4943E+01	1.5987E-01	1.7547E+01	5.8657E+05	8.2970E+02
1.5080E+01	1.5720E-01	1.7255E+01	5.7679E+05	8.2220E+02
1.5202E+01	1.5187E-01	1.6670E+01	5.5724E+05	8.1560E+02
1.5333E+01	1.4921E-01	1.6377E+01	5.4747E+05	8.0860E+02
1.5450E+01	1.4566E-01	1.5988E+01	5.3443E+05	8.0250E+02
1.5498E+01	1.4211E-01	1.5598E+01	5.2140E+05	8.0000E+02
1.5623E+01	1.4832E-01	1.6280E+01	5.4421E+05	7.9360E+02
1.5814E+01	1.5276E-01	1.6767E+01	5.6050E+05	7.8400E+02
1.5963E+01	1.5809E-01	1.7352E+01	5.8005E+05	7.7670E+02
1.6173E+01	1.7319E-01	1.9010E+01	6.3545E+05	7.6660E+02
1.6342E+01	1.7141E-01	1.8815E+01	6.2893E+05	7.5870E+02
1.6531E+01	1.9273E-01	2.1154E+01	7.0714E+05	7.5000E+02
1.6709E+01	1.7763E-01	1.9497E+01	6.5175E+05	7.4200E+02
1.6880E+01	1.9362E-01	2.1252E+01	7.1040E+05	7.3450E+02
1.7153E+01	1.9362E-01	2.1252E+01	7.1040E+05	7.2280E+02
1.7712E+01	1.9007E-01	2.0862E+01	6.9737E+05	7.0000E+02
1.8233E+01	1.9023E-01	2.0879E+01	6.9795E+05	6.8000E+02
1.8785E+01	1.9228E-01	2.1105E+01	7.0548E+05	6.6000E+02

Table II. Oscillator-strength density,  $df/dE$ , photoabsorption cross section,  $\sigma_a$ , and mass absorption coefficient,  $\mu_m$ . (Continued)

Energy (eV)	$f_n$ (eV <sup>-1</sup> )	$\sigma_a$ (Mb)	$\mu_m$ (cm <sup>2</sup> g <sup>-1</sup> )	$\lambda$ (Å)
1.9373E+01	1.9228E-01	2.1105E+01	7.0548E+05	6.4000E+02
1.9997E+01	1.9165E-01	2.1035E+01	7.0317E+05	6.2000E+02
2.0664E+01	1.8786E-01	2.0620E+01	6.8929E+05	6.0000E+02
2.2500E+01	1.9219E-01	2.1095E+01	7.0518E+05	5.5104E+02
2.5000E+01	1.7531E-01	1.9243E+01	6.4324E+05	4.9594E+02
2.7500E+01	1.5811E-01	1.7354E+01	5.8012E+05	4.5085E+02
3.0000E+01	1.4196E-01	1.5581E+01	5.2086E+05	4.1328E+02
3.5000E+01	1.1442E-01	1.2559E+01	4.1982E+05	3.5424E+02
4.0000E+01	9.3078E-02	1.0216E+01	3.4151E+05	3.0996E+02
4.5000E+01	7.6699E-02	8.4185E+00	2.8141E+05	2.7552E+02
5.0000E+01	6.4046E-02	7.0298E+00	2.3499E+05	2.4797E+02
6.0000E+01	4.6311E-02	5.0831E+00	1.6992E+05	2.0664E+02
7.0000E+01	3.4886E-02	3.8292E+00	1.2800E+05	1.7712E+02
8.0000E+01	2.7158E-02	2.9809E+00	9.9647E+04	1.5498E+02
9.0000E+01	2.1711E-02	2.3830E+00	7.9659E+04	1.3776E+02
1.0000E+02	1.7737E-02	1.9468E+00	6.5078E+04	1.2398E+02
1.2500E+02	1.0323E-02	1.1330E+00	3.7874E+04	9.9187E+01
1.5000E+02	6.9341E-03	7.6109E-01	2.5442E+04	8.2656E+01
1.7500E+02	4.8812E-03	5.3576E-01	1.7909E+04	7.0848E+01
2.0000E+02	3.5513E-03	3.8980E-01	1.3030E+04	6.1992E+01
2.2500E+02	2.6532E-03	2.9122E-01	9.7350E+03	5.5104E+01
2.5000E+02	2.0270E-03	2.2249E-01	7.4373E+03	4.9594E+01
2.7500E+02	1.5785E-03	1.7325E-01	5.7915E+03	4.5085E+01
3.0000E+02	1.2497E-03	1.3717E-01	4.5853E+03	4.1328E+01
3.5000E+02	8.1667E-04	8.9639E-02	2.9964E+03	3.5424E+01
4.0000E+02	5.5840E-04	6.1291E-02	2.0488E+03	3.0996E+01
4.5000E+02	3.9582E-04	4.3446E-02	1.4523E+03	2.7552E+01
5.0000E+02	2.8890E-04	3.1710E-02	1.0600E+03	2.4797E+01
5.3300E+02	2.3788E-04	2.6110E-02	8.7279E+02	2.3262E+01
5.3300E+02	1.4254E-03	1.5645E-01	5.2299E+03	2.3262E+01
5.3340E+02	6.3599E-03	6.9807E-01	2.3335E+04	2.3244E+01
5.3402E+02	1.3183E-02	1.4470E+00	4.8370E+04	2.3217E+01
5.3454E+02	8.9079E-03	9.7774E-01	3.2684E+04	2.3195E+01
5.3504E+02	4.0979E-03	4.4979E-01	1.5036E+04	2.3173E+01
5.3541E+02	1.1206E-02	1.2300E+00	4.1115E+04	2.3157E+01
5.3567E+02	1.9116E-02	2.0982E+00	7.0137E+04	2.3146E+01

Table II. Oscillator-strength density,  $df/dE$ , photoabsorption cross section,  $\sigma_a$ , and mass absorption coefficient,  $\mu_m$ . (Continued)

Energy (eV)	$f_n$ (eV <sup>-1</sup> )	$\sigma_a$ (Mb)	$\mu_m$ (cm <sup>2</sup> g <sup>-1</sup> )	$\lambda$ (Å)
5.3618E+02	1.4573E-02	1.5995E+00	5.3468E+04	2.3124E+01
5.3651E+02	9.6380E-03	1.0579E+00	3.5363E+04	2.3109E+01
5.3696E+02	1.2595E-02	1.3825E+00	4.6213E+04	2.3090E+01
5.3730E+02	1.0467E-02	1.1488E+00	3.8404E+04	2.3075E+01
5.3751E+02	8.9427E-03	9.8156E-01	3.2812E+04	2.3066E+01
5.3798E+02	8.4089E-03	9.2297E-01	3.0853E+04	2.3046E+01
5.3840E+02	8.9079E-03	9.7774E-01	3.2684E+04	2.3028E+01
5.3930E+02	8.3909E-03	9.2100E-01	3.0787E+04	2.2990E+01
5.3958E+02	8.4975E-03	9.3269E-01	3.1178E+04	2.2978E+01
5.4000E+02	7.9423E-03	8.7176E-01	2.9141E+04	2.2960E+01
5.4200E+02	7.3233E-03	8.0381E-01	2.6870E+04	2.2875E+01
5.4400E+02	6.6067E-03	7.2515E-01	2.4240E+04	2.2791E+01
5.4600E+02	6.1906E-03	6.7948E-01	2.2714E+04	2.2708E+01
5.4800E+02	5.9259E-03	6.5043E-01	2.1743E+04	2.2625E+01
5.5000E+02	5.8373E-03	6.4071E-01	2.1418E+04	2.2543E+01
5.5200E+02	6.1289E-03	6.7271E-01	2.2487E+04	2.2461E+01
5.5400E+02	6.1031E-03	6.6988E-01	2.2393E+04	2.2380E+01
5.5600E+02	6.0493E-03	6.6397E-01	2.2195E+04	2.2299E+01
5.5800E+02	5.8900E-03	6.4649E-01	2.1611E+04	2.2219E+01
5.6000E+02	5.7846E-03	6.3492E-01	2.1224E+04	2.2140E+01
5.6200E+02	5.3416E-03	5.8630E-01	1.9599E+04	2.2061E+01
5.6400E+02	5.3069E-03	5.8249E-01	1.9471E+04	2.1983E+01
5.6600E+02	5.2362E-03	5.7473E-01	1.9212E+04	2.1905E+01
5.8000E+02	4.3838E-03	4.8117E-01	1.6084E+04	2.1377E+01
5.9000E+02	4.2102E-03	4.6212E-01	1.5448E+04	2.1014E+01
6.0000E+02	4.0454E-03	4.4403E-01	1.4843E+04	2.0664E+01
7.0000E+02	2.7806E-03	3.0520E-01	1.0202E+04	1.7712E+01
8.0000E+02	1.9879E-03	2.1819E-01	7.2938E+03	1.5498E+01
9.0000E+02	1.4687E-03	1.6121E-01	5.3888E+03	1.3776E+01
1.0000E+03	1.1154E-03	1.2242E-01	4.0924E+03	1.2398E+01
1.2500E+03	6.1604E-04	6.7617E-02	2.2603E+03	9.9187E+00
1.5000E+03	3.7620E-04	4.1292E-02	1.3803E+03	8.2656E+00
1.7500E+03	2.4696E-04	2.7106E-02	9.0610E+02	7.0848E+00
2.0000E+03	1.7116E-04	1.8786E-02	6.2799E+02	6.1992E+00
2.2500E+03	1.2374E-04	1.3582E-02	4.5401E+02	5.5104E+00
2.5000E+03	9.2531E-05	1.0156E-02	3.3950E+02	4.9594E+00

Table II. Oscillator-strength density,  $df/dE$ , photoabsorption cross section,  $\sigma_a$ , and mass absorption coefficient,  $\mu_m$ . (Continued)

Energy (eV)	$f_n$ (eV <sup>-1</sup> )	$\sigma_a$ (Mb)	$\mu_m$ (cm <sup>2</sup> g <sup>-1</sup> )	$\lambda$ (Å)
2.7500E+03	6.8694E-05	7.5399E-03	2.5204E+02	4.5085E+00
3.0000E+03	5.3417E-05	5.8630E-03	1.9599E+02	4.1328E+00
3.5000E+03	3.3990E-05	3.7308E-03	1.2471E+02	3.5424E+00
4.0000E+03	2.2846E-05	2.5076E-03	8.3824E+01	3.0996E+00
4.5000E+03	1.6030E-05	1.7595E-03	5.8815E+01	2.7552E+00
5.0000E+03	1.1642E-05	1.2778E-03	4.2716E+01	2.4797E+00
6.0000E+03	6.6520E-06	7.3013E-04	2.4407E+01	2.0664E+00
7.0000E+03	4.1180E-06	4.5200E-04	1.5109E+01	1.7712E+00
8.0000E+03	2.7046E-06	2.9686E-04	9.9234E+00	1.5498E+00
9.0000E+03	1.8586E-06	2.0400E-04	6.8193E+00	1.3776E+00
1.0000E+04	1.2947E-06	1.4211E-04	4.7505E+00	1.2398E+00
1.2500E+04	6.3555E-07	6.9759E-05	2.3319E+00	9.9187E-01
1.5000E+04	3.5511E-07	3.8977E-05	1.3029E+00	8.2656E-01
1.7500E+04	2.1708E-07	2.3827E-05	7.9650E-01	7.0848E-01
2.0000E+04	1.4174E-07	1.5558E-05	5.2007E-01	6.1992E-01
2.2500E+04	9.7320E-08	1.0682E-05	3.5708E-01	5.5104E-01
2.5000E+04	6.9551E-08	7.6340E-06	2.5519E-01	4.9594E-01
2.7500E+04	5.1157E-08	5.6151E-06	1.8770E-01	4.5085E-01
3.0000E+04	3.8478E-08	4.2233E-06	1.4118E-01	4.1328E-01
3.5000E+04	2.3223E-08	2.5490E-06	8.5207E-02	3.5424E-01
4.0000E+04	1.4997E-08	1.6461E-06	5.5025E-02	3.0996E-01
4.5000E+04	1.0197E-08	1.1193E-06	3.7415E-02	2.7552E-01
5.0000E+04	7.2219E-09	7.9268E-07	2.6498E-02	2.4797E-01
6.0000E+04	3.9753E-09	4.3633E-07	1.4586E-02	2.0664E-01
7.0000E+04	2.3998E-09	2.6340E-07	8.8050E-03	1.7712E-01
8.0000E+04	1.5491E-09	1.7003E-07	5.6838E-03	1.5498E-01
9.0000E+04	1.0521E-09	1.1548E-07	3.8602E-03	1.3776E-01
1.0000E+05	7.4389E-10	8.1650E-08	2.7294E-03	1.2398E-01

When photon energy,  $E$ , is higher than  $10^5$  eV, the photoabsorption cross section of each atom,  $\sigma_a$ , in Mb is given by

$$\sigma_a = 680 (Z - 0.3)^6 \left( \frac{Ry}{E} \right)^4 \frac{\exp[-4\chi \arctan(\chi^{-1})]}{1 - \exp(-2\pi\chi)} .$$

Here  $E$  is photon energy in eV and  $\chi$  is given by

$$\chi = \sqrt{\frac{E_K}{E - E_K}} ,$$

where  $E_K = 13.6$  and  $539.9$  eV for hydrogen and oxygen atoms, respectively.

