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NAG 5-484

DETERMINATION OF BAND OSCILLATOR STRENGTHS OF ATMOSPHERIC MOLECULES FROM HIGH RESOLUTION VACUUM ULTRAVIOLET CROSS SECTION MEASUREMENTS

Grant NAG 5-484

Semiannual Status Report No. 1

For the period 1 November 1984 through 30 April 1985

Principal Investigator
W.H. Parkinson

August 1985

Prepared for
National Aeronautics and Space Administration
Greenbelt, Maryland 20771

Smithsonian Institution
Astrophysical Observatory
Cambridge, MA 02138

The Smithsonian Astrophysical Observatory
is a member of the
Harvard-Smithsonian Center for Astrophysics

The NASA Technical Officer for this grant is Dr. Igor J. Eberstein, Code 616, Goddard Space Flight Center, Greenbelt, Maryland 20771.

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Abstract

An account is given of progress during the six month period 1/11/84 - 4/30/85 in work on (a) rovibronic assignments of the Schumann-Runge bands of $^{18}O_2$; and (b) optical depth measurements of the Schumann-Runge bands of $^{18}O_2$. The work summarized above is part of a comprehensive spectroscopic investigation of the absorption wavelengths, rotational line assignments, cross sections, and band oscillator strengths of the Schumann-Runge bands of $^{18}O_2$ and $^{18}O^{16}O$ in the wavelength region 175-205 nm. The investigation is conducted at high resolution with a 6.65 m scanning spectrometer/spectrograph which is, by reason of its small instrumental width (FWHM = 0.0013 nm), uniquely suitable for cross section measurements of molecular bands with discrete rotational structure. Absolute cross sections, which are independent of the instrumental function and from which band oscillator strengths are directly determined, will be measured for the absorption bands that are most predissociated. Such measurements are needed for (a) accurate calculations of the stratospheric production of atomic oxygen and heavy ozone formed following the photopredissociation of $^{18}O^{16}O$ by solar radiation penetrating between the absorption lines of $^{16}O_2$; and (b) elucidation of the mechanism of predissociation of the upper state of the Schumann-Runge bands.

Progress Report for the Period 11/1/84 - 4/30/85

(a) Rovibronic Assignments of the Schumann-Runge Bands of $^{18}O_2$.

From high resolution photographic spectra of $^{18}O_2$ rotational line assignments have been completed for the (2,0)-(19,0) bands. The spectrograms were obtained for $^{18}O_2$ at 300 K and at 79 K. These assignments for $^{18}O_2$ at 300 K

are presented in Table I.

(b) Optical Depth Measurements of the Schumann-Runge Bands of $^{18}O_2$.

Photoelectric scans of the optical depth have been completed for the (2,0)-(15,0) Schumann-Runge bands of $^{18}O_2$ at 79 K. For values of $v' > 15$ these bands are subject to less predissociation and become sufficiently sharp that absolute cross section measurements are not possible even with our small instrumental full width at half-maximum of 0.0013 nm. The analogous point was reacned with $^{16}O_2$ at $v' > 12$. Reduction of the optical depth data of the (2,0)-(15,0) bands to cross sections remains to be done.

(c) Publications and Presentations

The following are supported by the current NASA grant:

K. Yoshino, D.E.Freeman, and W.H. Parkinson, "Atlas of the Schumann-Runge Absorption Bands of O_2 in the Wavelength Region 175-205 nm." J. Phys. Chem. Ref. Data 13, 207-227 (1984).

K. Yoshino, D.E. Freeman, A.S.-C. Cheung, and W.H. Parkinson, "Schumann-Runge Absorption Bands of $^{18}O_2$." Presented at the Symposium on Molecular Spectroscopy at the Ohio State University in June 1985.

P.L. Smith, H.E. Griesinger, J.H. Black, K. Yoshino, and D.E. Freeman, "Interstellar O_2. II. VUV Oscillator Strengths of Schumann-Runge Lines and Prospects for Space Telescope Observations." The Astrophysical Journal, 277, 569-575 (1984)

TABLE I. WAVENUMBER MEASUREMENTS AND LINE ASSIGNMENTS OF THE SCHUMANN-RUNGE ABSORPTION BANDS (2,0)-(19,0) OF $^{18}O_2$ AT 300 K

Wavenumbers of the B(2)-X(0) band

N	R(N)	P(N)
1	50663.419	
3	50660.474	
5	50652.698	50637.408
7	50640.541	50619.557
9	50623.676	50597.138
11	50602.178	50570.087
13	50576.031	50538.402

Wavenumbers of the B(3)-X(0) band

N	R(N)	P(N)
1	51271.533	
3	51268.393	51259.110
5	51260.565	51245.523
7	51248.015	51227.497
9	51230.608	51204.627
11	51208.559	51177.083
13	51181.904	51144.757
15	51150.111	51107.761
17	51114.139	51066.079
19	51072.883	

Wavenumbers of the B(4)-X(0) band

N	R(N)	P(N)
1	51858.02	
3	51855.60	51846.74R
5	51846.74P	51833.46R
7	51833.46P	51814.54
9	51815.90	51790.99
11	51793.38	51762.98
13	51766.00	51730.03
15	51733.61	51691.97
17	51696.46	51650.05
19	51654.86	51602.54

Wavenumbers of the B(5)-X(0) band

N	R(N)	P(N)
1	52422.84	
3	52420.84	52411.92R
5	52411.92P	52398.26R
7	52398.26P	52379.70R
9	52379.70P	52355.54
11	52356.62	52327.32
13	52328.52	52293.48
15	52295.10	52254.97
17	52256.97	52211.42
19	52214.16	52163.27
21	52165.87	52109.75
23	52113.19	52051.62
25	52055.69	

Wavenumbers of the B(6)-X(0) band

N	R(N)	P(N)
1	52962.75	52961.04
3	52959.10	52959.10R
5	52950.31P	52936.34R
7	52936.34P	52917.33R
9	52917.33P	52893.34R
11	52893.34P	52864.08R
13	52864.08P	52829.88R
15	52829.88P	52790.68R
17	52790.68P	52746.19R
19	52746.19P	52696.69
21	52697.08	52642.15
23	52642.76	52582.61R
25	52582.61P	52517.91R
27	52517.91P	52447.82R
29	52447.82P	

Wavenumbers of the B(7)-X(0) band

N	R(N)	P(N)
1	53476.23	53472.82R
3	53472.82P	53463.60R
5	53463.60P	53449.37R
7	53449.37P	53429.90R
9	53429.90P	53405.36R
11	53405.36P	53375.48R
13	53375.48P	53340.56R
15	53340.56P	53300.76
17	53299.94	53255.33
19	53254.09	53204.89
21	53203.90	53149.35
23	53147.71	53088.34
25	53086.06	53022.45
27	53019.64	

Wavenumbers of the B(8)-X(0) band

N	R(N)		P(N)	
1	53961.94			
3	53957.85		53949.07	
5	53948.49		53934.74	
7	53933.52		53915.03	
9	53913.19		53889.95	
11	53887.66		53859.58	
13	53856.70		53823.81	
15	53820.41		53782.75	
17	53778.87		53736.29	
19	53731.77	53732.37	53684.60	
21	53679.52	53679.94	53627.38	53628.00
23	53621.77	53622.48	53564.82	
25	53558.60		53496.94	
27	53490.11		53423.64	
29	53416.18			

Wavenumbers of the B(9)-X(0) band

N	R(N)		P(N)	
1	54418.44			
3	54414.20		54405.60	
5	54404.18		54391.13	
7	54388.70		54370.95	
9	54367.75		54345.26	
11	54341.25		54314.09	
13	54309.22		54277.44	
15	54271.73		54235.22	
17	54228.62		54187.56	
19	54180.14	54180.62	54134.37	54134.91
21	54126.12	54126.65	54075.63	54076.11
23	54066.40	54068.61	54011.43	54012.15
25	54001.26		53941.62	53942.19
27			53866.39	53866.97
31	53771.86		53698.84	53699.52

Wavenumbers of the B(10)-X(0) band

N	R(N)	P(N)
1	54842.28	
3	54838.05	54829.83
5	54827.64	54814.96
7	54811.51	54794.36
9	54789.76	54768.07
11	54762.36	54736.09
13	54729.19	54698.47
15	54690.38	54655.18
17	54645.87	54606.23
19	54595.68	54551.57
21	54539.55	54491.18
23	54478.03	54425.04
25		54353.71
27	54337.24	
29	54258.79	54192.21

Wavenumbers of the B(11)-X(0) band

N	R1(N)	R2(N)	R3(N)	P1(N)	P2(N)	P3(N)
1	55232.38					
3	55227.65			55219.76		
5	55216.46	55216.84		55204.51	55204.79	
7	55199.60	55199.94		55183.28	55183.49	
9	55177.10	55177.28		55156.33	55156.51	
11	55148.46	55148.68		55123.40	55123.58	
13	55113.91	55114.26		55084.48	55084.84	
15	55073.49	55073.98		55039.78	55040.16	55040.38
17	55027.16	55027.74	55028.02	54989.24	54989.79	
19	54974.95	54975.68	54976.05	54932.88	54933.47	
21	54916.83	54917.71			54871.01	
23	54852.83	54854.03		54802.50	54803.19	
25	54782.77	54784.11				
27	54706.91	54707.82				
29	54625.74	54627.15		54561.92	54563.25	

Wavenumbers of the B(12)-X(0) band

N	R1(N)	R2(N)	R3(N)	P1(N)	P2(N)	P3(N)
1	55586.05	55586.87		55582.69		
3	55580.66	55581.46		55573.36	55574.06	55574.61
5	55569.12	55569.93		55557.72	55558.49	
7	55551.48	55552.33		55535.94	55536.69	
9	55527.74	55528.63		55508.07	55508.88	
11	55497.91	55498.91		55474.11	55475.02	
13	55461.98	55462.99	55463.30	55434.08	55435.10	
15	55419.92	55420.98	55421.40	55387.97	55388.97	55389.29
17	55371.73	55372.86	55373.39	55335.72	55336.76	55337.16
19	55317.38	55318.57	55319.19	55277.40	55278.46	55278.94
21	55256.86	55258.17	55258.87	55212.82	55214.13	55214.60
23	55190.07	55191.43	55192.30	55142.15	55143.44	55144.14
25	55117.10	55118.66	55119.60	55065.34	55066.72	55067.56
27	55037.91			54982.31	54983.79	54984.74
29	54952.41	54954.19	54955.34	54893.00	54894.60	54895.67

Wavenumbers of the B(13)-X(0) band

N	R1(N)	R2(N)	R3(N)	P1(N)	P2(N)	P3(N)
1	55900.78			55897.61		
3	55895.07	55896.12		55888.14	55889.06	
5	55882.83	55883.86		55872.11	55873.05	
7	55864.28	55865.48		55849.65	55850.68	
9	55839.41	55840.69		55820.89	55821.99	
11	55808.22	55809.65		55785.83	55787.06	
13	55770.64	55772.20	55772.48	55744.40	55745.79	
15	55726.72	55728.28	55728.64	55696.64	55698.20	
17	55676.40	55678.03	55678.57	55642.52	55644.03	55644.44
19	55619.63	55621.40	55622.09			
21	55556.45			55515.15	55516.88	55517.62
23	55486.75	55488.75	55489.77	55441.79	55443.66	55444.56
25	55410.57	55412.73	55413.95	55362.02	55363.96	55365.12
27	55327.77	55329.98	55331.31	55275.68		
29	55234.67	55238.26	55240.67			55186.15
31				55079.15	55082.26	55084.84B

Wavenumbers of the B(14)-X(0) band

N	R1(N)	R2(N)	R3(N)	P1(N)	P2(N)	P3(N)
1	56175.04	56176.35		56171.95		
3	56168.77	56170.13		56162.40	56163.37	
5	56155.83	56157.28		56145.83	56147.15	
7	56136.27	56137.89		56122.66	56124.04	
9	56110.15	56111.93		56092.87	56094.44	
11	56077.39	56079.25	56079.48	56056.53	56058.25	
13	56038.01	56040.21		56013.57	56015.43	56015.60
15	55992.01	55994.10	55994.64	55963.98	55965.99	55966.30
17	55939.28	55941.56	55942.37	55907.79	55909.88	55910.35
19	55879.82	55882.83B	55883.86B	55844.87	55847.18	55847.93
21	55813.62	55816.26	55817.52	55775.31	55777.73	55775.31
23	55740.64			55698.20	55701.60	55702.83
25	55660.77	55663.79	55665.48	55615.81	55618.62	
27	55574.06B	55577.30q	55579.66q	55525.99	55528.63B	55530.54
29	55480.16	55483.72	55485.99	55429.01	55432.26	55435.00q

Wavenumbers of the B(15)-X(0) band

N	R1(N)	R2(N)	R3(N)	P1(N)	P2(N)	P3(N)
1	56408.37	56410.28		56405.40		
3	56401.57	56403.91B		56395.52	56397.59	56398.29B
5	56387.82	56389.89		56378.59	56380.38B	
7	56367.17	56369.45		56354.63	56356.70	
9	56339.61	56342.08	56342.24	56323.77	56326.04	
11	56305.16	56307.71	56308.12	56285.99	56288.51	
13	56263.78	56266.50	56267.22	56241.33	56243.91	56244.29
15	56215.41	56218.38	56219.36	56189.76	56192.45	56193.17
17	56160.04	56163.37B	56164.30	56131.20	56134.16	56135.25
19	56097.67	56101.12	56102.62	56065.70	56068.93	56070.10
21	56028.16	56032.00	55918.98	55993.19	55996.43	55998.04
23	55951.49	55955.55	55957.58	55913.42	55917.21	55918.98
25	55867.62	55872.11B		55826.69	55830.77	55832.78
27				55732.70	55737.17	55739.46

Wavenumbers of the B(16)-X(0) band

N	R1(N)	R2(N)	R3(N)	P1(N)	P2(N)	P3(N)
1	56601.86	56604.80B		56599.21		
3	56594.59	56597.71		56589.18	56592.01	56592.71
5	56579.96	56583.21		56571.64	56574.59	
7	56558.16	56561.43	56561.65	56546.80	56549.94	56550.19B
9	56529.19B	56532.48	56533.04	56514.74	56517.97	56518.19
11	56492.77	56496.46	56497.36	56475.47	56478.83	56479.37
13	56449.25	56453.24	56454.32	56428.98	56432.63	56433.44
15	56398.22B	56402.79	56403.91B	56375.22	56379.12	56380.38B
17		56344.85	56346.60	56314.18	56318.47	56319.79
19	56274.57	56279.69	56281.74	55245.80	56250.50	56252.18
21	56201.50	56207.05	56209.48	56170.12B	56175.04B	56177.06
23	56120.89	56127.02	56129.71	56086.81	56092.87B	56094.44B
25				55996.43B	56002.06	56004.87

Wavenumbers of the B(17)-X(0) band

N	R1(N)	R2(N)	R3(N)	P1(N)	P2(N)	P3(N)
1	56758.45	56762.93				
3	56750.68	56754.85B	56755.58B	56745.78	56750.13	
5	56735.17	56739.93		56727.69	56732.22	
7	56712.11	56716.97	56717.28	56701.97	56706.46B	56706.65
9	56681.42	56686.66	56687.30	56668.65	56673.47	56673.88
11	56643.20	56648.83B	56649.85	56627.83	56632.96	56633.62
13	56597.38	56603.49	56604.80B	56579.37	56584.95	56586.01
15	56543.85	56550.19B	56552.27	56523.35	56529.19B	56530.86
17	56482.66	56489.68	56492.08	56459.67	56466.18	56468.04
19	56413.66	56421.20	56424.08	56388.10	56395.52B	56397.59B
21	56336.76	56344.85B	56348.30	56309.03	56316.67	56319.79B
23		56260.01		56222.12	56230.11	56233.58

Wavenumbers of the B(18)-X(0) band

N	R1(N)	R2(N)	R3(N)	P1(N)	P2(N)	P3(N)
1	56882.01	56888.99				
3	56873.90	56880.49	56880.97	56869.56	56876.21	56877.26
5	56857.47B	56864.29	56864.63	56850.80	56857.47B	56857.84
7	56833.11	56840.30	56840.82	56824.18	56831.08	56831.39
9	56800.82	56808.38	56809.37	56789.61	56796.86	56797.37
11	56760.62	56768.62	56770.09	56747.19	56754.85B	56755.58B
13	56712.27	56720.89	56722.93	56696.74	56704.81	56706.46B
15	56656.23	56664.85	56666.94	56638.43	56646.85	56648.83B
17				56571.89	56580.50	56583.21B

Wavenumbers of the B(19)-X(0) band

N	R1(N)	R2(N)	R3(N)	P1(N)	P2(N)	P3(N)
1	56977.10	56987.38	56989.42			
3	56968.64	56977.91	56979.00	56964.55	56974.54	56975.74
5	56951.25	56961.69	56962.41	56945.49	56954.94	56955.98
7	55925.88	56936.56	56937.15	56918.08	56928.45	56929.19
9	56892.75	56903.33	56903.73	56882.39	56892.96	56893.75
11	56849.06	56861.81	56862.24	56839.11	56849.62	56850.16
13	56799.19	56811.68	56812.52	56785.29	56797.85	56798.48
15				56723.15	56737.55	56738.52