MEASUREMENTS OF LINE INTENSITIES IN THE TWO-MICRON BAND OF AMMONIA†

SUNIL SARANGI
Infrared Astronomy Group, Physical Research Laboratory, Navrangpura, Ahmedabad-380 009, India

Abstract—Intensities of about four hundred lines of ammonia in the 2μ region have been measured using Doppler-broadened lines. Comparison with rigid-rotor calculations gives fair agreement between theory and experiment. The total integrated intensity of the $\nu_3+\nu_4$ (perpendicular) band has been estimated to be 17.19 cm^{-2} atm^{-1} at 296 K.

INTRODUCTION

THE ANALYSIS of the 2μ band of ammonia has been reported in a previous publication.[1] This band has recently been observed in Jupiter[2] and an interpretation of the spectrum requires the absolute intensities of the individual transitions. Most of the strong lines in this region belong to the $\nu_3+\nu_4$ (perpendicular) band.[1] The intensity distribution in a combination band is quite complex and depends on the interacting levels. KWAN[3] has studied this distribution in the combination of a parallel and a perpendicular band. But theoretical investigation of the combination of two perpendicular bands has not been attempted yet. Because of the inadequacy of the theoretical calculations, it is necessary to measure absolute line intensities in the laboratory.

EXPERIMENTAL STUDIES

The spectra were taken with an 1.8 m Ebert–Fastie spectrometer[1] with a resolution of 0.05–0.06 cm^{-1}. Two sample cells were used. One had a fixed path length of 42.16 cm, and the other was a White cell of base length 2 m used with a total path length of 810 cm. Research-grade ammonia was used at pressures between 1 and 2 torr in the White cell and between 3 and 6 torr in the single-pass cell. The pressure was measured with an accuracy of better than 2% with an oil manometer and a Datamatrix precision pressure gauge. At such low pressures, the pressure broadening is small and lines are essentially Doppler-broadened. Since the wing absorption is negligible, it was possible to draw the base lines (100% transmission) by joining the far wings of the lines.

The areas under the lines gave the equivalent widths. These were further corrected[4] to include the contribution from the far wings, which were not included in the measurement. The self-broadened line widths of ammonia have been given by MARGOLIS and SARANGI[5] and BENEDICT *et al.*[7] Those for unidentified lines have been assumed to be 0.35 cm^{-1} atm^{-1}. Since the lines are only weakly broadened, an error in the assumed pressure-broadened width has a negligible effect on the calculated absolute intensities. The intensities were calculated by reverse interpolation from the tables of JANSSON and KORB.[6]

RESULTS

The absolute intensities of 412 lines have been measured and reported in Table 1. These intensities are the averages of one to six independent measurements, the reported error being the standard deviation. Three fourths of the values have an error of less than 10% of the mean, which is adequate for most astronomical purposes. The rather high uncertainty of these results is partly due to blending with neighbouring lines because of instrumental broadening.

Two hundred and ninety-one of these lines have been identified in Ref. (1). Some of these are blends of two closely spaced lines and the reported intensities contain some systematic error

†Part of this work was carried out at the Jet Propulsion Laboratory, California Institute of Technology, U.S.A., under Contract Number NAS7-100 sponsored by the National Aeronautics and Space Administration (U.S.A.) while the author was an NAS-NRC Resident Research Associate.

Table 1. Line intensities in the 2μ band of ammonia†

Line	Intensity Mean	Std. Dev.	Line	Intensity Mean	Std. Dev.
341	0.603	0.038 (3)	511	3.314	0.147 (5)
344	1.049	0.084 (3)	512	5.179	0.536 (5)
345	0.506	(1)	550	4.964	0.190 (4)
346	1.385	0.161 (3)	551	5.040	0.350 (4)
347	0.381	(1)	554	6.953	0.436 (4)
349	0.339	(1)	555	10.730	0.683 (4)
351	0.307	(1)	556	2.028	0.166 (4)
354	0.617	0.118 (3)	557	4.217	0.183 (4)
355	0.440	0.077 (3)	558	7.787	0.613 (4)
356	1.523	0.094 (3)	561	2.898	0.221 (2)
360	0.371	0.005 (2)	598	0.496	0.039 (3)
361	1.103	0.032 (2)	602	0.565	0.050 (3)
362	0.941	0.038 (3)	603	0.571	0.013 (2)
363	0.704	0.005 (2)	604	7.485	0.293 (5)
364	1.742	0.272 (3)	605	3.079	0.224 (4)
365	0.895	0.052 (3)	606	8.564	0.884 (5)
366	1.540	0.159 (3)	608	1.855	0.163 (5)
367	0.222	(1)	609	19.390	2.050 (4)
373	0.585	0.045 (3)	610	11.020	0.322 (4)
375	2.194	0.018 (2)	611	6.749	0.474 (4)
376	0.526	0.030 (3)	618	0.393	(1)
385	1.187	0.020 (2)	620	0.514	0.030 (3)
386	1.160	0.015 (3)	622	0.847	0.084 (3)
394	0.902	0.047 (3)	623	0.302	0.062 (2)
395	2.426	0.092 (4)	624	0.870	0.033 (3)
396	1.046	0.008 (4)	625	1.181	0.135 (3)
400	1.115	0.062 (3)	627	0.516	0.023 (3)
401	0.203	(1)	630	0.220	0.041 (2)
402	0.684	0.041 (3)	632	0.635	0.049 (3)
403	1.257	0.134 (3)	635	0.523	0.041 (3)
404	2.970	0.929 (4)	638	0.696	0.033 (3)
405	1.461	0.180 (4)	646	21.380	1.360 (3)
406	1.440	0.064 (5)	647	18.480	2.550 (4)
408	1.253	0.106 (5)	648	10.420	1.500 (4)
431	0.447	0.075 (3)	650	8.306	0.552 (4)
432	0.495	0.040 (3)	651	4.303	0.634 (4)
434	0.572	0.035 (4)	675	1.087	0.083 (3)
435	0.433	0.013 (2)	677	1.320	0.173 (3)
436	1.797	0.114 (3)	679	1.209	0.042 (3)
437	1.930	0.112 (3)	681	0.939	0.141 (3)
438	0.543	0.033 (3)	683	0.609	0.017 (3)
439	0.561	0.023 (3)	691	0.615	0.013 (3)
440	0.295	(1)	692	0.758	0.019 (4)
445	0.344	0.010 (3)	693	3.932	0.363 (7)
446	2.443	0.372 (5)	694	15.950	1.400 (4)
450	2.149	0.172 (6)	695	16.220	1.330 (4)
451	0.810	0.090 (4)	696	11.570	0.505 (4)
452	6.924	0.460 (4)	697	14.660	0.324 (4)
454	0.321	(1)	718	1.699	0.197 (4)
455	2.176	0.270 (5)	719	1.594	0.117 (6)
456	3.415	0.301 (5)	720	1.520	0.192 (5)
457	1.546	0.272 (6)	723	1.833	0.115 (5)
459	4.808	0.367 (4)	724	1.182	0.007 (3)
460	0.252	0.003 (2)	727	0.662	0.015 (4)
461	1.646	0.270 (6)	729	0.664	0.115 (4)
489	0.856	0.014 (2)	730	1.213	0.109 (4)
490	1.172	0.200 (2)	732	0.715	0.045 (4)
491	0.897	0.077 (2)	733	4.477	0.360 (5)
493	1.616	0.048 (2)	736	0.500	(1)
494	1.132	0.060 (3)	738	23.010	3.400 (4)
497	6.417	0.422 (5)	739	19.830	1.360 (4)
499	6.634	0.661 (5)	762	4.637	0.282 (4)
501	0.979	0.014 (2)	763	4.900	0.455 (4)
502	1.588	0.017 (2)	764	5.415	0.234 (4)
503	0.903	0.072 (4)	765	6.027	0.151 (4)
504	1.711	0.106 (5)	767	4.291	0.455 (4)
505	5.331	0.409 (5)	768	3.871	0.276 (4)
506	3.730	0.260 (5)	769	5.892	0.548 (4)
508	3.278	0.282 (4)	770	3.551	0.352 (4)
510	3.268	0.192 (5)	771	22.900	3.180 (4)

Table 1. (*Contd*)

Line	Intensity Mean	Intensity Std. Dev.	Line	Intensity Mean	Intensity Std. Dev.
772	21.280	1.820 (4)	998	1.411	0.025 (3)
773	2.604	0.400 (5)	1000	0.785	0.028 (3)
774	0.595	0.021 (3)	1008	0.898	0.003 (3)
775	1.184	0.063 (3)	1010	0.483	(1)
779	1.452	0.041 (3)	1012	0.615	0.044 (3)
781	1.434	0.063 (2)	1014	12.350	0.952 (4)
782	1.378	0.065 (3)	1017	3.978	0.342 (4)
788	0.681	0.005 (2)	1018	3.545	0.223 (4)
810	3.402	0.188 (4)	1019	7.448	0.374 (4)
813	3.667	0.155 (3)	1023	5.219	0.436 (3)
814	3.055	0.474 (4)	1025	0.571	0.018 (3)
816	3.746	0.325 (4)	1026	2.598	0.189 (5)
818	11.080	0.780 (3)	1027	1.584	0.137 (5)
819	7.733	0.538 (4)	1030	1.958	0.078 (3)
821	2.141	0.143 (6)	1032	0.465	(1)
825	1.209	0.097 (3)	1033	0.482	(1)
828	1.178	0.050 (3)	1047	0.789	0.007 (2)
830	0.400	0.067 (3)	1056	2.106	0.166 (3)
838	0.719	0.016 (2)	1057	1.615	0.087 (2)
850	0.859	0.059 (2)	1059	0.265	0.023 (2)
851	0.806	0.093 (2)	1062	0.663	0.030 (3)
854	4.081	0.319 (5)	1065	1.351	0.134 (3)
856	10.050	0.469 (4)	1067	1.420	0.137 (5)
857	5.366	0.280 (5)	1068	13.860	0.833 (4)
858	4.660	0.392 (6)	1069	8.866	0.479 (4)
859	2.770	0.229 (6)	1070	6.333	0.314 (4)
862	3.300	0.156 (4)	1071	8.550	0.590 (4)
864	3.723	0.364 (4)	1073	7.336	0.160 (4)
867	1.236	0.136 (5)	1074	8.459	0.317 (4)
868	2.250	0.262 (6)	1075	9.616	0.910 (4)
869	2.329	0.242 (6)	1098	0.350	(1)
870	1.952	0.176 (6)	1103	0.579	0.026 (2)
872	1.230	0.110 (5)	1104	0.177	(1)
873	5.393	0.133 (4)	1105	0.206	0.008 (2)
877	0.527	(1)	1109	0.364	0.018 (2)
878	5.882	0.659 (4)	1111	0.456	0.009 (2)
879	1.987	(1)	1114	12.730	0.487 (4)
880	1.134	0.112 (2)	1115	15.430	0.823 (4)
881	1.208	0.071 (2)	1116	0.685	0.012 (2)
883	0.262	(1)	1117	0.827	0.124 (3)
903	23.200	0.696 (5)	1118	1.364	0.167 (5)
904	39.590	2.960 (4)	1121	27.020	1.340 (4)
907	21.740	2.180 (4)	1122	3.297	0.070 (4)
910	9.815	0.650 (5)	1126	6.172	0.631 (4)
914	12.920	1.240 (5)	1129	0.369	(1)
916	6.207	0.311 (5)	1131	0.603	0.010 (2)
938	0.779	0.011 (3)	1134	1.004	0.059 (3)
939	0.246	0.005 (2)	1143	0.462	0.068 (4)
940	3.167	0.326 (8)	1144	0.468	0.070 (3)
941	0.682	0.019 (3)	1145	1.255	0.120 (4)
943	1.650	0.152 (7)	1151	0.715	0.041 (4)
945	1.423	0.066 (6)	1165	27.410	1.500 (4)
947	2.687	0.259 (8)	1166	26.360	1.240 (4)
949	2.817	0.237 (3)	1173	7.869	0.483 (4)
951	4.399	0.129 (4)	1174	7.601	0.121 (4)
953	4.398	0.312 (5)	1176	2.610	0.096 (4)
954	6.600	0.418 (5)	1178	3.283	0.466 (2)
956	12.480	0.523 (3)	1179	4.134	0.324 (2)
974	0.670	0.039 (3)	1180	2.096	0.288 (2)
975	0.764	0.071 (3)	1181	2.403	0.248 (2)
976	0.713	0.021 (3)	1212	13.060	1.190 (4)
981	0.670	0.052 (3)	1214	13.260	0.928 (4)
982	0.328	0.036 (3)	1215	1.396	0.025 (3)
984	0.631	0.080 (3)	1219	0.367	(1)
985	0,312	0.039 (2)	1220	0.282	(1)
987	2.359	0.254 (2)	1221	0.726	(1)
989	0.432	0.066 (3)	1222	0.482	(1)
993	3.164	0.204 (3)	1223	8.876	0.480 (4)
994	0.462	0.049 (3)	1225	9.512	0.876 (4)
995	0.299	0.036 (2)	1229	2.007	0.113 (3)

Table 1. (*Contd*)

Line	Intensity Mean	Intensity Std. Dev.	Line	Intensity Mean	Intensity Std. Dev.
1230	0.724	0.008 (2)	1523	3.720	0.144 (2)
1231	0.677	0.058 (2)	1527	4.030	0.128 (5)
1232	2.849	0.194 (5)	1530	0.472	0.077 (2)
1233	26.790	1.810 (4)	1531	0.357	0.011 (2)
1234	1.489	0.085 (2)	1534	0.436	0.013 (2)
1236	5.188	0.335 (4)	1536	0.605	0.006 (2)
1260	11.510	1.040 (4)	1537	0.788	0.034 (3)
1262	11.560	0.889 (4)	1542	2.309	0.274 (7)
1269	18.780	0.539 (4)	1546	0.181	(1)
1272	19.740	1.100 (4)	1548	0.418	(1)
1276	0.777	0.031 (3)	1550	2.340	0.200 (6)
1277	6.155	0.483 (4)	1554	2.191	0.129 (4)
1279	2.723	0.134 (2)	1555	2.364	0.180 (4)
1282	6.999	0.548 (4)	1561	3.278	0.140 (4)
1283	2.329	0.237 (3)	1565	0.404	0.007 (3)
1302	4.427	0.320 (3)	1566	2.010	0.216 (3)
1307	2.582	0.229 (4)	1572	1.117	0.065 (3)
1308	14.030	0.483 (4)	1573	0.323	0.043 (3)
1312	15.200	0.968 (4)	1576	0.700	0.050 (3)
1321	4.836	0.319 (4)	1577	1.644	0.104 (3)
1323	7.313	0.130 (4)	1578	1.576	0.031 (4)
1326	8.420	0.418 (4)	1579	5.335	0.326 (4)
1334	6.757	0.347 (4)	1582	0.443	0.023 (3)
1339	6.624	0.358 (3)	1589	0.961	0.043 (3)
1342	0.285	(1)	1592	0.438	0.025 (3)
1345	0.456	0.046 (3)	1596	1.199	0.074 (3)
1346	0.346	0.040 (3)	1597	1.425	0.117 (2)
1349	0.766	0.027 (3)	1600	1.714	0.083 (3)
1353	14.520	0.982 (4)	1601	0.362	0.030 (3)
1369	6.879	0.268 (4)	1605	2.484	0.104 (2)
1372	6.770	0.228 (4)	1609	0.471	0.031 (3)
1382	6.607	0.253 (4)	1610	2.773	0.314 (3)
1383	6.641	0.421 (4)	1612	2.149	0.142 (2)
1391	11.360	0.381 (4)	1613	0.629	0.017 (2)
1396	17.380	0.863 (4)	1614	0.381	0.016 (2)
1397	0.694	(1)	1616	1.317	0.058 (3)
1398	2.144	0.218 (3)	1621	1.263	0.030 (3)
1399	5.076	0.373 (4)	1623	0.987	0.028 (3)
1402	4.507	0.132 (4)	1633	0.466	(1)
1406	4.774	0.288 (4)	1639	1.805	0.077 (3)
1409	1.800	0.366 (3)	1640	1.130	0.084 (2)
1410	4.574	0.240 (4)	1647	0.534	0.031 (2)
1415	6.481	0.138 (3)	1648	0.374	0.019 (2)
1420	8.262	0.400 (4)	1650	0.385	0.055 (2)
1421	2.335	0.298 (4)	1652	0.496	0.036 (2)
1439	4.971	0.289 (4)	1653	0.875	0.056 (2)
1446	4.118	0.277 (4)	1655	0.322	0.036 (2)
1452	4.413	0.247 (4)	1658	0.548	0.036 (2)
1454	3.003	0.230 (4)	1660	0.712	0.047 (2)
1455	5.612	0.097 (3)	1662	0.762	(1)
1459	5.978	0.140 (4)	1665	0.613	0.049 (2)
1462	10.330	0.541 (4)	1666	0.408	0.009 (2)
1467	3.322	0.216 (4)	1671	0.723	0.016 (3)
1472	2.957	0.128 (4)	1672	1.797	0.089 (3)
1486	2.872	0.104 (3)	1677	0.266	0.028 (2)
1496	3.113	0.144 (5)	1679	0.351	0.009 (2)
1497	1.909	0.260 (5)	1680	0.446	0.049 (2)
1498	2.260	0.262 (5)	1682	0.461	0.047 (2)
1499	8.840	0.629 (4)	1687	0.341	(1)
1500	7.080	0.533 (3)	1688	0.907	0.044 (3)
1501	1.631	0.208 (4)	1689	2.817	0.347 (2)
1502	2.230	0.139 (4)	1690	0.782	0.039 (2)
1505	2.726	0.228 (4)	1701	1.488	0.067 (3)
1508	2.765	0.118 (4)	1704	1.277	0.028 (3)
1510	1.849	0.150 (3)	1709	1.289	0.051 (3)
1516	5.849	0.413 (5)	1712	1.641	0.077 (3)

†The lines are identified by their serial numbers in Ref. (1). The intensities are given in units of (10^{-2} cm^{-2} atm^{-1}) at 296 K and the figures in the parentheses denote the number of independent measurements for each line.

due to the use of single line curve of growth in data reduction. The distribution of intensities in the $\nu_3 + \nu_4$ (perpendicular) band has been computed using the rigid-rotor approximation.[7] The 291 identified lines, with a combined strength of 14.67 cm^{-2} atm^{-1}, account for 85.4% of the integrated intensity of this band. This result leads to an estimate of 17.19 cm^{-2}-atm^{-1} for the total integrated intensity at 296 K, the estimated error being a few per cent of this value. The computed absolute intensities based on this band strength agree fairly well with the experimental values. However, the differences are, still, quite large and warrant a detailed calculation including local interactions.

Since most of the strong lines in this region belong to the $\nu_3 + \nu_4$ (perpendicular) band and the parallel component of this band is very weak, all of the other bands contribute only a small fraction of the total intensity. For practical calculations, these almost randomly-distributed lines may be accounted for by a suitable band model.

Acknowledgement—The author is grateful to Dr J. S. MARGOLIS of the Jet Propulsion Laboratory for many helpful discussions during the course of this work.

REFERENCES

1. S. SARANGI, *JQSRT* **18**, 257 (1977).
2. T. Z. MARTIN, Dissertation, University of Hawaii, Honolulu (1975).
3. Y. Y. KWAN, *J. Molec. Spectrosc.* **49**, 27 (1974).
4. C. L. KORB, R. H. HUNT and E. K. PLYLER, *J. Chem. Phys.* **48**, 4252 (1968).
5. J. S. MARGOLIS and S. SARANGI, *JQSRT* **16**, 405 (1976).
6. P. A. JANSSON and C. L. KORB, *JQSRT* **8**, 1399 (1968).
7. W. S. BENEDICT, E. K. PLYLER and E. D. TIDWELL, *J. Res. N.B.S.* **61**, 123 (1958).