

# Enhanced sensitivity to a possible variation of the proton-to-electron mass ratio in ammonia

## Supplementary Material

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Here we provide comprehensive tables of all investigated transitions between the  $2\nu_2$  and  $\nu_4$  vibrational states of  $^{14}\text{NH}_3$ . All rotation-vibration energy levels have a vibrational state ( $v$ ), symmetry ( $\Gamma$ ), parity ( $p$ ), rotational quantum number ( $J$ ), and projection onto the molecule-fixed  $z$  axis ( $K$ ) label. For all transitions we give a TROVE computed frequency  $\nu_{\text{calc}}$  and corresponding sensitivity coefficient  $T_{\text{calc}}$ , and a MARVEL substituted experimental frequency  $\nu_{\text{exp}}$  and corresponding sensitivity coefficient  $T_{\text{exp}}$  where possible. Upper and lower states are labelled with a ' and '', respectively. Aside from Table 1 which contains the observed frequencies from Ref. [1, 2], transitions have been grouped together according to Einstein A coefficient in Tables 2, 3 and 4. Note that in relation to the standard Herzberg convention [3] which uses the normal mode quantum numbers  $v_1$ ,  $v_2$ ,  $v_3$ ,  $v_4$ ,  $l_3$  and  $l_4$ , the  $2\nu_2$  state corresponds to the doubly excited inversion mode  $v_2 = 2$ , whilst  $\nu_4$  is the singly excited asymmetric bending mode  $v_4 = |l_4| = 1$  (see Down et al. [4] for more details).

Table 1: Observed vibration-rotation-inversion frequencies ( $\nu$ ), Einstein A coefficients ( $A$ ) and sensitivity coefficients ( $T$ ) of  $^{14}\text{NH}_3$  for transitions between the  $2\nu_2$  and  $\nu_4$  vibrational states. Experimental frequencies are from Ref. [2] unless stated otherwise.

$v'$	$\Gamma'$	$p'$	$J'$	$K'$	$v''$	$\Gamma''$	$p''$	$J''$	$K''$	$\nu_{\text{calc}}/\text{MHz}$	$\nu_{\text{exp}}/\text{MHz}$	$A/\text{s}^{-1}$	$T_{\text{calc}}$	$T_{\text{exp}}$
$\nu_4$	$E''$	+	9	9	$2\nu_2$	$E'$	+	9	8	132 031.60	124 829.13 <sup>a,b</sup>	2.167E-5	-29.98	-31.71
$\nu_4$	$E'$	+	8	8	$2\nu_2$	$E''$	+	8	7	160 886.62	154 415.54 <sup>a</sup>	3.036E-5	-28.97	-30.19
$\nu_4$	$E'$	+	9	8	$2\nu_2$	$E''$	+	9	7	185 115.85	177 312.18	4.845E-5	-22.66	-23.66
$\nu_4$	$A''_2$	+	7	7	$2\nu_2$	$A'_2$	+	7	6	204 389.50	198 997.44	4.284E-5	-26.52	-27.24
$\nu_4$	$A''_2$	+	9	7	$2\nu_2$	$A'_2$	+	9	6	214 465.53	206 314.26	5.749E-5	-20.53	-21.34
$2\nu_2$	$A''_2$	+	10	9	$\nu_4$	$A'_2$	+	10	10	205 993.39	210 104.63	9.220E-5	14.34	14.06
$\nu_4$	$A''_2$	+	8	7	$2\nu_2$	$A'_2$	+	8	6	220 233.54	213 191.30	6.121E-5	-22.26	-22.99
$2\nu_2$	$E'$	+	10	4	$\nu_4$	$E''$	+	10	5	215 008.15	219 719.96	2.321E-5	14.39	14.09
$\nu_4$	$E'$	+	9	6	$2\nu_2$	$E''$	+	9	5	232 288.19	223 905.49	5.161E-5	-19.94	-20.68
$2\nu_2$	$E''$	+	2	1	$\nu_4$	$E'$	+	1	0	233 283.50	231 528.17	1.180E-6	27.70	27.91
$\nu_4$	$E''$	+	9	5	$2\nu_2$	$E'$	+	9	4	244 124.00	235 545.72	3.788E-5	-20.19	-20.92
$2\nu_2$	$E'$	+	11	10	$\nu_4$	$E''$	+	11	11	234 782.46	240 987.16	1.228E-4	13.70	13.34
$\nu_4$	$A'_2$	+	9	4	$2\nu_2$	$A''_2$	+	9	3	252 734.04	243 884.52	2.227E-5	-21.14	-21.91
$\nu_4$	$E''$	+	9	3	$2\nu_2$	$E'$	+	9	2	257 497.74	248 518.72	9.251E-6	-22.53	-23.35
$2\nu_2$	$E'$	+	10	8	$\nu_4$	$E''$	+	10	9	247 568.61	251 505.03	1.272E-4	12.71	12.51
$\nu_4$	$E'$	+	8	6	$2\nu_2$	$E''$	+	8	5	260 843.42	253 418.53	7.117E-5	-19.97	-20.55
$2\nu_2$	$E''$	+	10	5	$\nu_4$	$E'$	+	10	6	250 530.56	255 218.89	5.420E-5	13.24	13.00
$\nu_4$	$E'$	+	6	6	$2\nu_2$	$E''$	+	6	5	265 487.21	261 535.38	5.745E-5	-22.94	-23.29
$\nu_4$	$E'$	+	7	6	$2\nu_2$	$E''$	+	7	5	272 436.40	266 540.95	7.700E-5	-20.74	-21.20
$2\nu_2$	$E''$	+	12	11	$\nu_4$	$E'$	+	12	12	258 846.80	267 188.68	1.536E-4	12.87	12.47
$2\nu_2$	$E''$	+	10	7	$\nu_4$	$E'$	+	10	8	266 662.39	270 799.22	1.222E-4	12.40	12.21
$2\nu_2$	$A'_2$	+	10	6	$\nu_4$	$A''_2$	+	10	7	267 702.67	272 146.04	9.216E-5	12.61	12.41
$\nu_4$	$E''$	+	8	5	$2\nu_2$	$E'$	+	8	4	294 171.35	286 489.22	6.298E-5	-18.94	-19.45
$2\nu_2$	$A''_2$	+	11	9	$\nu_4$	$A'_2$	+	11	10	285 705.21	291 851.94	1.775E-4	12.20	11.95
$2\nu_2$	$E''$	+	14	13	$\nu_4$	$E'$	+	14	14	291 137.45	303 522.59	2.101E-4	11.11	10.66
$\nu_4$	$A'_2$	+	8	4	$2\nu_2$	$A''_2$	+	8	3	325 490.67	317 688.65	4.406E-5	-18.41	-18.86
$\nu_4$	$E''$	+	7	5	$2\nu_2$	$E'$	+	7	4	328 122.85	321 934.98	8.437E-5	-18.27	-18.62
$2\nu_2$	$E'$	+	11	8	$\nu_4$	$E''$	+	11	9	317 129.46	323 758.48	1.849E-4	11.91	11.67
$2\nu_2$	$E'$	+	12	10	$\nu_4$	$E''$	+	12	11	318 361.60	326 815.17	2.298E-4	11.57	11.27
$\nu_4$	$E''$	+	6	5	$2\nu_2$	$E'$	+	6	4	344 695.37	340 322.94	9.137E-5	-18.29	-18.52
$2\nu_2$	$E''$	+	11	7	$\nu_4$	$E'$	+	11	8	333 147.37	340 449.73	1.570E-4	12.05	11.79
$2\nu_2$	$A'_2$	+	11	6	$\nu_4$	$A''_2$	+	11	7	332 808.60	340 787.72	1.099E-4	12.50	12.21
$\nu_4$	$E''$	+	5	5	$2\nu_2$	$E'$	+	5	4	345 142.06	342 797.10	7.054E-5	-19.09	-19.22
$\nu_4$	$E''$	+	8	3	$2\nu_2$	$E'$	+	8	2	353 734.11	346 476.00	2.037E-5	-16.96	-17.32
$2\nu_2$	$A''_2$	+	12	9	$\nu_4$	$A'_2$	+	12	10	362 254.22	371 521.86	2.544E-4	11.28	11.00
$\nu_4$	$A'_2$	+	7	4	$2\nu_2$	$A''_2$	+	7	3	381 473.91	375 174.47	6.887E-5	-16.71	-16.99
$2\nu_2$	$A'_2$	+	14	12	$\nu_4$	$A''_2$	+	14	13	363 477.37	376 477.33	3.281E-4	10.34	9.98
$\nu_4$	$E'$	+	0	0	$2\nu_2$	$E''$	+	1	1	376 860.11	379 596.53	4.703E-6	-18.84	-18.70

<sup>a</sup> Ref. [1]. <sup>b</sup> MARVEL analysis [5] reports a frequency of 123 705.91 MHz resulting in  $T = -32.00$ .

Table 2: Vibration-rotation-inversion frequencies ( $\nu$ ), Einstein A coefficients ( $A$ ) and sensitivity coefficients ( $T$ ) of  $^{14}\text{NH}_3$  for transitions between the  $2\nu_2$  and  $\nu_4$  vibrational states. Experimental frequencies have been obtained using energy levels from the MARVEL analysis [5].

$v'$	$\Gamma'$	$p'$	$J'$	$K'$	$v''$	$\Gamma''$	$p''$	$J''$	$K''$	$\nu_{\text{calc}}/\text{MHz}$	$\nu_{\text{exp}}/\text{MHz}$	$A/\text{s}^{-1}$	$T_{\text{calc}}$	$T_{\text{exp}}$
$\nu_4$	$E'$	+	12	12	$2\nu_2$	$E''$	+	12	11	98 604.7		1.232E-5	-28.19	
$\nu_4$	$E''$	+	15	15	$2\nu_2$	$E'$	+	15	14	105 113.2		1.498E-5	-24.50	
$2\nu_2$	$E'$	-	11	5	$\nu_4$	$E''$	-	12	6	114 532.7	116 719.3	1.236E-6	1.32	1.29
$\nu_4$	$E'$	-	10	3	$2\nu_2$	$E''$	-	9	4	122 078.5	113 519.2	1.211E-6	-10.89	-11.71
$2\nu_2$	$A''_2$	-	10	0	$\nu_4$	$A'_2$	+	11	2	135 815.0	143 327.4	1.120E-6	11.78	11.17
$\nu_4$	$E'$	+	13	12	$2\nu_2$	$E''$	+	13	11	142 611.3		3.425E-5	-19.76	
$\nu_4$	$E''$	+	10	3	$2\nu_2$	$E'$	+	10	2	151 734.0	142 903.4	2.438E-6	-30.51	-32.40
$\nu_4$	$A''_2$	-	10	2	$2\nu_2$	$A'_2$	-	9	3	158 134.5	148 964.7	3.712E-6	-8.29	-8.80
$\nu_4$	$E''$	+	10	9	$2\nu_2$	$E'$	+	10	8	162 964.2		4.001E-5	-22.28	
$2\nu_2$	$A''_2$	+	10	3	$\nu_4$	$A'_2$	+	10	4	165 035.7	169 236.3	6.421E-6	16.36	15.95
$\nu_4$	$E''$	+	11	9	$2\nu_2$	$E'$	+	11	8	166 276.9		4.090E-5	-19.42	
$2\nu_2$	$E'$	+	9	8	$\nu_4$	$E''$	+	9	9	174 047.5		6.374E-5	14.47	
$\nu_4$	$E'$	-	10	1	$2\nu_2$	$E''$	-	9	2	174 877.9	165 720.4	6.185E-6	-7.11	-7.51
$\nu_4$	$E''$	-	10	0	$2\nu_2$	$E'$	-	9	1	186 039.2	176 739.5	9.006E-6	-5.91	-6.22
$\nu_4$	$E'$	+	10	6	$2\nu_2$	$E''$	+	10	5	190 719.0		2.944E-5	-20.13	
$2\nu_2$	$E''$	+	9	5	$\nu_4$	$E'$	+	9	6	203 574.1		4.550E-5	12.45	
$\nu_4$	$A''_2$	-	12	4	$2\nu_2$	$A'_2$	-	11	3	217 415.5	213 858.1	5.839E-6	-5.96	-6.06
$2\nu_2$	$A''_2$	+	11	3	$\nu_4$	$A'_2$	+	11	4	222 988.6	232 096.7	6.801E-6	17.97	17.27
$\nu_4$	$E'$	+	9	2	$2\nu_2$	$E''$	+	9	1	262 162.5	252 726.0	2.652E-6	-24.30	-25.20
$2\nu_2$	$E''$	-	10	2	$\nu_4$	$E'$	-	11	3	263 484.6	272 824.7	1.490E-6	4.33	4.18
$2\nu_2$	$E'$	+	11	2	$\nu_4$	$E''$	+	11	3	272 133.6	284 989.4	2.189E-6	14.28	13.64
$2\nu_2$	$E'$	+	11	4	$\nu_4$	$E''$	+	11	5	278 363.3	287 246.1	2.573E-5	14.93	14.47
$2\nu_2$	$E'$	+	12	2	$\nu_4$	$E''$	+	12	3	294 309.3	308 379.8	8.639E-6	14.56	13.90
$2\nu_2$	$E'$	+	15	14	$\nu_4$	$E''$	+	15	15	299 984.3		2.345E-4	10.22	
$2\nu_2$	$E'$	+	12	2	$\nu_4$	$E''$	+	12	3	302 808.4	312 803.4	1.413E-6	13.25	12.83
$\nu_4$	$A'_2$	-	15	13	$2\nu_2$	$A''_2$	-	14	12	309 565.7	304 019.2	1.384E-5	3.67	3.73
$2\nu_2$	$E''$	+	11	5	$\nu_4$	$E'$	+	11	6	314 599.2	323 076.1	6.149E-5	13.37	13.02
$2\nu_2$	$E'$	-	10	1	$\nu_4$	$E''$	-	11	2	326 336.1	326 806.8	4.222E-5	-0.61	-0.61
$2\nu_2$	$A''_2$	-	11	6	$\nu_4$	$A'_2$	-	12	7	332 994.5	334 687.7	3.212E-5	-1.55	-1.54
$\nu_4$	$E'$	-	12	3	$2\nu_2$	$E''$	-	11	2	333 920.8		1.505E-5	-5.53	
$2\nu_2$	$A''_2$	+	12	3	$\nu_4$	$A'_2$	+	12	4	342 021.2	355 894.6	6.644E-6	15.02	14.43
$\nu_4$	$A''_2$	-	9	2	$2\nu_2$	$A'_2$	+	9	0	351 803.5	339 058.1	3.077E-6	-18.80	-19.51
$\nu_4$	$A''_2$	-	11	2	$2\nu_2$	$A'_2$	+	11	0	367 917.3	350 853.0	6.345E-6	-14.65	-15.36
$2\nu_2$	$E''$	+	15	13	$\nu_4$	$E'$	+	15	14	375 768.9	390 891.3	3.693E-4	9.77	9.39
$2\nu_2$	$E'$	+	12	4	$\nu_4$	$E''$	+	12	5	376 818.1	390 488.2	2.550E-5	13.38	12.92
$\nu_4$	$E'$	+	8	2	$2\nu_2$	$E''$	+	8	1	380 133.8	372 905.3	7.163E-6	-16.73	-17.06
$\nu_4$	$A''_2$	-	15	2	$2\nu_2$	$A'_2$	+	15	0	389 106.6	376 629.1	5.421E-6	-6.98	-7.21
$2\nu_2$	$E'$	+	12	8	$\nu_4$	$E''$	+	12	9	394 583.8	404 951.6	2.354E-4	11.28	10.99
$2\nu_2$	$E'$	+	13	10	$\nu_4$	$E''$	+	13	11	399 548.4	411 594.9	3.240E-4	10.67	10.36
$2\nu_2$	$E''$	+	12	5	$\nu_4$	$E'$	+	12	6	405 328.4	418 467.6	6.459E-5	12.35	11.97
$2\nu_2$	$E''$	+	12	7	$\nu_4$	$E'$	+	12	8	413 941.4	425 387.4	1.852E-4	11.43	11.12

Table 2: (*Continued*)

$v'$	$\Gamma'$	$p'$	$J'$	$K'$	$v''$	$\Gamma''$	$p''$	$J''$	$K''$	$\nu_{\text{calc}}/\text{MHz}$	$\nu_{\text{exp}}/\text{MHz}$	$A/\text{s}^{-1}$	$T_{\text{calc}}$	$T_{\text{exp}}$
$2\nu_2$	$E''$	+	12	1	$\nu_4$	$E'$	+	12	2	415 167.6		1.147E-6	9.59	
$2\nu_2$	$E''$	-	15	8	$\nu_4$	$E'$	+	15	4	416 085.0	432 973.2	6.532E-6	4.17	4.00
$2\nu_2$	$A'_2$	+	12	6	$\nu_4$	$A''_2$	+	12	7	417 976.6	430 386.5	1.219E-4	11.76	11.42
$\nu_4$	$A'_2$	+	6	4	$2\nu_2$	$A''_2$	+	6	3	418 270.4	413 748.1	9.006E-5	-15.80	-15.98
$\nu_4$	$E''$	-	12	2	$2\nu_2$	$E'$	-	11	1	424 005.5	411 879.2	1.470E-5	-5.76	-5.93
$\nu_4$	$A''_2$	-	13	2	$2\nu_2$	$A'_2$	+	13	0	431 191.5	410 204.9	2.552E-5	-5.95	-6.25
$2\nu_2$	$E''$	-	10	2	$\nu_4$	$E'$	-	11	3	432 930.3	432 248.1	1.132E-4	-1.72	-1.72
$2\nu_2$	$E''$	+	14	11	$\nu_4$	$E'$	+	14	12	433 760.7	448 408.6	4.013E-4	9.79	9.47
$\nu_4$	$E''$	+	7	3	$2\nu_2$	$E'$	+	7	2	436 515.8	430 468.6	4.113E-5	-15.08	-15.29
$\nu_4$	$A'_2$	+	5	4	$2\nu_2$	$A''_2$	+	5	3	437 616.0	434 941.1	9.782E-5	-15.50	-15.59
$\nu_4$	$A'_2$	+	4	4	$2\nu_2$	$A''_2$	+	4	3	442 676.5	441 874.1	7.796E-5	-15.66	-15.68
$2\nu_2$	$A''_2$	+	13	9	$\nu_4$	$A'_2$	+	13	10	448 069.8	461 549.9	3.198E-4	10.55	10.25
$2\nu_2$	$A'_2$	+	15	12	$\nu_4$	$A''_2$	+	15	13	452 668.6	469 935.8	4.668E-4	9.62	9.27
$2\nu_2$	$E'$	-	14	13	$\nu_4$	$E''$	+	14	11	453 538.0		1.459E-4	5.23	
$2\nu_2$	$A''_2$	+	13	3	$\nu_4$	$A'_2$	+	13	4	471 333.7	489 078.7	2.981E-6	10.89	10.49
$\nu_4$	$E'$	+	7	2	$2\nu_2$	$E''$	+	7	1	484 698.5	478 994.6	1.719E-5	-14.13	-14.29
$2\nu_2$	$E'$	+	13	8	$\nu_4$	$E''$	+	13	9	488 083.1	503 099.1	2.741E-4	10.45	10.14
$2\nu_2$	$A''_2$	+	3	3	$\nu_4$	$A'_2$	+	2	2	491 165.0	489 672.2	4.360E-6	12.69	12.72
$\nu_4$	$A'_2$	-	13	7	$2\nu_2$	$A''_2$	-	12	6	491 180.0	485 978.4	6.061E-5	-2.69	-2.72
$\nu_4$	$E''$	+	6	3	$2\nu_2$	$E'$	+	6	2	493 089.6	488 661.3	6.308E-5	-13.99	-14.12
$2\nu_2$	$A''_2$	-	15	12	$\nu_4$	$A'_2$	+	15	10	494 630.6	512 454.4	1.437E-5	3.19	3.08
$2\nu_2$	$E'$	+	14	2	$\nu_4$	$E''$	-	14	2	508 969.6	524 718.7	8.777E-6	9.69	9.40
$2\nu_2$	$E'$	+	13	4	$\nu_4$	$E''$	+	13	5	512 279.4	530 229.9	2.025E-5	10.59	10.23
$\nu_4$	$A''_2$	+	7	1	$2\nu_2$	$A'_2$	+	7	0	512 816.0	507 179.0	9.573E-6	-13.86	-14.01
$2\nu_2$	$E''$	+	13	7	$\nu_4$	$E'$	+	13	8	516 209.6		2.015E-4	10.36	
$2\nu_2$	$E''$	+	13	5	$\nu_4$	$E'$	+	13	6	527 994.5	545 753.3	5.975E-5	10.38	10.05
$2\nu_2$	$A'_2$	+	13	6	$\nu_4$	$A''_2$	+	13	7	529 772.2	546 912.7	1.235E-4	10.32	10.00
$\nu_4$	$E''$	+	5	3	$2\nu_2$	$E'$	+	5	2	530 045.1	527 333.3	8.219E-5	-13.25	-13.31
$2\nu_2$	$E'$	-	14	13	$\nu_4$	$E''$	+	14	11	532 701.2	548 704.9	2.808E-4	4.61	4.48
$\nu_4$	$A''_2$	-	14	10	$2\nu_2$	$A'_2$	-	13	9	532 974.0	529 031.5	6.325E-5	-0.59	-0.59
$2\nu_2$	$E''$	+	15	11	$\nu_4$	$E'$	+	15	12	534 682.8	554 512.8	5.162E-4	9.28	8.95
$2\nu_2$	$A''_2$	+	14	9	$\nu_4$	$A'_2$	+	14	10	545 853.1	564 260.5	3.434E-4	9.50	9.19
$\nu_4$	$E''$	+	4	3	$2\nu_2$	$E'$	+	4	2	549 801.4	548 781.8	9.102E-5	-12.92	-12.94
$2\nu_2$	$E''$	+	13	1	$\nu_4$	$E'$	+	13	2	551 357.3	568 811.3	4.039E-6	8.08	7.83
$2\nu_2$	$E''$	+	11	1	$\nu_4$	$E'$	-	11	3	552 562.5	557 067.9	1.128E-6	2.65	2.63
$\nu_4$	$E''$	+	3	3	$2\nu_2$	$E'$	+	3	2	556 807.5	557 275.3	7.623E-5	-12.88	-12.87
$\nu_4$	$E'$	+	10	2	$2\nu_2$	$E''$	-	9	4	560 587.9	557 554.9	1.270E-6	-3.67	-3.69
$\nu_4$	$E'$	+	6	2	$2\nu_2$	$E''$	+	6	1	563 310.0	559 214.0	3.027E-5	-12.64	-12.73
$2\nu_2$	$A'_2$	-	12	9	$\nu_4$	$A''_2$	+	12	5	566 089.1	577 705.1	2.592E-6	1.75	1.72
$\nu_4$	$A'_2$	-	15	13	$2\nu_2$	$A''_2$	+	14	9	566 272.0	557 190.6	3.342E-6	-6.55	-6.66
$2\nu_2$	$A'_2$	-	10	3	$\nu_4$	$A''_2$	-	11	4	568 097.7	567 172.6	2.545E-4	-1.87	-1.88
$\nu_4$	$E'$	+	12	2	$2\nu_2$	$E''$	-	11	2	574 213.5		9.890E-5	-2.48	
$2\nu_2$	$E'$	-	11	7	$\nu_4$	$E''$	-	12	8	589 721.7	591 039.0	1.809E-4	-2.16	-2.16

Table 2: (*Continued*)

$v'$	$\Gamma'$	$p'$	$J'$	$K'$	$v''$	$\Gamma''$	$p''$	$J''$	$K''$	$\nu_{\text{calc}}/\text{MHz}$	$\nu_{\text{exp}}/\text{MHz}$	$A/\text{s}^{-1}$	$T_{\text{calc}}$	$T_{\text{exp}}$
$2\nu_2$	$E'$	+	14	8	$\nu_4$	$E''$	+	14	9	602 274.1	622 391.0	2.893E-4	9.28	8.98
$\nu_4$	$E'$	+	14	6	$2\nu_2$	$E''$	-	14	10	604 954.2	588 757.6	4.244E-6	-4.21	-4.33
$2\nu_2$	$E'$	+	15	10	$\nu_4$	$E''$	+	15	11	619 826.9	641 982.3	5.033E-4	8.66	8.36
$\nu_4$	$E'$	+	5	2	$2\nu_2$	$E''$	+	5	1	621 217.9	618 776.8	4.583E-5	-11.62	-11.66
$\nu_4$	$E'$	-	11	9	$2\nu_2$	$E''$	-	10	10	624 116.9	615 826.8	3.863E-6	-1.35	-1.37
$\nu_4$	$A_2''$	+	11	1	$2\nu_2$	$A_2'$	-	10	3	632 208.3		4.048E-5	-3.70	
$2\nu_2$	$A_2''$	+	13	9	$\nu_4$	$A_2'$	-	12	5	639 466.3	653 650.6	1.787E-6	6.71	6.57
$2\nu_2$	$E''$	-	8	2	$\nu_4$	$E'$	+	9	0	639 730.1	646 252.4	1.557E-6	1.88	1.86
$2\nu_2$	$E''$	+	14	7	$\nu_4$	$E'$	+	14	8	643 933.2	665 196.4	1.991E-4	8.90	8.62
$2\nu_2$	$A_2''$	-	13	12	$\nu_4$	$A_2'$	-	14	13	647 671.6	651 484.6	1.246E-4	-4.68	-4.66
$\nu_4$	$E''$	-	15	4	$2\nu_2$	$E'$	+	15	4	653 373.7		2.997E-6	-8.94	
$2\nu_2$	$E''$	+	12	1	$\nu_4$	$E'$	-	12	3	655 460.2	669 113.6	2.964E-6	6.72	6.58
$\nu_4$	$E'$	+	4	2	$2\nu_2$	$E''$	+	4	1	658 707.0	657 787.0	6.078E-5	-11.06	-11.07
$2\nu_2$	$A_2'$	+	14	6	$\nu_4$	$A_2''$	+	14	7	670 120.1	691 897.2	1.111E-4	8.52	8.25
$2\nu_2$	$E'$	+	3	2	$\nu_4$	$E''$	+	2	1	673 351.8	672 644.4	3.223E-5	8.89	8.89
$\nu_4$	$A_2''$	+	5	1	$2\nu_2$	$A_2'$	+	5	0	674 404.1	672 376.5	2.542E-5	-10.83	-10.86
$2\nu_2$	$A_2'$	-	8	3	$\nu_4$	$A_2''$	-	9	2	674 766.9	679 711.7	1.384E-4	0.94	0.93
$2\nu_2$	$E'$	+	14	4	$\nu_4$	$E''$	+	14	5	676 784.5	698 111.4	1.154E-5	7.88	7.64
$\nu_4$	$E'$	+	3	2	$2\nu_2$	$E''$	+	3	1	678 679.2	679 163.4	6.964E-5	-10.80	-10.79
$2\nu_2$	$E''$	+	14	5	$\nu_4$	$E'$	+	14	6	680 837.7	702 457.3	4.641E-5	8.17	7.92
$2\nu_2$	$E'$	-	10	1	$\nu_4$	$E''$	+	11	3	681 314.3	686 273.1	4.382E-6	2.05	2.03
$\nu_4$	$E''$	-	13	6	$2\nu_2$	$E'$	-	12	5	685 946.1	680 012.7	1.377E-4	-2.85	-2.88
$\nu_4$	$E'$	+	2	2	$2\nu_2$	$E''$	+	2	1	686 189.0	687 852.5	6.318E-5	-10.73	-10.70
$2\nu_2$	$E''$	-	14	8	$\nu_4$	$E'$	+	14	4	688 887.1	661 641.0	5.510E-5	0.58	0.60
$\nu_4$	$A_2'$	-	12	1	$2\nu_2$	$A_2''$	+	12	3	694 772.0		9.461E-6	-8.76	
$2\nu_2$	$E''$	-	9	2	$\nu_4$	$E'$	+	10	2	698 999.1	702 125.4	1.683E-5	1.47	1.47
$\nu_4$	$E''$	-	15	2	$2\nu_2$	$E'$	+	15	4	701 865.1	686 876.9	4.513E-5	-8.78	-8.97
$2\nu_2$	$E''$	-	12	10	$\nu_4$	$E'$	-	13	11	706 269.1	708 727.7	2.235E-4	-3.36	-3.35
$2\nu_2$	$E'$	+	15	2	$\nu_4$	$E''$	-	15	2	707 705.1	720 609.5	1.218E-5	6.38	6.27
$2\nu_2$	$A_2''$	+	15	9	$\nu_4$	$A_2'$	+	15	10	711 914.2	735 227.6	4.144E-4	7.20	6.97
$2\nu_2$	$A_2''$	-	8	0	$\nu_4$	$A_2'$	-	9	1	712 843.5	721 065.6	5.050E-4	0.11	0.11
$2\nu_2$	$E'$	-	8	1	$\nu_4$	$E''$	-	9	0	714 033.7	722 303.2	4.761E-4	0.17	0.17
$2\nu_2$	$E''$	-	8	2	$\nu_4$	$E'$	-	9	1	716 965.7	724 899.9	3.951E-4	0.34	0.33
$2\nu_2$	$E'$	+	15	8	$\nu_4$	$E''$	+	15	9	724 328.6	748 607.8	2.274E-4	7.41	7.17
$\nu_4$	$A_2''$	-	11	8	$2\nu_2$	$A_2'$	-	10	9	735 774.6	727 288.4	2.146E-5	-1.89	-1.91
$2\nu_2$	$E''$	-	10	4	$\nu_4$	$E'$	-	11	5	735 948.5	734 922.7	5.368E-4	-1.95	-1.95
$\nu_4$	$E''$	-	15	12	$2\nu_2$	$E'$	-	14	11	741 087.0	734 546.6	1.865E-4	-0.25	-0.25
$2\nu_2$	$E''$	-	8	4	$\nu_4$	$E'$	-	9	3	742 169.2	749 245.6	2.163E-4	0.47	0.47
$2\nu_2$	$E''$	+	14	1	$\nu_4$	$E'$	+	14	2	745 838.7	759 442.8	1.168E-5	5.74	5.64
$2\nu_2$	$E'$	-	8	5	$\nu_4$	$E''$	-	9	4	757 599.5	764 122.9	1.374E-4	0.41	0.40
$\nu_4$	$E''$	+	13	3	$2\nu_2$	$E'$	-	12	1	770 619.5	761 683.1	2.912E-6	-4.32	-4.37
$\nu_4$	$A_2''$	+	3	1	$2\nu_2$	$A_2'$	+	3	0	774 058.1	774 889.5	4.660E-5	-9.60	-9.59
$2\nu_2$	$A_2''$	-	8	6	$\nu_4$	$A_2'$	-	9	5	785 351.3	791 493.8	8.082E-5	0.18	0.18

Table 2: (*Continued*)

$v'$	$\Gamma'$	$p'$	$J'$	$K'$	$v''$	$\Gamma''$	$p''$	$J''$	$K''$	$\nu_{\text{calc}}/\text{MHz}$	$\nu_{\text{exp}}/\text{MHz}$	$A/\text{s}^{-1}$	$T_{\text{calc}}$	$T_{\text{exp}}$
$2\nu_2$	$E''$	+	15	7	$\nu_4$	$E'$	+	15	8	795 136.5	820 833.3	1.733E-4	7.30	7.07
$\nu_4$	$E'$	+	12	2	$2\nu_2$	$E''$	-	11	2	800 805.6		1.586E-4	-3.13	
$2\nu_2$	$A''_2$	-	14	12	$\nu_4$	$A'_2$	+	14	10	802 556.4	817 431.8	5.121E-5	0.42	0.42
$2\nu_2$	$A'_2$	-	8	3	$\nu_4$	$A''_2$	+	9	1	817 078.3	821 302.6	1.975E-4	0.42	0.42
$2\nu_2$	$E''$	+	13	1	$\nu_4$	$E'$	-	13	3	819 449.7	837 081.4	5.860E-6	5.82	5.70
$\nu_4$	$E'$	-	11	7	$2\nu_2$	$E''$	-	10	8	820 370.1	811 608.6	6.793E-5	-2.21	-2.23
$\nu_4$	$A''_2$	+	1	1	$2\nu_2$	$A'_2$	+	1	0	822 000.9	824 624.2	6.427E-5	-9.16	-9.13
$2\nu_2$	$E'$	-	13	13	$\nu_4$	$E''$	+	13	11	824 474.2	838 064.7	8.400E-6	-1.17	-1.16
$2\nu_2$	$E'$	-	8	7	$\nu_4$	$E''$	-	9	6	829 606.7	835 209.1	4.188E-5	-0.16	-0.16
$2\nu_2$	$A'_2$	+	15	6	$\nu_4$	$A''_2$	+	15	7	835 632.5	861 357.9	8.630E-5	6.74	6.54
$2\nu_2$	$A'_2$	-	11	9	$\nu_4$	$A''_2$	+	11	5	836 453.9	845 821.7	1.129E-6	0.40	0.40
$2\nu_2$	$E'$	-	15	7	$\nu_4$	$E''$	+	15	3	838 738.4	857 668.9	1.272E-5	2.64	2.59
$\nu_4$	$E'$	-	14	9	$2\nu_2$	$E''$	-	13	8	839 029.2	831 788.8	2.630E-4	-1.75	-1.76
$\nu_4$	$A''_2$	+	10	1	$2\nu_2$	$A'_2$	-	9	3	841 574.4	833 197.0	1.540E-6	-3.43	-3.46
$2\nu_2$	$E''$	+	3	1	$\nu_4$	$E'$	+	2	0	843 046.4	842 667.6	1.210E-4	6.91	6.91
$\nu_4$	$E'$	-	13	5	$2\nu_2$	$E''$	-	12	4	845 468.7	838 820.7	2.002E-4	-2.95	-2.98
$2\nu_2$	$A'_2$	+	15	0	$\nu_4$	$A''_2$	+	15	1	855 355.8		4.298E-6	0.33	
$2\nu_2$	$E''$	+	15	5	$\nu_4$	$E'$	+	15	6	857 007.7	880 193.2	2.848E-5	6.21	6.05
$2\nu_2$	$E'$	+	15	4	$\nu_4$	$E''$	+	15	5	858 045.0	881 947.1	3.491E-6	5.59	5.44
$\nu_4$	$E'$	+	15	0	$2\nu_2$	$E''$	+	15	1	865 195.0		1.230E-5	-7.66	
$\nu_4$	$E'$	+	15	6	$2\nu_2$	$E''$	-	15	10	876 629.1	857 387.9	2.319E-5	-3.65	-3.73
$\nu_4$	$E''$	-	11	6	$2\nu_2$	$E'$	-	10	7	884 234.9	875 140.7	1.594E-4	-2.38	-2.41
$2\nu_2$	$E''$	-	11	8	$\nu_4$	$E'$	-	12	9	887 979.3	888 965.3	5.942E-4	-2.40	-2.40
$2\nu_2$	$E''$	-	8	8	$\nu_4$	$E'$	-	9	7	895 998.7	902 654.5	1.557E-5	-0.59	-0.58
$\nu_4$	$E''$	+	15	1	$2\nu_2$	$E'$	+	15	2	898 460.0		6.512E-5	-7.43	
$\nu_4$	$E''$	-	14	2	$2\nu_2$	$E'$	+	14	4	898 879.7	880 934.1	1.336E-4	-7.61	-7.77

Table 3: Vibration-rotation-inversion frequencies ( $\nu$ ), Einstein A coefficients ( $A$ ) and sensitivity coefficients ( $T$ ) of  $^{14}\text{NH}_3$  for transitions between the  $2\nu_2$  and  $\nu_4$  vibrational states. Experimental frequencies have been obtained using energy levels from the MARVEL analysis [5].

$v'$	$\Gamma'$	$p'$	$J'$	$K'$	$v''$	$\Gamma''$	$p''$	$J''$	$K''$	$\nu_{\text{calc}}/\text{MHz}$	$\nu_{\text{exp}}/\text{MHz}$	$A/\text{s}^{-1}$	$T_{\text{calc}}$	$T_{\text{exp}}$
$\nu_4$	$E'$	—	14	3	$2\nu_2$	$E''$	—	14	8	6223.7		5.840E-11	-217.22	
$2\nu_2$	$E''$	—	12	8	$\nu_4$	$E'$	—	13	9	17 103.2	20 755.7	3.391E-9	-17.35	-14.30
$\nu_4$	$E''$	—	10	6	$2\nu_2$	$E'$	—	9	7	19 036.8	11 683.4	9.298E-10	-51.85	-84.48
$2\nu_2$	$E''$	+	15	11	$\nu_4$	$E'$	—	14	7	27 634.9	46 788.8	2.313E-11	191.99	113.40
$\nu_4$	$E'$	+	11	2	$2\nu_2$	$E''$	—	10	2	32 848.3	28 291.4	4.250E-9	-57.62	-66.90
$\nu_4$	$E'$	—	8	3	$2\nu_2$	$E''$	+	8	1	33 250.0	25 603.0	5.274E-9	-160.99	-209.07
$2\nu_2$	$E'$	+	8	2	$\nu_4$	$E''$	+	8	3	39 392.7	49 374.3	6.298E-11	156.58	124.93
$\nu_4$	$E''$	+	12	3	$2\nu_2$	$E'$	—	11	1	45 301.6	38 428.3	7.179E-10	-52.51	-61.91
$2\nu_2$	$E''$	—	9	8	$\nu_4$	$E'$	—	10	7	45 829.3	53 966.1	6.295E-9	13.90	11.80
$\nu_4$	$E'$	+	12	6	$2\nu_2$	$E''$	—	12	10	48 053.7	37 036.2	5.298E-9	-24.87	-32.27
$\nu_4$	$E''$	+	12	3	$2\nu_2$	$E'$	—	11	1	53 797.8	42 851.8	2.761E-10	-49.29	-61.89
$2\nu_2$	$E'$	+	9	2	$\nu_4$	$E''$	+	9	3	56 597.8	68 679.3	3.476E-10	101.43	83.59
$\nu_4$	$A'_2$	+	13	4	$2\nu_2$	$A''_2$	—	12	0	60 738.0	51 342.8	2.565E-10	-44.17	-52.26
$2\nu_2$	$E''$	+	9	1	$\nu_4$	$E'$	—	9	1	63 289.2		5.474E-9	79.00	
$2\nu_2$	$E'$	+	2	2	$\nu_4$	$E''$	+	1	1	63 924.7	61 712.7	1.042E-8	104.21	107.95
$2\nu_2$	$E'$	+	10	2	$\nu_4$	$E''$	+	10	3	64 989.0	77 575.0	6.839E-10	71.99	60.31
$\nu_4$	$A'_2$	—	10	5	$2\nu_2$	$A''_2$	—	9	6	65 933.4	58 158.6	7.357E-8	-18.50	-20.97
$\nu_4$	$E''$	+	14	5	$2\nu_2$	$E'$	—	13	1	66 655.9		2.448E-11	-44.25	
$\nu_4$	$E'$	—	12	5	$2\nu_2$	$E''$	—	11	4	68 478.6	65 641.3	2.187E-7	-10.90	-11.37
$2\nu_2$	$E'$	+	13	2	$\nu_4$	$E''$	—	13	2	71 605.4		4.559E-9	70.67	
$\nu_4$	$E''$	—	12	2	$2\nu_2$	$E'$	+	12	2	75 895.5	60 647.6	4.231E-9	-53.72	-67.22
$2\nu_2$	$E'$	—	13	13	$\nu_4$	$E''$	—	12	6	75 925.4	89 116.6	1.724E-11	-3.08	-2.62
$2\nu_2$	$A'_2$	+	11	0	$\nu_4$	$A''_2$	+	11	1	76 408.1		7.566E-9	69.42	
$2\nu_2$	$E'$	+	12	8	$\nu_4$	$E''$	+	11	3	82 910.6	89 509.4	1.362E-11	56.90	52.70
$2\nu_2$	$E''$	+	11	1	$\nu_4$	$E'$	+	11	2	86 783.9	96 528.3	1.320E-8	47.28	42.51
$2\nu_2$	$E'$	+	15	14	$\nu_4$	$E''$	—	14	12	96 401.3		2.589E-11	13.55	
$\nu_4$	$E''$	—	10	4	$2\nu_2$	$E'$	—	9	5	99 908.8	91 668.2	4.346E-7	-13.36	-14.56
$\nu_4$	$E'$	+	15	12	$2\nu_2$	$E''$	—	15	14	104 471.7	86 839.9	1.426E-7	-5.36	-6.45
$\nu_4$	$E''$	+	15	7	$2\nu_2$	$E'$	—	14	5	104 981.3	87 564.5	1.117E-10	-30.73	-36.84
$2\nu_2$	$E''$	—	13	4	$\nu_4$	$E'$	+	14	6	108 998.5	124 181.3	1.328E-10	26.25	23.04
$\nu_4$	$E'$	—	7	3	$2\nu_2$	$E''$	+	7	1	117 602.6	110 957.2	9.461E-8	-51.03	-54.08
$\nu_4$	$E'$	+	13	2	$2\nu_2$	$E''$	—	13	8	119 041.6	109 711.6	4.915E-11	-9.75	-10.58
$\nu_4$	$A'_2$	+	8	4	$2\nu_2$	$A''_2$	—	7	6	122 869.9	120 732.7	1.752E-11	-6.46	-6.57
$\nu_4$	$E'$	—	15	1	$2\nu_2$	$E''$	—	15	8	125 130.4	111 510.3	1.255E-7	-17.01	-19.09
$\nu_4$	$E'$	+	10	2	$2\nu_2$	$E''$	+	10	1	133 512.6	123 427.8	4.745E-7	-40.78	-44.11
$2\nu_2$	$A'_2$	—	9	9	$\nu_4$	$A''_2$	—	10	8	135 065.5	141 945.6	4.751E-8	1.22	1.16
$2\nu_2$	$E''$	—	13	8	$\nu_4$	$E'$	—	13	3	149 050.8	158 558.5	1.436E-8	9.91	9.32
$2\nu_2$	$E''$	—	8	4	$\nu_4$	$E'$	+	9	2	160 418.9	162 319.1	5.872E-9	7.00	6.91
$2\nu_2$	$E''$	+	10	1	$\nu_4$	$E'$	—	10	1	161 435.2	168 626.8	3.602E-8	19.48	18.65
$2\nu_2$	$E'$	+	11	2	$\nu_4$	$E''$	+	11	3	165 899.2	174 547.8	8.989E-7	22.32	21.21
$\nu_4$	$E'$	—	6	3	$2\nu_2$	$E''$	+	6	1	174 647.1	169 341.3	2.539E-8	-36.43	-37.57
$\nu_4$	$E''$	—	10	4	$2\nu_2$	$E'$	+	11	8	178 151.7		6.768E-10	-17.61	
$2\nu_2$	$E''$	+	12	1	$\nu_4$	$E'$	+	12	2	188 575.5		4.254E-9	26.85	
$\nu_4$	$E''$	—	11	2	$2\nu_2$	$E'$	+	11	2	189 082.1	184 918.5	3.358E-8	-11.16	-11.41
$2\nu_2$	$E''$	+	8	7	$\nu_4$	$E'$	—	7	5	198 702.4	203 766.3	8.527E-11	16.21	15.80

Table 3: (*Continued*)

$v'$	$\Gamma'$	$p'$	$J'$	$K'$	$v''$	$\Gamma''$	$p''$	$J''$	$K''$	$\nu_{\text{calc}}/\text{MHz}$	$\nu_{\text{exp}}/\text{MHz}$	$A/\text{s}^{-1}$	$T_{\text{calc}}$	$T_{\text{exp}}$
$\nu_4$	$E'$	-	5	3	$2\nu_2$	$E''$	+	5	1	209 318.1	205 609.0	8.205E-9	-31.22	-31.78
$\nu_4$	$A_2''$	+	9	1	$2\nu_2$	$A_2'$	+	9	0	209 489.0	197 467.1	7.478E-8	-30.17	-32.01
$\nu_4$	$E'$	+	10	0	$2\nu_2$	$E''$	-	9	2	219 921.8	211 671.7	4.588E-7	-10.52	-10.93
$2\nu_2$	$E''$	-	7	4	$\nu_4$	$E'$	+	8	0	221 192.9	226 050.6	1.446E-9	4.95	4.84
$\nu_4$	$E'$	-	3	3	$2\nu_2$	$E''$	+	3	1	221 639.6	221 261.9	2.673E-10	-30.81	-30.86
$\nu_4$	$E'$	-	4	3	$2\nu_2$	$E''$	+	5	5	222 383.0	221 629.8	2.688E-11	-30.49	-30.60
$\nu_4$	$E'$	-	4	3	$2\nu_2$	$E''$	+	4	1	223 276.4	221 209.4	2.001E-9	-29.92	-30.20
$2\nu_2$	$E''$	-	11	10	$\nu_4$	$E'$	+	11	6	228 058.1	236 952.0	4.881E-7	2.22	2.14
$\nu_4$	$A_2''$	-	3	2	$2\nu_2$	$A_2'$	+	3	0	231 898.5	231 697.2	4.217E-10	-30.10	-30.12
$2\nu_2$	$E''$	+	10	7	$\nu_4$	$E'$	-	11	11	232 641.9	231 001.8	1.039E-10	0.57	0.58
$\nu_4$	$A_2''$	-	5	2	$2\nu_2$	$A_2'$	+	5	0	240 790.3	236 429.8	4.767E-10	-28.56	-29.09
$2\nu_2$	$A_2''$	+	10	9	$\nu_4$	$A_2'$	-	9	7	246 042.7	245 788.3	1.394E-9	1.18	1.18
$\nu_4$	$A_2''$	-	7	2	$2\nu_2$	$A_2'$	+	7	0	256 343.5	246 617.0	9.753E-9	-26.06	-27.09
$\nu_4$	$E'$	-	10	1	$2\nu_2$	$E''$	-	9	4	265 637.1	265 500.3	2.065E-8	0.91	0.91
$2\nu_2$	$E'$	+	15	2	$\nu_4$	$E''$	+	15	3	271 177.3	295 527.8	1.948E-7	19.97	18.33
$\nu_4$	$E''$	-	11	2	$2\nu_2$	$E'$	+	12	8	272 070.6	269 956.9	1.176E-11	-11.49	-11.58
$\nu_4$	$A_2''$	-	5	4	$2\nu_2$	$A_2'$	+	6	6	273 695.5	271 413.1	1.013E-10	-23.91	-24.11
$\nu_4$	$A_2'$	-	14	1	$2\nu_2$	$A_2''$	+	14	3	284 161.3	262 580.4	6.415E-7	-21.29	-23.04
$\nu_4$	$E''$	+	9	7	$2\nu_2$	$E'$	+	8	2	289 050.9	278 543.2	1.050E-11	-21.95	-22.78
$\nu_4$	$E''$	-	15	4	$2\nu_2$	$E'$	+	15	4	293 553.8	273 373.9	3.777E-7	-15.55	-16.69
$2\nu_2$	$E''$	+	7	5	$\nu_4$	$E'$	-	6	1	299 067.0	306 213.1	1.727E-10	16.65	16.26
$2\nu_2$	$A_2'$	+	7	6	$\nu_4$	$A_2''$	-	6	4	299 741.5	304 232.2	2.560E-10	14.71	14.50
$\nu_4$	$A_2''$	+	15	13	$2\nu_2$	$A_2'$	-	15	15	310 977.7	292 218.4	8.819E-7	0.42	0.44
$2\nu_2$	$E'$	-	14	13	$\nu_4$	$E''$	-	13	6	370 468.5	386 366.5	1.634E-7	6.52	6.25
$2\nu_2$	$E''$	+	11	1	$\nu_4$	$E'$	-	11	3	383 116.8	397 644.4	7.878E-7	8.74	8.43
$2\nu_2$	$E'$	-	9	1	$\nu_4$	$E''$	+	10	1	391 133.2	399 006.5	5.035E-8	4.54	4.46
$\nu_4$	$E''$	-	14	4	$2\nu_2$	$E'$	+	14	4	391 573.9	369 051.4	9.071E-9	-13.83	-14.68
$\nu_4$	$E'$	-	8	3	$2\nu_2$	$E''$	+	9	7	393 819.4	386 248.0	7.438E-10	-11.20	-11.42
$\nu_4$	$A_2''$	-	10	4	$2\nu_2$	$A_2'$	-	10	9	395 977.9	399 753.4	1.409E-11	7.58	7.51
$\nu_4$	$E''$	-	12	4	$2\nu_2$	$E'$	+	12	4	400 546.7	382 835.1	2.160E-10	-13.26	-13.88
$2\nu_2$	$E''$	-	12	2	$\nu_4$	$E'$	-	13	5	404 821.7	411 541.5	3.784E-11	3.60	3.55
$2\nu_2$	$E''$	+	2	1	$\nu_4$	$E'$	-	1	1	411 785.9	410 294.2	2.933E-10	15.50	15.56
$\nu_4$	$E''$	-	13	4	$2\nu_2$	$E'$	+	13	4	412 766.2	391 603.0	1.298E-9	-13.63	-14.37
$2\nu_2$	$E'$	+	3	2	$\nu_4$	$E''$	-	2	0	418 312.4	418 044.7	3.347E-10	15.03	15.04
$2\nu_2$	$E'$	+	5	4	$\nu_4$	$E''$	-	4	2	426 211.9	427 780.8	2.998E-10	13.77	13.72
$2\nu_2$	$A_2'$	+	13	0	$\nu_4$	$A_2''$	+	13	1	427 273.2	444 607.4	8.633E-7	5.14	4.94
$\nu_4$	$E'$	-	13	3	$2\nu_2$	$E''$	-	13	8	432 732.4	422 088.3	1.336E-9	-3.24	-3.32
$\nu_4$	$E''$	-	7	6	$2\nu_2$	$E'$	+	8	8	436 285.0	429 917.9	1.476E-9	-12.77	-12.96
$2\nu_2$	$A_2''$	-	14	12	$\nu_4$	$A_2'$	+	13	4	436 303.0	447 998.1	1.222E-10	1.36	1.32
$\nu_4$	$E''$	+	8	1	$2\nu_2$	$E'$	-	7	5	449 011.2	444 718.8	4.822E-9	-3.44	-3.48
$2\nu_2$	$E''$	-	10	8	$\nu_4$	$E'$	-	10	1	471 678.5		3.126E-10	-3.36	
$\nu_4$	$E''$	+	11	1	$2\nu_2$	$E'$	-	10	1	472 739.7	462 948.4	1.469E-7	-6.20	-6.33
$2\nu_2$	$E'$	+	13	2	$\nu_4$	$E''$	+	13	3	473 783.0	488 310.8	6.262E-11	9.78	9.49
$2\nu_2$	$E'$	+	11	2	$\nu_4$	$E''$	+	12	9	477 572.4	489 990.1	1.758E-11	7.19	7.01
$\nu_4$	$E''$	-	13	0	$2\nu_2$	$E'$	-	13	7	479 838.8	467 282.5	6.591E-9	-2.32	-2.38
$2\nu_2$	$E''$	-	8	4	$\nu_4$	$E'$	-	9	1	485 870.6		5.687E-9	-0.51	
$\nu_4$	$E''$	+	14	5	$2\nu_2$	$E'$	+	15	10	486 677.1	467 668.0	8.877E-10	-12.98	-13.51

Table 3: (*Continued*)

$v'$	$\Gamma'$	$p'$	$J'$	$K'$	$v''$	$\Gamma''$	$p''$	$J''$	$K''$	$\nu_{\text{calc}}/\text{MHz}$	$\nu_{\text{exp}}/\text{MHz}$	$A/\text{s}^{-1}$	$T_{\text{calc}}$	$T_{\text{exp}}$
$2\nu_2$	$E''$	—	11	8	$\nu_4$	$E'$	—	11	3	490 061.7	490 267.1	2.737E-9	-3.19	-3.19
$2\nu_2$	$E''$	—	10	10	$\nu_4$	$E'$	+	10	6	492 622.0	499 709.3	7.714E-8	-0.36	-0.35
$\nu_4$	$A_2''$	—	11	10	$2\nu_2$	$A_2'$	+	10	6	494 681.5	496 832.3	8.060E-9	-1.76	-1.76
$2\nu_2$	$E''$	+	12	7	$\nu_4$	$E'$	+	11	0	495 889.7	509 581.8	7.614E-11	8.86	8.62
$2\nu_2$	$E'$	+	13	8	$\nu_4$	$E''$	—	12	2	498 381.0	515 446.1	3.328E-11	9.41	9.10
$\nu_4$	$E''$	+	14	9	$2\nu_2$	$E'$	+	13	4	502 008.5	481 006.5	1.541E-11	-13.17	-13.74
$\nu_4$	$E''$	—	3	0	$2\nu_2$	$E'$	+	4	4	509 875.0	509 939.3	2.820E-11	-14.19	-14.19
$2\nu_2$	$E'$	—	14	1	$\nu_4$	$E''$	—	15	6	513 775.3	529 792.8	2.948E-10	4.18	4.05
$2\nu_2$	$E''$	+	12	7	$\nu_4$	$E'$	—	11	1	518 473.1		7.981E-11	8.20	
$2\nu_2$	$A_2'$	+	9	6	$\nu_4$	$A_2''$	—	8	2	520 115.9	530 125.8	6.108E-9	6.67	6.54
$\nu_4$	$A_2''$	—	11	10	$2\nu_2$	$A_2'$	+	12	12	527 967.5	522 798.6	5.244E-9	-6.89	-6.96
$\nu_4$	$A_2''$	+	14	5	$2\nu_2$	$A_2'$	—	13	3	529 679.3	519 268.7	2.848E-8	-6.78	-6.92
$\nu_4$	$E'$	—	9	1	$2\nu_2$	$E''$	—	8	4	544 495.1	536 665.8	5.798E-11	-2.32	-2.36
$\nu_4$	$A_2'$	—	8	7	$2\nu_2$	$A_2''$	+	9	9	547 699.8	541 374.3	4.911E-9	-8.93	-9.03
$2\nu_2$	$E'$	—	10	7	$\nu_4$	$E''$	—	10	0	551 917.9	562 160.3	2.505E-11	-0.39	-0.39
$\nu_4$	$E''$	+	8	5	$2\nu_2$	$E'$	—	7	7	553 180.0	550 518.3	1.517E-9	-1.67	-1.68
$2\nu_2$	$E''$	—	11	2	$\nu_4$	$E'$	+	12	4	554 034.4		4.035E-8	3.69	
$2\nu_2$	$E'$	+	11	10	$\nu_4$	$E''$	—	10	8	556 948.4	552 032.8	6.561E-11	-0.65	-0.66
$2\nu_2$	$A_2''$	—	14	6	$\nu_4$	$A_2'$	+	15	8	558 315.5	575 254.6	1.019E-8	4.32	4.20
$2\nu_2$	$A_2''$	+	12	9	$\nu_4$	$A_2'$	—	13	13	563 019.2	565 112.9	7.362E-9	1.73	1.73
$2\nu_2$	$E'$	—	15	13	$\nu_4$	$E''$	—	14	6	566 197.0	583 213.0	1.775E-8	0.14	0.13
$\nu_4$	$A_2'$	+	12	8	$2\nu_2$	$A_2''$	+	11	3	574 312.4	561 928.1	8.085E-11	-8.53	-8.72
$\nu_4$	$E''$	—	10	0	$2\nu_2$	$E'$	+	10	2	588 510.6	581 667.0	9.235E-8	-6.84	-6.92

Table 4: Vibration-rotation-inversion frequencies ( $\nu$ ), Einstein A coefficients ( $A$ ) and sensitivity coefficients ( $T$ ) of  $^{14}\text{NH}_3$  for transitions between the  $2\nu_2$  and  $\nu_4$  vibrational states. Experimental frequencies have been obtained using energy levels from the MARVEL analysis [5].

$v'$	$\Gamma'$	$p'$	$J'$	$K'$	$v''$	$\Gamma''$	$p''$	$J''$	$K''$	$\nu_{\text{calc}}/\text{MHz}$	$\nu_{\text{exp}}/\text{MHz}$	$A/\text{s}^{-1}$	$T_{\text{calc}}$	$T_{\text{exp}}$
$2\nu_2$	$A'_2$	—	14	9	$\nu_4$	$A''_2$	+	14	5	2869.0	13 943.5	2.496E-12	770.89	158.62
$\nu_4$	$E''$	+	5	3	$2\nu_2$	$E'$	+	5	2	3540.5	389.9	1.894E-15	-1843.25	-16,737.52
$2\nu_2$	$A''_2$	—	13	12	$\nu_4$	$A'_2$	+	12	4	3654.5	12 450.3	2.167E-18	125.08	36.71
$2\nu_2$	$E'$	+	6	2	$\nu_4$	$E''$	+	6	3	7362.9	12 687.9	6.231E-14	877.49	509.21
$2\nu_2$	$A''_2$	+	13	9	$\nu_4$	$A'_2$	—	14	13	8783.9	13 385.9	7.203E-13	260.35	170.84
$\nu_4$	$E''$	+	4	3	$2\nu_2$	$E'$	+	4	2	10 441.8	9235.5	9.301E-15	-630.49	-712.84
$\nu_4$	$E''$	+	12	7	$2\nu_2$	$E'$	—	11	7	13 244.8	3258.0	5.271E-18	-131.57	-534.87
$\nu_4$	$E''$	+	3	3	$2\nu_2$	$E'$	+	3	2	13 727.5	14 116.6	2.066E-15	-484.00	-470.66
$\nu_4$	$A'_2$	—	11	5	$2\nu_2$	$A''_2$	+	12	9	18 889.9	9313.7	3.659E-12	-233.82	-474.24
$\nu_4$	$E'$	+	13	8	$2\nu_2$	$E''$	+	14	11	21 809.9	10 121.4	5.243E-21	-222.12	-478.64
$2\nu_2$	$E'$	+	7	2	$\nu_4$	$E''$	+	7	3	22 031.7	29 771.2	4.761E-12	288.71	213.65
$\nu_4$	$E'$	+	13	10	$2\nu_2$	$E''$	—	12	10	22 511.4	11 390.1	1.900E-17	-45.36	-89.65
$2\nu_2$	$E''$	—	11	8	$\nu_4$	$E'$	+	11	2	24 283.2	29 727.5	6.991E-17	44.14	36.05
$\nu_4$	$A''_2$	—	7	2	$2\nu_2$	$A'_2$	+	8	6	33 193.0	25 452.1	3.082E-13	-140.17	-182.79
$\nu_4$	$E''$	—	12	8	$2\nu_2$	$E'$	—	12	11	37 009.4	34 972.4	5.319E-20	45.86	48.53
$\nu_4$	$E'$	+	5	2	$2\nu_2$	$E''$	+	6	5	37 758.9	35 875.2	4.280E-17	-158.57	-166.89
$\nu_4$	$E'$	+	10	8	$2\nu_2$	$E''$	+	9	1	42 879.3	29 604.5	3.786E-15	-142.81	-206.85
$\nu_4$	$E''$	+	14	1	$2\nu_2$	$E'$	—	14	7	44 774.0	26 546.7	6.005E-13	-65.86	-111.08
$2\nu_2$	$A''_2$	—	15	6	$\nu_4$	$A'_2$	—	15	1	47 199.3	59 449.2	9.114E-12	17.21	13.67
$2\nu_2$	$E''$	+	10	7	$\nu_4$	$E'$	+	9	2	47 382.2	47 660.4	1.134E-16	74.98	74.55
$2\nu_2$	$E''$	+	8	7	$\nu_4$	$E'$	+	7	4	49 067.0	53 771.1	3.235E-19	96.03	87.62
$2\nu_2$	$E'$	—	14	11	$\nu_4$	$E''$	—	13	0	50 673.9	64 280.5	1.837E-17	-4.85	-3.82
$\nu_4$	$E''$	+	10	7	$2\nu_2$	$E'$	+	11	10	53 258.1	49 792.6	7.021E-19	-73.12	-78.21
$2\nu_2$	$E''$	+	8	1	$\nu_4$	$E'$	—	9	7	55 815.4	66 964.1	2.485E-14	106.98	89.17
$2\nu_2$	$E'$	+	5	4	$\nu_4$	$E''$	—	4	0	60 051.4	63 043.9	5.157E-14	102.78	97.90
$\nu_4$	$E''$	+	9	3	$2\nu_2$	$E'$	—	8	5	64 134.6	58 861.4	5.937E-16	-21.57	-23.50
$2\nu_2$	$A''_2$	+	10	3	$\nu_4$	$A'_2$	+	11	8	65 303.8	72 587.6	2.485E-13	43.28	38.94
$\nu_4$	$E''$	—	9	8	$2\nu_2$	$E'$	+	8	2	66 883.7	57 708.2	7.717E-17	-47.24	-54.75
$\nu_4$	$E'$	+	15	6	$2\nu_2$	$E''$	—	14	2	67 144.5	53 783.2	3.293E-12	-47.41	-59.18
$\nu_4$	$E'$	—	10	1	$2\nu_2$	$E''$	+	11	7	68 862.3	59 127.9	2.090E-15	-53.67	-62.51
$\nu_4$	$E''$	—	7	0	$2\nu_2$	$E'$	—	6	5	69 644.8	64 096.1	4.241E-15	-3.43	-3.73
$2\nu_2$	$E'$	+	9	8	$\nu_4$	$E''$	—	8	6	72 271.0	78 005.7	3.767E-12	26.51	24.56
$\nu_4$	$E''$	+	10	1	$2\nu_2$	$E'$	—	11	11	73 958.8	64 546.6	5.011E-17	-7.00	-8.02
$2\nu_2$	$E'$	+	12	4	$\nu_4$	$E''$	+	13	9	77 781.2	94 457.9	1.745E-14	70.00	57.64
$\nu_4$	$E''$	—	15	10	$2\nu_2$	$E'$	+	15	10	79 259.1	57 282.5	9.514E-16	-76.85	-106.33
$2\nu_2$	$E'$	+	15	8	$\nu_4$	$E''$	—	14	0	82 460.9	103 540.2	4.726E-15	49.65	39.54
$\nu_4$	$E'$	—	15	7	$2\nu_2$	$E''$	+	15	7	82 880.6	56 099.2	2.551E-16	-76.46	-112.96
$\nu_4$	$E''$	+	13	9	$2\nu_2$	$E'$	+	12	2	86 193.3	72 994.5	3.558E-14	-52.03	-61.44
$2\nu_2$	$A''_2$	+	15	9	$\nu_4$	$A'_2$	—	14	1	89 976.7	111 115.7	1.566E-18	60.20	48.75
$\nu_4$	$E''$	+	10	9	$2\nu_2$	$E'$	+	9	4	93 115.5	81 629.4	3.945E-20	-49.44	-56.40
$2\nu_2$	$E'$	+	10	8	$\nu_4$	$E''$	+	9	5	96 563.2	97 613.4	7.541E-20	35.95	35.56
$\nu_4$	$E''$	—	8	2	$2\nu_2$	$E'$	—	7	5	104 453.7	103 325.9	2.312E-13	-7.79	-7.87
$\nu_4$	$E'$	—	14	7	$2\nu_2$	$E''$	+	14	7	110 323.6	87 142.1	9.221E-16	-56.88	-72.01
$\nu_4$	$E'$	+	10	0	$2\nu_2$	$E''$	+	11	7	113 903.1	105 079.2	3.443E-13	-41.85	-45.36
$\nu_4$	$A'_2$	—	14	1	$2\nu_2$	$A''_2$	—	15	12	127 303.9	111 657.5	3.416E-16	-14.68	-16.74

Table 4: (*Continued*)

$v'$	$\Gamma'$	$p'$	$J'$	$K'$	$v''$	$\Gamma''$	$p''$	$J''$	$K''$	$\nu_{\text{calc}}/\text{MHz}$	$\nu_{\text{exp}}/\text{MHz}$	$A/\text{s}^{-1}$	$T_{\text{calc}}$	$T_{\text{exp}}$
$\nu_4$	$E''$	—	12	0	$2\nu_2$	$E''$	—	12	7	128 808.8	116 841.5	2.621E-12	-5.35	-5.90
$\nu_4$	$E''$	—	14	10	$2\nu_2$	$E''$	—	14	13	129 717.2	113 927.7	2.815E-15	-24.72	-28.14
$\nu_4$	$E'$	—	13	7	$2\nu_2$	$E''$	+	13	7	137 931.5		2.502E-15	-42.72	
$2\nu_2$	$E''$	+	10	5	$\nu_4$	$E''$	—	11	9	143 648.6	150 832.9	6.730E-18	23.80	22.66
$2\nu_2$	$E''$	—	10	4	$\nu_4$	$E''$	+	11	4	147 482.9	156 281.9	2.428E-12	13.13	12.39
$\nu_4$	$A'_2$	—	2	1	$2\nu_2$	$A''_2$	+	3	3	147 719.7	149 449.7	1.315E-12	-47.21	-46.66

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