

The spectrum of $^{15}\text{NH}_3$ in the 66-2000 cm^{-1} region

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Overview of Presentation

1. Motivation for this spectroscopic study and the current status of knowledge
2. Experimental Details
3. Spectroscopic analysis
4. Data interpretation and comparisons with other studies
5. Conclusions and directions for future work
6. Acknowledgements

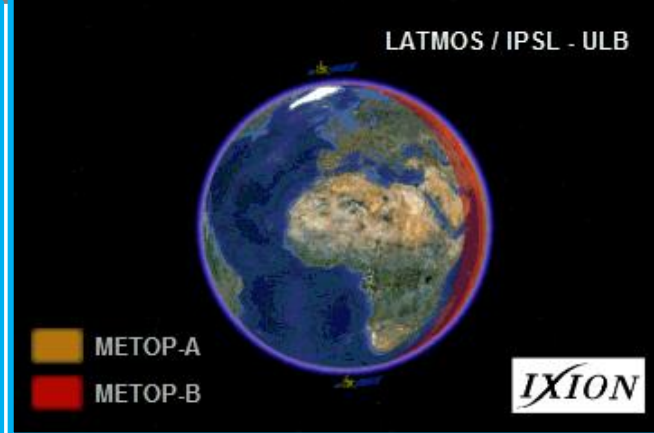
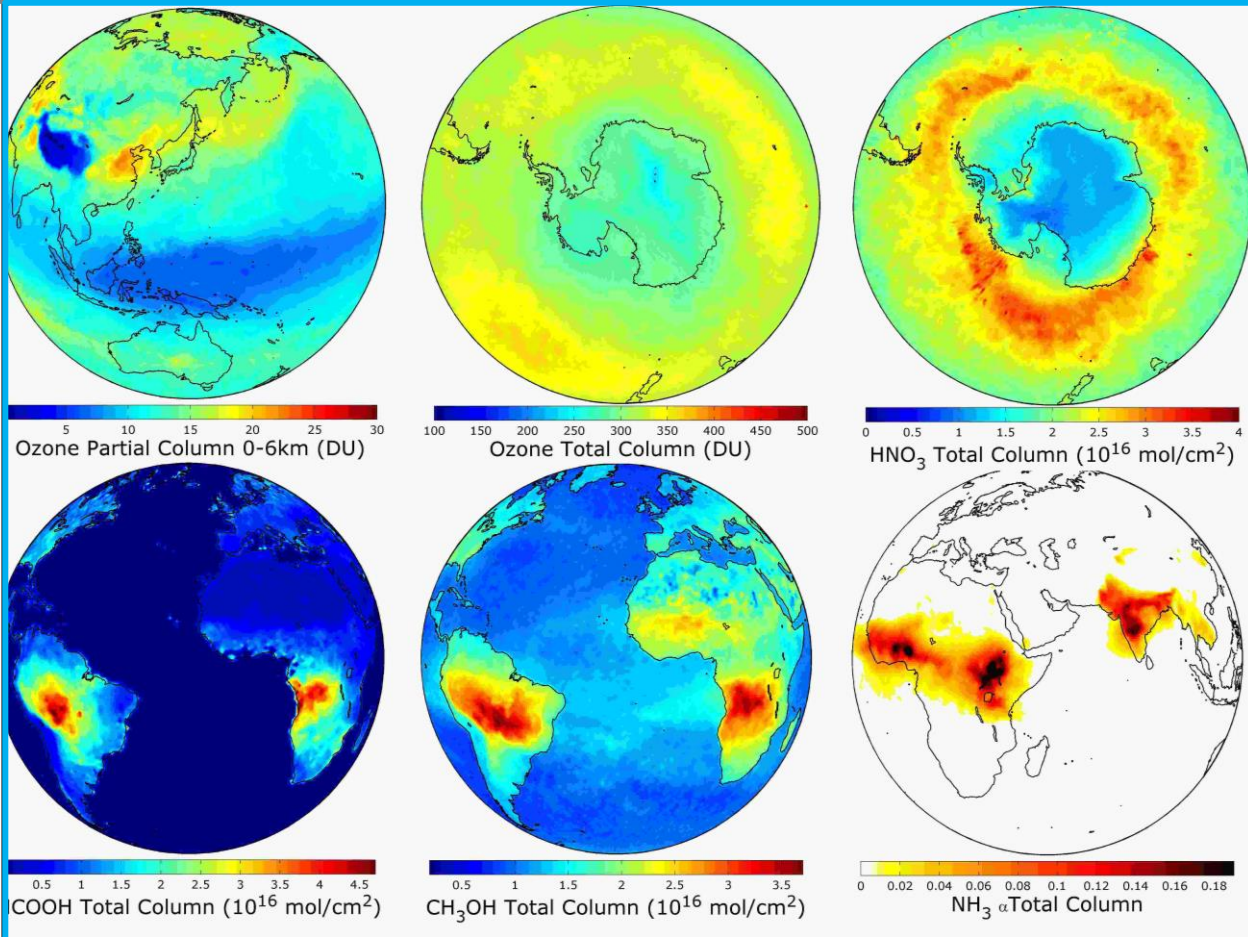
- Ammonia is a gas readily released into the air from a variety of biological sources, as well as from industrial and combustion processes.
- While NH_3 has many beneficial uses, it can detrimentally affect the quality of the environment through eutrophication of natural ecosystems, the associated loss of biodiversity, and the formation of secondary particles in the atmosphere, which can reduce visibility.
- Possible health effects of ammonia gas in the atmosphere include short-term irritation of the eyes and lungs and the long-term effects on the cardiovascular system through inhalation of fine particulate matter formed from ammonia in the atmosphere.
- The dominant source of NH_3 emissions in the Canada is agriculture (~85%), largely from animal waste and commercial fertilizer application.

Source: <http://nadp.sws.uiuc.edu/amon/>



AMoN (Ammonia Monitoring Network) field site at Sequoia National Park, USA

Monitoring Ammonia in the Atmosphere



Animation showing MetOp-A and MetOp-B flying simultaneously. Half an orbit (~50 minutes) is separating the two satellites. Image Credit: Maya George/LATMOS

IASI performs measurements covering the globe twice daily, which makes it an ideal instrument for monitoring the evolution of important compounds in the atmosphere.

Examples of different atmospheric compounds retrieved from the Infrared Atmospheric Sounding Interferometer (IASI) measurements: Ozone (for partial and total columns), nitric acid (HNO₃), formic acid (HCOOH), methanol (CH₃OH) and ammonia (NH₃). Image Credit: Maya George/LATMOS

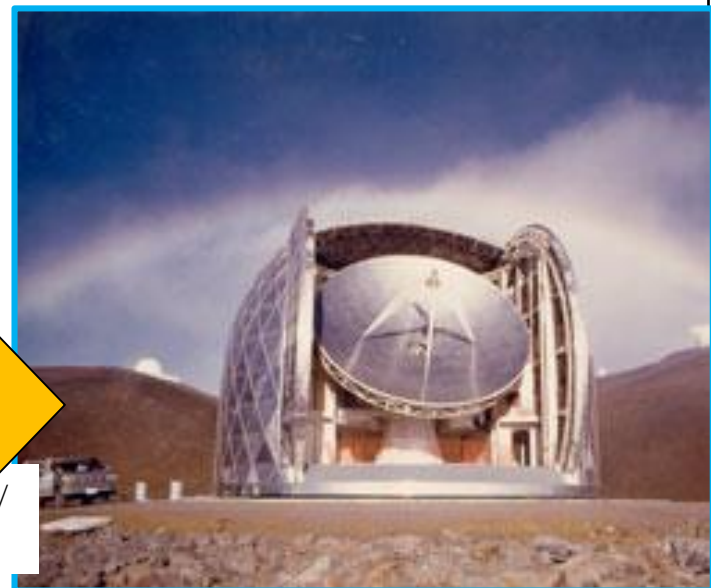
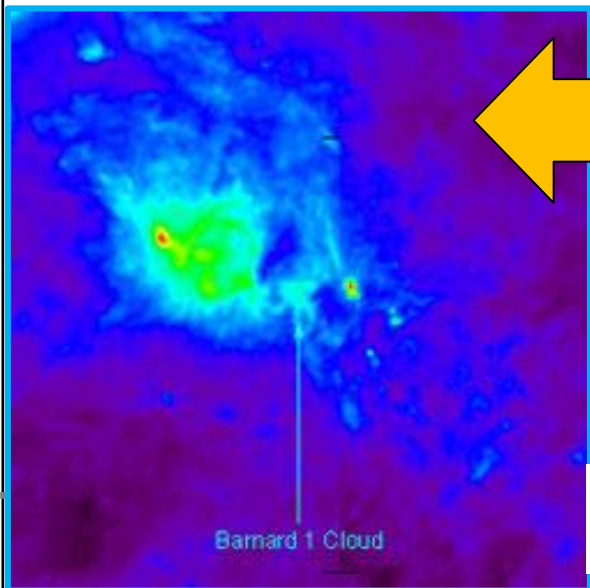
Interstellar Ammonia

- The composition of the interstellar medium determines the composition of the objects which form from it such as stars and planets. The information provided by the study of atoms and molecules in interstellar space is crucial to our understanding of star formation and galactic evolution.
- Interstellar molecules, such as water and ammonia and atoms such as oxygen and carbon are detected in the infrared in many parts of our galaxy. These molecules are found in the cool clouds of dust and gas within which new stars and planets are formed.
- Ammonia (NH_3) was the first polyatomic molecule detected in interstellar space. Since its initial discovery by Cheung *et al.* (1968), because of its large number of transitions sensitive to a wide range of excitation conditions and the fact that it can be detected in a great variety of regions, NH_3 is perhaps second only to carbon monoxide (CO) in importance. Ammonia is found on Pluto, Jupiter and, in small amounts, on Uranus.

IRAS image of the vicinity of the Barnard~1 cloud in the constellation Perseus, where triply deuterated ammonia was detected at the CSO.

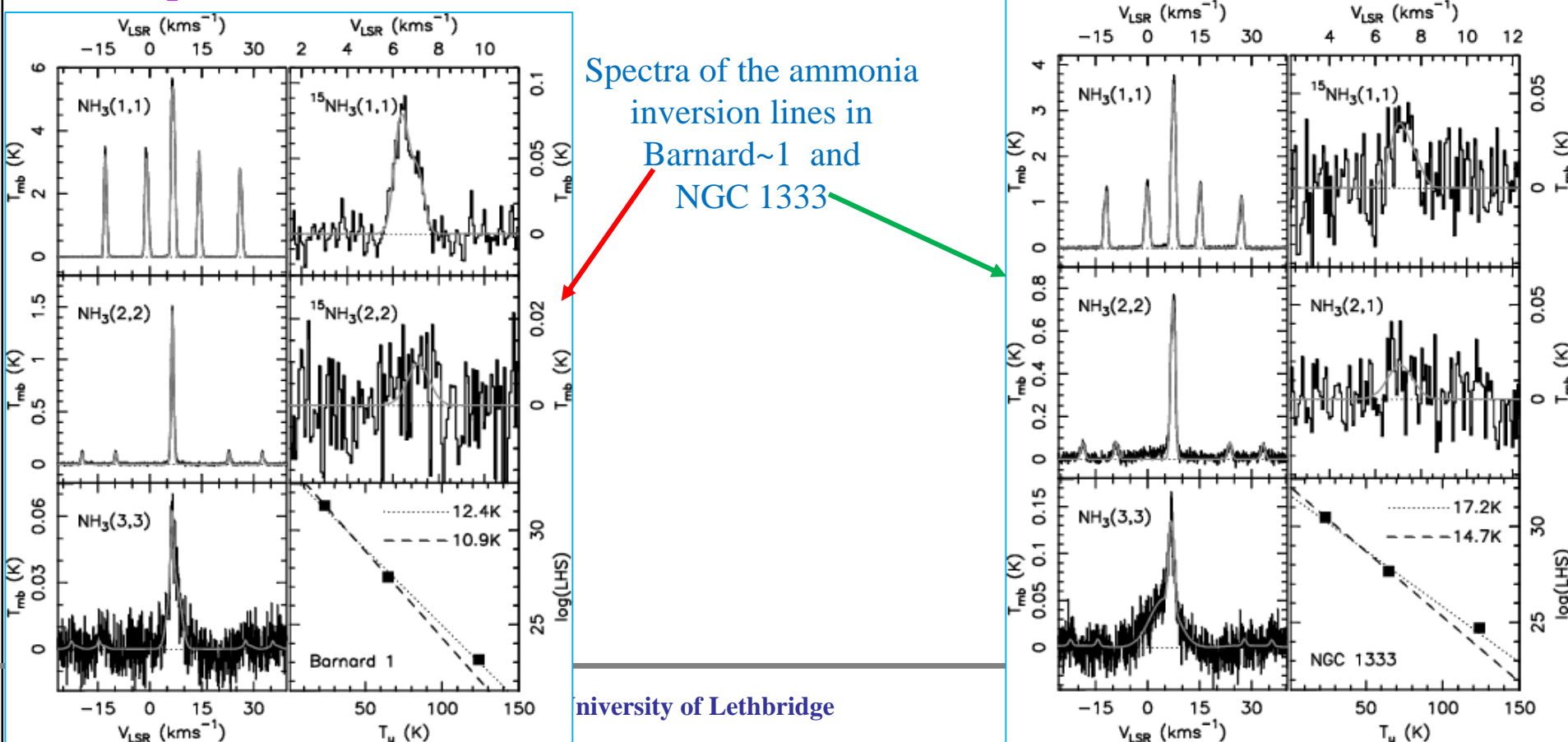
The 10.4-meter Leighton telescope of the Caltech Submillimeter Observatory (CSO) atop Mauna Kea, Hawaii.

Source: <http://www.spaceflightnow.com/news/n0205/31ammonia/>



Nitrogen Isotopic Fractionation in Interstellar Ammonia

Using the Green Bank Telescope (GBT), D.C. Lis *et al.* *Astrophys.J.* (2010) have obtained accurate measurements of the $^{14}\text{N}/^{15}\text{N}$ isotopic ratio in ammonia in two nearby cold, dense molecular clouds, **Barnard~1** and **NGC 1333**. The $^{14}\text{N}/^{15}\text{N}$ ratio in Barnard~1, 334 ± 50 , is particularly well constrained and falls in between the **local interstellar medium/proto-solar value of ~ 450** and the **terrestrial atmospheric value of 272**.



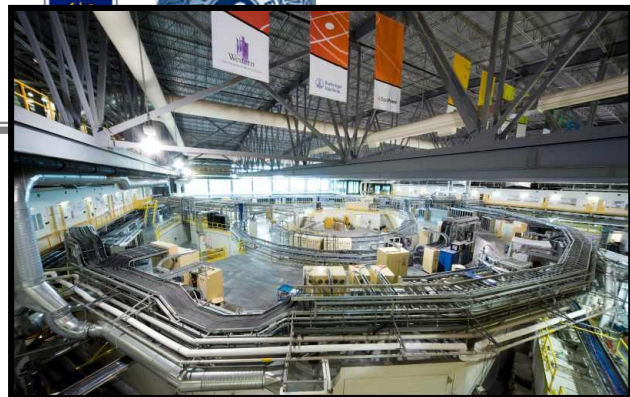
Current status of Spectroscopic Knowledge On Ammonia

- Ammonia is a well studied molecule owing to its importance as a model molecule possessing internal inversion motion which can be characterized by infrared spectroscopy.
- Until recently, the available data in the far-infrared region were marginal. Indeed previous studies were performed only at low/medium resolution (up to $R \sim 0.1 \text{ cm}^{-1}$).
- For this reason the atmospheric retrievals of ammonia performed by infrared techniques use only cross section parameters to analyze the observed atmospheric spectra.
- Among the isotopically substituted molecules, $^{15}\text{NH}_3$ received little attention in comparison with the parent main isotope $^{14}\text{NH}_3$. $^{15}\text{NH}_3$ has an energy pattern very similar to that of $^{14}\text{NH}_3$ and represents a suitable test to check the assignment of the transitions and the adequacy of the Hamiltonian for the description of the spectrum, in particular at very high J values.
- While recently the ground state transitions of $^{14}\text{NH}_3$ [1] has been reinvestigated by means of several high resolution techniques, only two studies were devoted to the analogous spectra in $^{15}\text{NH}_3$ [2,3]. Of these, the most recent was performed in 1994 and rotation-inversion transitions were measured only up to $J = 6$. The bending states of $^{15}\text{NH}_3$ were also analysed using spectra recorded at moderate resolution [4].

Spectroscopic Goals for this study

- The use of infrared techniques to retrieve tropospheric species is a very powerful technique, provided that accurate spectroscopic parameters are used to analyze the observed spectra.
- The goal of the present study is to perform the first detailed infrared study of $^{15}\text{NH}_3$ in the far-infrared region. The target task, in the near future, will be to provide a precise and consistent list of $^{15}\text{NH}_3$ lines involving accurate line position, intensity and air-broadening parameters.
- Since the knowledge of the ground state energy pattern is essential to investigate the vibrationally excited states we recorded the far infrared spectrum of the molecule at very high resolution and path length in order to observe very high J transitions and also the rotation-inversion spectrum in the lowest excited vibrational states.
- We aimed to observe perturbation allowed transitions, which are essential to better characterize the rotation and distortion parameters related to the axis of symmetry, C , D_K , H_K ,
- The spectral range we aim to investigate extends from 60 to 2000 cm^{-1} allowing the observation of transitions $\nu_2 \leftarrow \text{GS}$, $\nu_4 \leftarrow \text{GS}$, $2\nu_2 \leftarrow \text{GS}$ and the hot bands $2\nu_2 \leftarrow \nu_2$, $\nu_4 \leftarrow \nu_2$ and $2\nu_2 \leftarrow \nu_4$.

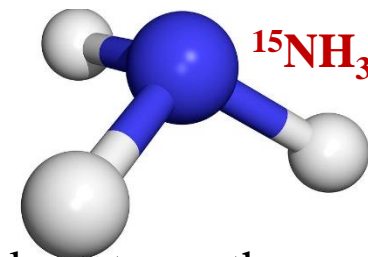
Experimental Conditions



- The high resolution of the Bruker Fourier transform spectrometer at the FIR beamline, coupled with the high brightness of the synchrotron in the difficult $60\text{-}400\text{ cm}^{-1}$ region, represented a powerful capability for this study.
- In the FIR region, Doppler broadening of the spectral lines is small, so that the high-resolution of the spectrometer was exploited to the full, while the high brightness gives greatly improved SNR ratio.
- The sample was supplied by Sigma-Aldrich with a purity of 98% and used without any further purification.

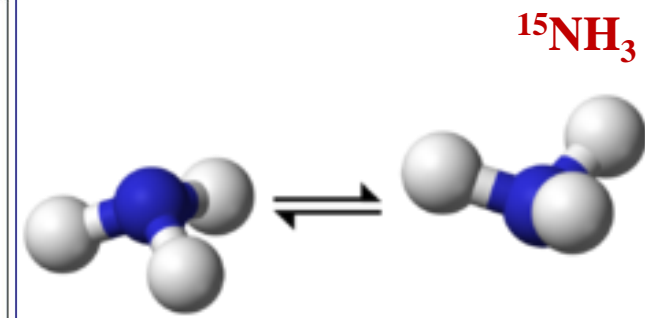
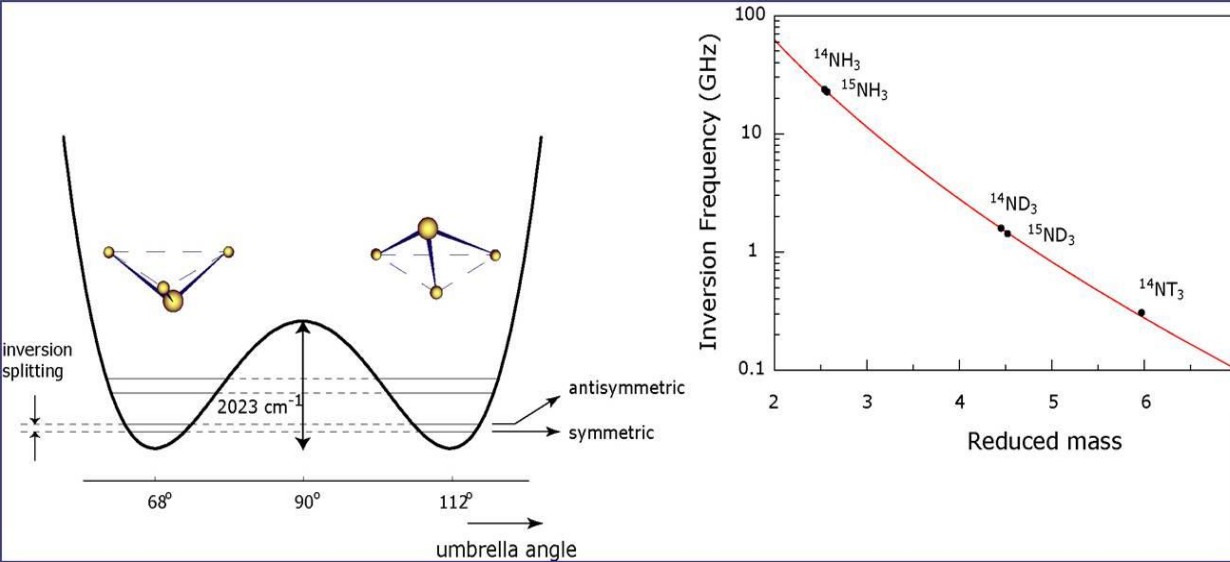
Range (cm^{-1})	Pressure (Torr)	Pathlength (m)	Temperature (K)	Resolution (cm^{-1})	Source
60-370	0.002	8	298	0.00096	Synchrotron
60-370	1	72	298	0.00096	Synchrotron
60-370	0.05	72	298	0.00096	Synchrotron
896-1149	0.05	72	298	0.003	Global
1100-1700	0.05	72	298	0.003	Global
1100-1700	0.005	72	298	0.003	Global
1600- 2085	0.005	72	298	0.003	Global

- The pyramidal NH_3 molecule is a symmetric top with inversion, well understood in laboratory microwave spectroscopy (Townes & Schawlow 1955, Kukolich 1967).
- Several important properties make NH_3 particularly interesting in astrophysical conditions: the existence of metastable and non-metastable states, ortho- and para- species, **inversion motion of the molecule**, and hyperfine structures.
- The rotational energy of NH_3 is a function of the two principal quantum numbers (J , K), corresponding to the total angular momentum and its projection along the molecular axis.
- The molecule has an electric dipole moment only along the molecular axis, and the dipole selection rules are $\Delta K = 0$, $\Delta J = 0, \pm 1$. Hence, *dipole transitions between K -ladders are normally forbidden*.
- Interaction between rotational and vibrational motions, induces a small dipole moment perpendicular to the rotation axis, giving rise to very slow $\Delta k = \pm 3$ ($K = |k|$) transitions (Oka *et al.* 1971). The K -ladders are essentially independent of each other. Normal intermolecular collisions (not involving weak magnetic effects) also produce only transitions in which Δk is a multiple of 3 (including 0). Within each K -ladder, the upper states ($J > K$) are called non-metastable because they can decay rapidly via the far-infrared $\Delta J = 1$ transitions. The lowest states can only decay via the much slower $\Delta k = \pm 3$ transitions and are called metastable.



Source: PT Ho, C. Townes, Ann. Rev. Astron. Astrophys. 1983. 21: 239-70

The Inversion Motion of Ammonia Molecule



- The N atom can tunnel quantum mechanically through the plane of the H atoms. The potential barrier due to the H atoms is low enough that such tunneling occurs rapidly, resulting in the two lowest vibrational states providing a transition frequency that falls in the microwave range.
- All (J, K) rotational states are thus split into *inversion doublets* (except for K = 0, where nuclear spin statistics and symmetry considerations eliminate half of the inversion doublet). The $\Delta J = 0, \Delta K = 0$ inversion transitions across the doublets are allowed from symmetry considerations (Townes & Schawlow 1955). The inversion doublets are further split by hyperfine interactions.

Source: P.T. Ho, C. Townes, *Ann. Rev. Astron. Astrophys.* 1983. 21: 239-70

Energy levels in $^{15}\text{NH}_3$

Energy diagram of the rotation-inversion energy levels of NH_3 . J is the total angular-momentum quantum number, and K is the projected angular momentum along the molecular axis.

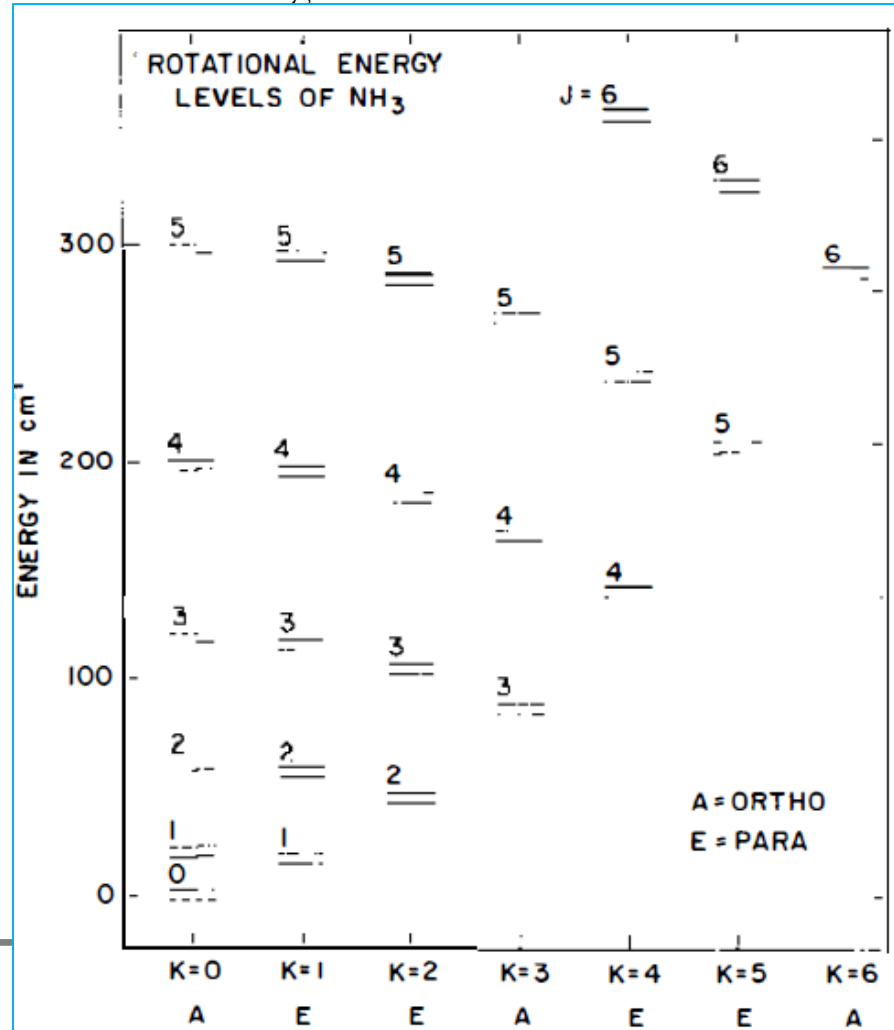
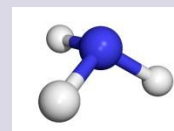
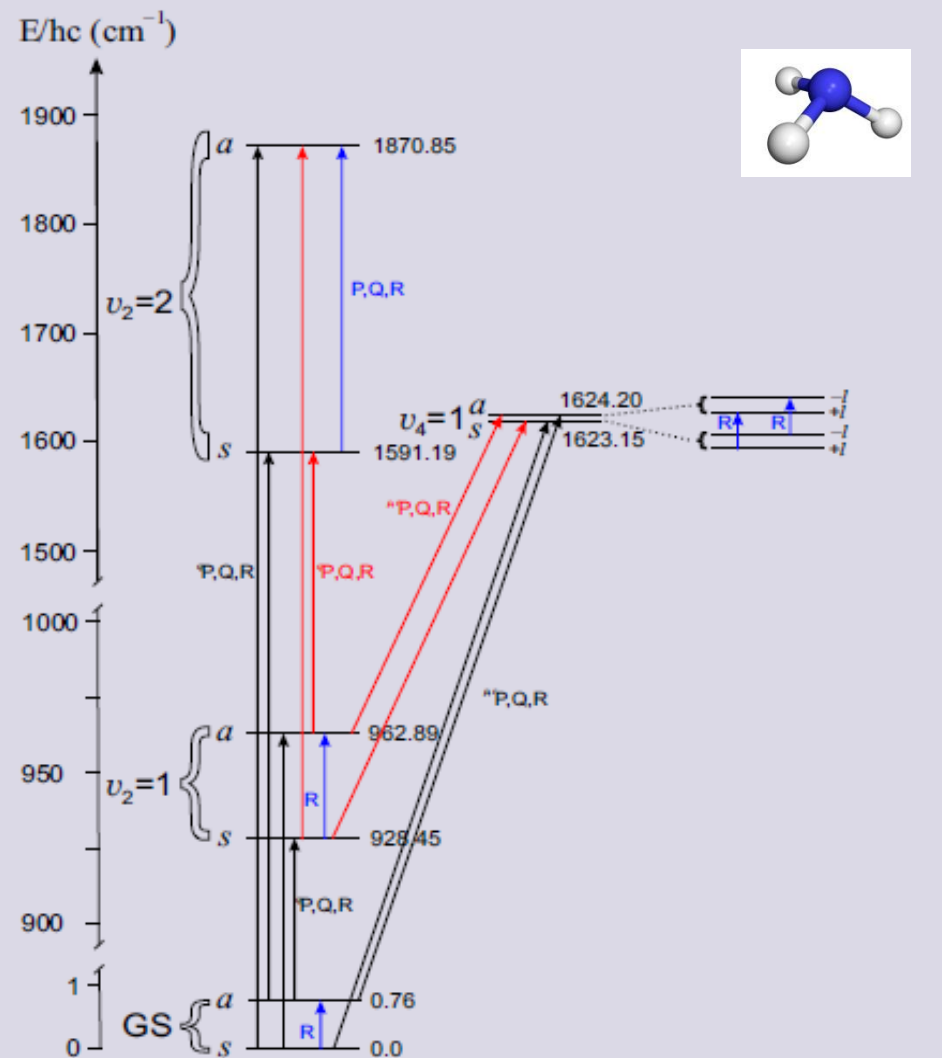


Diagram of energy levels in $^{15}\text{NH}_3$. Shown by arrows are observed transitions. The blue arrows correspond to inversion-rotation transitions. The red arrows correspond to hot band transitions starting from the v_2 level. The black arrows correspond to vibration-rotation transitions from the ground state (GS).



- In the region below 2000 cm^{-1} three bands involving the states $\nu_2 = 1$, $\nu_4 = 1$ and $\nu_2 = 2$ are observed.
- Because of the inversion motion each level is split into two sublevels whose wavefunctions are symmetric (s) or antisymmetric (a) with respect to the plane of inversion. Furthermore each (s) and (a) level of the double degenerate $\nu_4 = 1$ state contains stacks of levels characterized by the $l = 1$ and $l = -1$ vibrational angular momentum.
- Here we report on the observation and the analysis of the inversion rotation spectrum in the ground, $\nu_2 = 1$, $\nu_4 = 1$ and $\nu_2 = 2$ states. All the allowed and forbidden inversion-rotation transitions belonging to the ground state, together with the pure inversion transitions present in the literature, were fitted simultaneously on the basis of an inversion-rotational Hamiltonian which includes the centrifugal distortion constants up to 12^{th} power and the $\Delta k = \pm 3$ and $\Delta k = \pm 6$ interaction terms. 651 transitions with J up to 23 were fitted to 54 parameters, with a RMS value for 534 FIR lines of $0.98 \times 10^{-4} \text{ cm}^{-1}$ (3.3 MHz).

Molecular Hamiltonian for the ground state containing diagonal, and $\Delta K = \pm 3, 6$ off-diagonal terms.

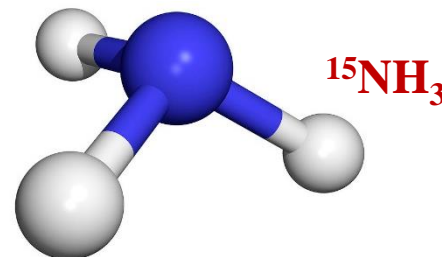
$$\begin{aligned}
 {}^{(i)}E(J, K) = & {}^{(i)}E^0 + {}^{(i)}B[J(J+1) - K^2] + {}^{(i)}CK^2 - {}^{(i)}D_J[J(J+1)]^2 - {}^{(i)}D_{JK}[J(J+1)]K^2 - {}^{(i)}D_KK^4 \\
 & + {}^{(i)}H_J[J(J+1)]^3 + {}^{(i)}H_{JK}[J(J+1)]^2K^2 + {}^{(i)}H_{JKK}[J(J+1)]K^4 + {}^{(i)}H_KK^6 \\
 & + {}^{(i)}L_J[J(J+1)]^4 + {}^{(i)}L_{JJK}[J(J+1)]^3K^2 + {}^{(i)}L_{JJKK}[J(J+1)]^2K^4 + {}^{(i)}L_{JJKK}[J(J+1)]K^6 + {}^{(i)}L_KK^8 \\
 & + {}^{(i)}M_J[J(J+1)]^5 + {}^{(i)}M_{JJJK}[J(J+1)]^4K^2 + {}^{(i)}M_{JJKK}[J(J+1)]^3K^4 \\
 & + {}^{(i)}M_{JJKK}[J(J+1)]^2K^6 + {}^{(i)}M_{JKKK}[J(J+1)]K^8 + {}^{(i)}M_KK^{10} \\
 & + {}^{(i)}N_J[J(J+1)]^6 + {}^{(i)}N_{JJJK}[J(J+1)]^5K^2 + {}^{(i)}N_{JJJKK}[J(J+1)]^4K^4 \\
 & + {}^{(i)}N_{JJJKK}[J(J+1)]^3K^6 + {}^{(i)}N_{JJKKK}[J(J+1)]^2K^8 + {}^{(i)}N_{JJKKKK}[J(J+1)]K^{10} + {}^{(i)}N_KK^{12}
 \end{aligned}$$

$$\begin{aligned}
 \left(\begin{smallmatrix} s \\ a \end{smallmatrix}\right) \langle v, J, K | H / hc | v, J, K \pm 3 \rangle \left(\begin{smallmatrix} a \\ s \end{smallmatrix}\right) = & \left\{ [\alpha + \alpha_J(J(J+1)) + \alpha_{JJ}(J(J+1))^2] \times (2K \pm 3) + [\alpha_K + \alpha_{JK}(J(J+1))] \right. \\
 & \left. \times [K^3 + (K \pm 3)^3] + \alpha_{KK} [K^5 + (K \pm 3)^5] \right\} F_{\pm 3}
 \end{aligned}$$

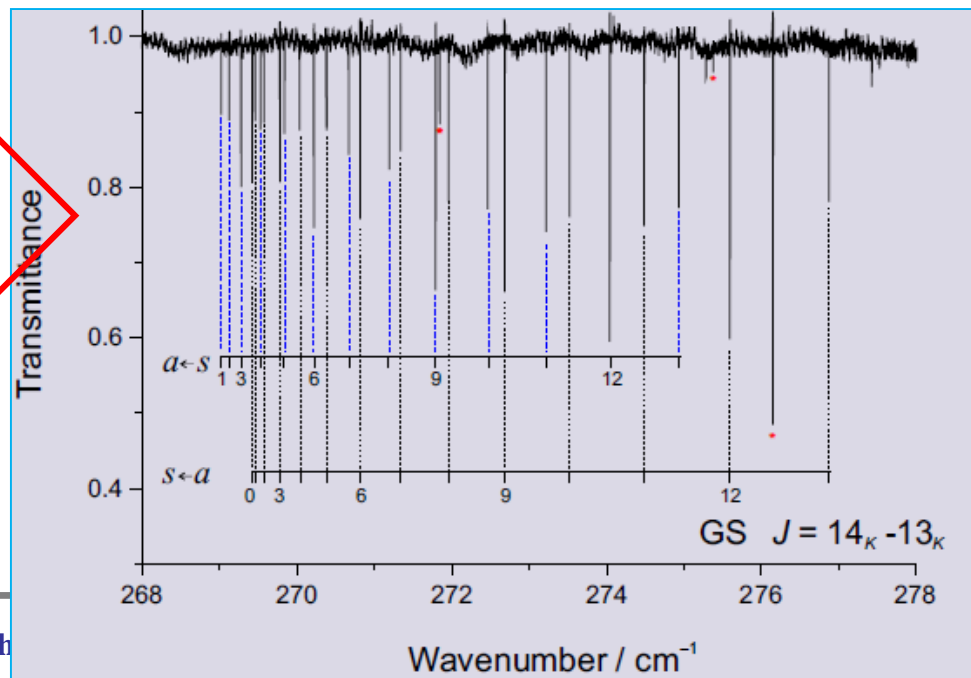
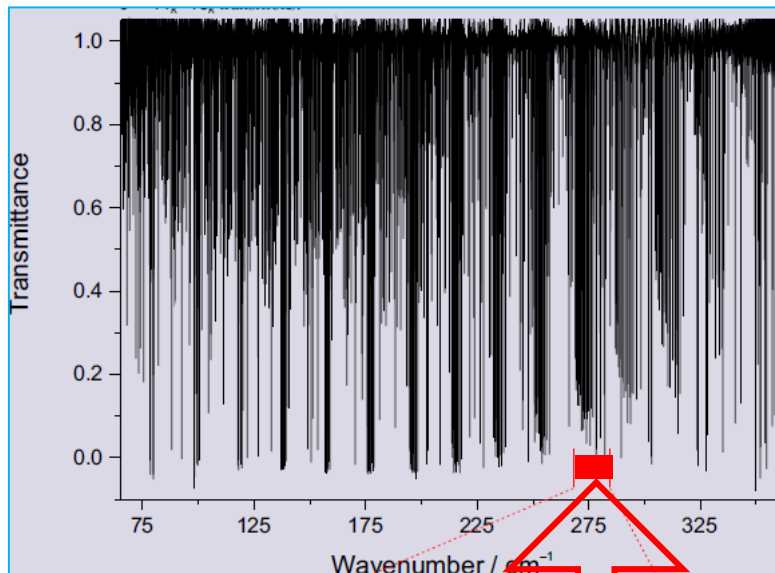
$$\left(\begin{smallmatrix} s \\ a \end{smallmatrix}\right) \langle v, J, K | H / hc | v, J, K \pm 6 \rangle \left(\begin{smallmatrix} s \\ a \end{smallmatrix}\right) = \left\{ {}^{(i)}\eta + {}^{(i)}\eta_J J(J+1) + {}^{(i)}\eta_K [K^2 + (K \pm 6)^2] \right\} F_{\pm 6}$$

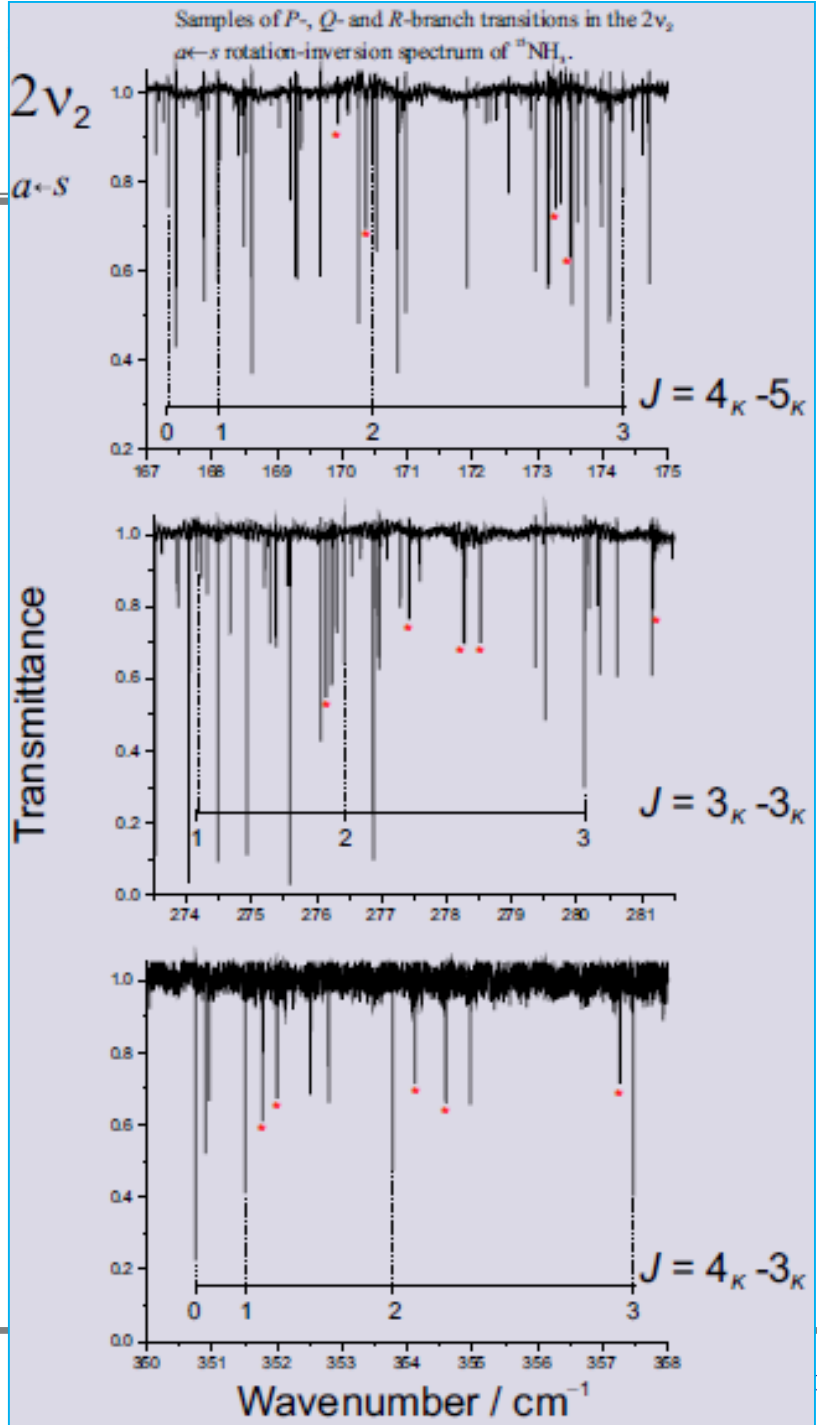
$${}^a F_{+n} = [J(J+1) - K(K \pm 1)]^{1/2} [J(J+1) - (K \pm 1)(K \pm 2)]^{1/2} \dots \{J(J+1) - [K \pm (n-1)](K \pm n)\}^{1/2}$$

Example of Spectra Analyzed in this Study

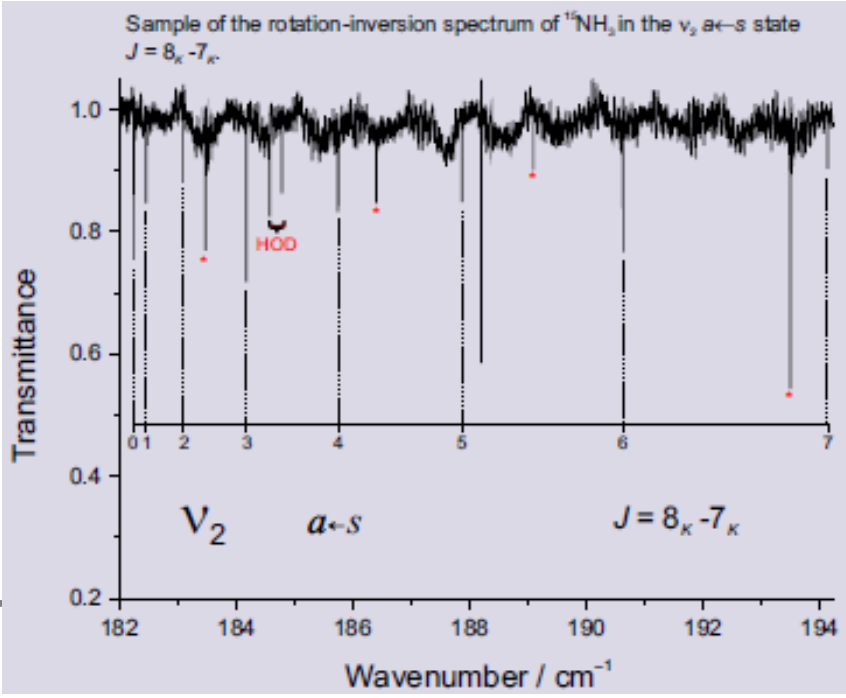
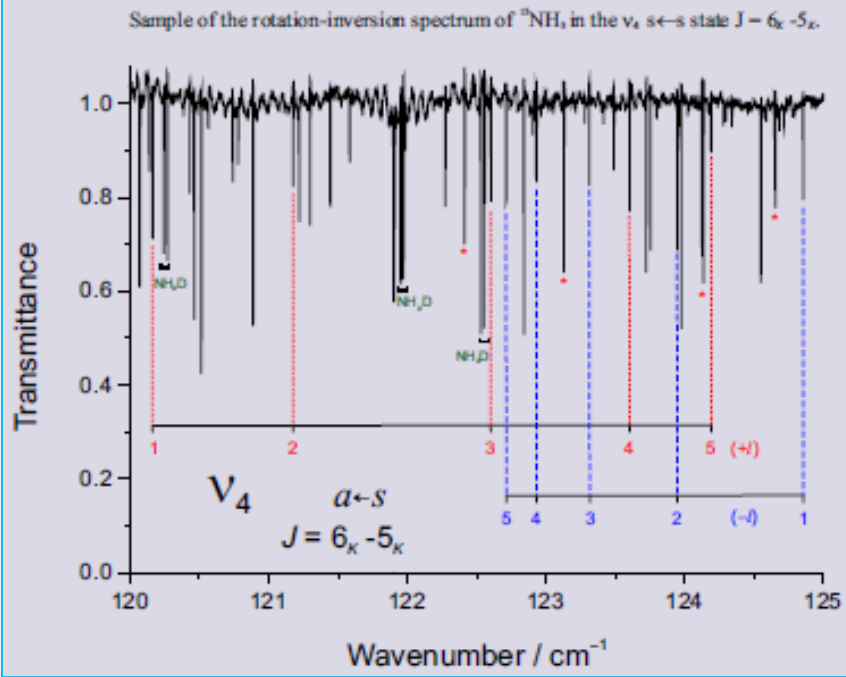


The far-infrared spectrum of $^{15}\text{NH}_3$, recorded using synchrotron radiation at the Canadian Light Source, Saskatoon, Canada. The bottom panel shows an enlarged section of the $J = 14_{\kappa} - 13_{\kappa}$ transitions.





**Examples
of
Spectra
Analyzed
in this
Study**





Observed Perturbation allowed $\Delta k = \pm 3$ transitions in the ground state up to $J = 10$



J	K	J	K		observed	J	K	J	K		observed	J	K	J	K		observed
4	0	3	3	a - a	112.2217	8	0	7	-3	a - a	189.5146	9	3	9	-6	s - s	97.11553
5	0	4	-3	s - s	131.8437	8	1	7	4	s - s	211.4348	9	-3	8	0	a - a	144.0887
5	1	4	2	a - a	109.7602	8	1	7	4	a - a	211.3065	9	4	8	1	s - s	122.6360
5	1	4	2	s - s	109.8208	8	1	7	2	a - a	167.8585	9	4	8	1	a - a	122.6451
5	-3	4	0	a - a	65.9114	8	2	8	5	s - s	75.80351	9	5	8	2	s - s	101.0645
6	0	5	-3	a - a	151.1470	8	2	7	1	s - s	146.3186	9	5	8	2	a - a	101.1013
6	1	5	4	s - s	173.3057	8	2	7	1	a - a	146.2798	9	6	8	3	a - a	79.39756
6	1	5	2	s - s	129.3188	8	2	7	5	a - a	233.2988	9	-3	9	6	a - a	96.98271
6	1	5	2	a - a	129.2549	8	3	7	6	a - a	255.5570	9	3	8	6	s - s	274.2817
6	-3	5	0	s - s	85.6074	8	-3	7	-6	s - s	255.7657	9	6	8	-3	s - s	79.33243
7	0	6	-3	s - s	170.5068	8	4	7	1	a - a	103.1120	10	0	9	-3	a - a	227.2037
7	1	6	2	s - s	148.6926	8	5	7	2	s - s	81.35313	10	1	9	4	s - s	248.8132
7	1	6	4	s - s	192.4580	8	-3	7	0	s - s	124.7274	10	1	9	2	s - s	205.9055
7	1	6	4	a - a	192.3235	9	0	8	-3	s - s	208.5423	10	1	9	2	a - a	205.8428
7	2	6	1	s - s	126.9523	9	1	8	2	s - s	187.0005	10	1	9	4	a - a	248.7005
7	2	6	1	a - a	126.9166	9	1	8	4	s - s	230.2241	10	2	9	5	s - s	270.5480
7	-3	6	-6	a - a	236.8087	9	1	8	2	a - a	186.9354	10	2	9	1	s - s	184.6119
7	-3	6	0	a - a	105.2169	9	1	8	4	a - a	230.1029	10	2	9	1	a - a	184.5708
7	4	6	1	s - s	83.4423	9	2	8	5	s - s	252.1149	10	2	9	5	a - a	270.4050
7	4	7	7	s - s	120.9681	9	2	8	5	a - a	251.9591	10	3	10	-6	a - a	96.22192
7	4	6	1	a - a	83.46845	9	2	8	1	s - s	165.5435	10	4	9	1	s - s	142.0483

Sample results ($^{15}\text{NH}_3$ Ground State)

Retrieved molecular ground state constants. The reported **uncertainties** in units of the last significant figure correspond to one standard deviation.

Parameters	Parameters	Parameters	Parameters
ΔE	0.75768574(119)		
$\Delta B \times 10^2$	-0.4928777(119)	B	9.92234818(258)
$\Delta C \times 10^2$	0.1921887(103)	C	6.22786179(482)
$\Delta D_J \times 10^4$	-0.1672699(392)	$D_J \times 10^3$	0.8517830(331)
$\Delta D_{JK} \times 10^4$	-0.4599043(839)	$D_{JK} \times 10^3$	-1.5845476(563)
$\Delta D_K \times 10^4$	-0.3140035(515)	$D_K \times 10^3$	0.917091(271)
$\Delta H_J \times 10^6$	-0.0393098(630)	$H_J \times 10^6$	0.241917(619)
$\Delta H_{JK} \times 10^6$	0.160910(203)	$H_{JK} \times 10^6$	-0.75800(558)
$\Delta H_{JKK} \times 10^6$	-0.217889(231)	$H_{JKK} \times 10^6$	0.83017(959)
$\Delta H_K \times 10^6$	0.0976399(911)	$H_K \times 10^6$	-0.31024(725)
$\Delta L_J \times 10^9$	0.069463(400)	$L_J \times 10^9$	-0.120960(579)
$\Delta L_{JK} \times 10^9$	-0.37864(173)	$L_{JK} \times 10^9$	0.45875(290)
$\Delta L_{JKK} \times 10^9$	0.76837(295)	$L_{JKK} \times 10^9$	-0.4914(134)
$\Delta L_{JKKK} \times 10^9$	-0.68721(226)	$L_{JKKK} \times 10^9$	0.975(191)
$\Delta L_K \times 10^9$	0.228450(667)	$L_K \times 10^9$	0.3520(441)
$\Delta M_J \times 10^{12}$	-0.08582(116)	$M_J \times 10^{12}$	0.046432(607)
$\Delta M_{JK} \times 10^{12}$	0.59092(621)	$M_{JK} \times 10^{12}$	0.0*
$\Delta M_{JKK} \times 10^{12}$	-1.6177(141)	$M_{JKK} \times 10^{12}$	-1.1071(291)
$\Delta M_{JKKK} \times 10^{12}$	-2.1912(167)	$M_{JKKK} \times 10^{12}$	2.828(110)
$\Delta M_K \times 10^{12}$	-1.4667(103)	$M_{KKK} \times 10^{12}$	-2.576(136)
$\Delta N_J \times 10^{15}$	0.38827(273)	$M_K \times 10^{12}$	0.0*
$\Delta N_{JK} \times 10^{15}$	0.05368(127)	N_J	0.0*
$\Delta N_{JKK} \times 10^{15}$	-0.4514(816)	N_{JKK}	0.0*
$\Delta N_{JKKK} \times 10^{15}$	1.5897(236)	N_{JKKK}	0.0*
$\Delta N_K \times 10^{15}$	-2.9286(385)	N_{JKKKK}	0.0*
$\Delta N_{KK} \times 10^{15}$	2.9918(378)	N_{JKKKK}	0.0*
$\Delta N_{KKK} \times 10^{15}$	-1.6085(221)	N_{KKKKK}	0.0*
$\Delta N_{KKKK} \times 10^{15}$	0.5600(616)	N_K	0.0*

Sample results ($^{15}\text{NH}_3$ v_2 state)

Retrieved molecular constants in the v_2 state. The reported **uncertainties** in units of the last significant figure correspond to one standard deviation.

Parameters	Parameters	Parameters	Parameters
ΔE	34.438608(397)		
ΔB	-0.1778174(235)	B	10.0489379(179)
ΔC	0.0696015(223)	C	6.1024541(795)
$\Delta D_J \times 10^3$	-0.438459(451)	$D_J \times 10^3$	1.141239(200)
$\Delta D_{JK} \times 10^3$	1.1196050(899)	$D_{JK} \times 10^3$	-2.448734(434)
$\Delta D_K \times 10^3$	-0.809650(613)	$D_K \times 10^3$	2.02175(702)
$\Delta H_J \times 10^6$	-0.64520(368)	$H_J \times 10^6$	0.582892(923)
$\Delta H_{JK} \times 10^6$	2.5596(112)	$H_{JK} \times 10^6$	-2.34591(350)
$\Delta H_{JKK} \times 10^6$	-3.3724(137)	$H_{JKK} \times 10^6$	3.09355(495)
$\Delta H_K \times 10^6$	1.46414(599)	$H_K \times 10^6$	-2.531(236)
$\Delta L_J \times 10^9$	0.5663(134)	$L_J \times 10^9$	-0.29598(165)
$\Delta L_{JK} \times 10^9$	-2.8098(562)	$L_{JK} \times 10^9$	1.7357(103)
$\Delta L_{JKK} \times 10^9$	5.262(101)	$L_{JKK} \times 10^9$	-3.4481(184)
$\Delta L_{JKKK} \times 10^9$	-4.2348(825)	$L_{JKKK} \times 10^9$	2.7781(132)
$\Delta L_K \times 10^9$	1.2118(285)	$L_K \times 10^9$	-38.50(290)
$\Delta M_J \times 10^{12}$	-0.2292(181)	$M_J \times 10^{12}$	0.0*
$\Delta M_{JK} \times 10^{12}$	1.2320(984)	$M_{JK} \times 10^{12}$	0.0*
$\Delta M_{JKK} \times 10^{12}$	-2.629(239)	$M_{JKK} \times 10^{12}$	0.0*
$\Delta M_{JKKK} \times 10^{12}$	2.172(302)	$M_{JKKK} \times 10^{12}$	0.0*
$\Delta M_{KKKK} \times 10^{12}$	-0.258(196)	$M_{KKKK} \times 10^{12}$	0.0*
$\Delta M_K \times 10^{12}$	0.2919(500)	$M_K \times 10^{12}$	39.67(749)

Results of Spectroscopic Analysis

- An analogous set of spectroscopic parameters was obtained for the inversion-rotation transitions in the $\nu_2 = 1$ state but the spectroscopic parameters must be considered as effective since the interaction of this state with $\nu_4 = 1$ was not taken into account. For the $\nu_4 = 1$ and $\nu_2 = 2$ states only a list of observed inversion-rotation transitions is reported.
- The analysis has been extended to all vibrational transitions falling below 2000 cm^{-1} , namely $\nu_2 \leftarrow \text{GS}$, $\nu_4 \leftarrow \text{GS}$ and $2\nu_2 \leftarrow \text{GS}$ and the hot bands $2\nu_2 \leftarrow \nu_2$, $\nu_4 \leftarrow \nu_2$ and $2\nu_2 \leftarrow \nu_4$.
- Transitions up to $J = 15$ have been identified and fitted, together with the rotation-inversion transition in all the excited states, using of a computer program based on an effective Hamiltonian which takes into account all symmetry allowed interactions between and within the excited states.
- About 6300 transitions have been observed, 5700 of these have been so far retained in the fit.

Conclusions and Directions for Future Work

- Transmission spectra in spectral range $60 - 2085 \text{ cm}^{-1}$ have been analyzed and the results for molecular constants are presented grouped by bands.
- We were also able to determine several molecular constants, among them are the rotational constant C and centrifugal distortion D_k and H_k parameters.
- Currently we are retrieving intensities for the newly assigned transitions. Of special interest are the observed forbidden transitions.

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