New Models of Ammonia Opacity Under Conditions Characteristic of the Jovian Atmosphere Using Strict Physical Principals

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March 11, 2016

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Introduction

- Several extensive laboratory studies have been conducted to measure the microwave opacity of ammonia.
- Both ammonia opacity models (Hanley et al. (2009) *Icarus* 202,316–335, Devaraj et al. (2014) *Icarus* 241, 165–179) give consistent results at temperatures up to 500 K (within 6%).
- Studies of the microwave emission made using these models indicate emission at 24– and 50–cm wavelengths originate from the deep atmosphere (T$>$ 600K).
- Both ammonia opacity models have been examined from a physical viewpoint and faults have been identified.
- A new model that addresses these physical faults has been developed.

Introduction

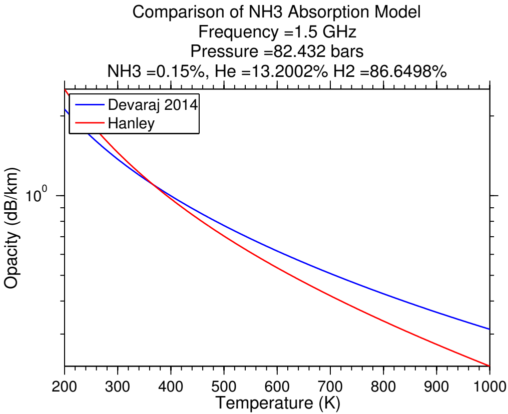


Figure: Comparison of the temperature dependence of the two different models for the microwave absorption of NH_3. Shown are the models from Hanley et al. (2009) and Devaraj et al. (2014).

Issues with the Hanley 2009 model

- No high pressure data was used in the model development.
  - Only pressures less than 12 bars are used in fitting the model.
- Only used one H_2/He mixing ratio (86.3%/13.7%)
  - While this is characteristic of Jupiter it does not fit for all outer planets.
  - Assumed Helium parameters are from Berge and Gulkis 1976 and were not directly measured.
- Uses an outdated line catalog.

Issues with the Devaraj 2014 model

- The temperature dependence of the coupling parameters (Z_i) are unnecessarily limited.
  - This limited the search space when minimizing the cost function
- The rotational line parameters are unnecessarily coupled to the inversion line parameters.
- In the high pressure inversion model, the shift parameter (δ_j) is positive.
  - This is nonphysical because inversion lines must be shifted negative with increasing pressure (Townes and Schawlow 1955).
- A significant discontinuity occurs at the pressure where the parameters are "switched".

Addressing these issues when creating a new model

- This new model uses all the data taken (Hanley et al. 2008, Devaraj et al. 2014, and our high temperature data from 2015).
    - This addresses the pressure and mixing ratio issues present in Hanley's model.
- The temperature dependence of the coupling parameters (Z_i) are unbounded (as suggested by P. Rosenkranz).
- The rotational line parameters are not coupled to those from the inversion lines when fitting the new model.
- The pressure switch present in the Devaraj model has been converted to a frequency switch with a **much** smaller discontinuity.
    - Two models have been created: one with a frequency switch and one without. This will be discussed later.

Fitting the Data

- The method used for data fitting was a L-BFGS-B optimization routine with a minimization function

$$\chi^2 = \frac{DW \times (\alpha_{measured} - \alpha_{model})^2}{\sigma^2_{measured}}$$

where

- DW is the data weight
- $\alpha_{measured}$ and α_{model} are the measured and modeled opacities
- $\sigma_{measured}$ is the measured uncertainty in opacity

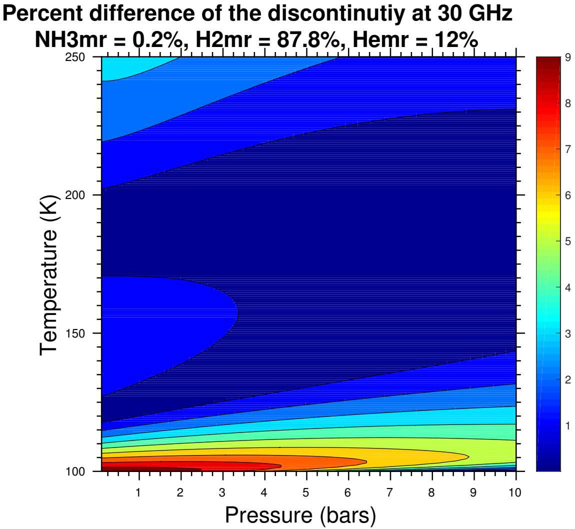
Fitting the Data for the Switch Model

- The data is split into two groups
  - Group I is all data where Frequency ≤ 24 GHz
  - Group II is all data where Frequency > 24 GHz
- The inversion lines are fit to a Ben-Reuven lineshape using data only from Group I.
- 2618 data points are used to fit the 14 free inversion parameters.
- The data in Group II was best fit with the low pressure model from Devaraj et al. 2014

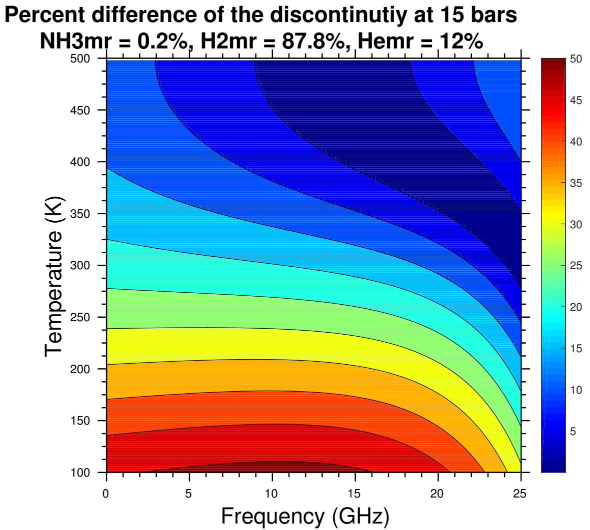
Optimizing the Frequency Switch

- It is necessary to find the frequency where the high frequency and low frequency models differ the least.
- Due to the asymmetry of the Ben-Reuven lineshape it was decided that the frequency switch should be in the range between 25–70 GHz.
- Using the weighting functions for the jovian planets at frequencies of 25–70 GHz the following parameter space was explored
  - Pressure: 0–7 bars
  - Temperature: 100–250 K
  - Ammonia Concentration: 0–0.2%
  - Helium Concentration: 10–20%
- A Monte-Carlo method was used to explore this search space and found that a 30 GHz switch had the smallest model discontinuity
  - On average the percent difference is on the order of 1.5%

Percent Difference at the Proposed Model's Switch



Percent Difference at the Devaraj Model's Switch



Fitting the Data for the No Switch Model

- The full data set is kept intact and not split into groups.
- The inversion lines are fit to a Ben-Reuven lineshape
- The rotational and roto-vibrational lines are fit to a modified Gross lineshape.
- 3631 data points are used to fit the 28 free parameters simultaneously.
    - 14 inversion parameters
    - 7 rotational parameters
    - 7 roto-vibrational parameters

Model Performance

Model	Cavity	FPR (22–40 GHz)	FPR (75–150 GHz)
Hanley 2009	95.88	86.0	13.03
Devaraj 2014	93.92	90.8	80.36
Bellotti Switch	95.94	89.2	80.36
Bellotti No Switch	90.57	84.8	76.70

Model	High Pressure	High Temperature	Total
Hanley 2009	65.14	100.00	64.31
Devaraj 2014	70.92	45.46	83.07
Bellotti Switch	70.32	100.00	83.68
Bellotti No Switch	70.23	81.82	80.39

The Statistical Difference Between the Switch and the No Switch Model

Model	All Data		Juno Data	
	Percent Fit	χ^2 Score	Percent Fit	χ^2 Score
Bellotti Switch	84.10%	38.10	84.45%	34.43
Bellotti No Switch	80.39%	41.42	81.40%	35.09

- A higher percent fit is better.
- A lower χ^2 score is better.

By both standards the model with a switch is better.

The Switch Model

Inversion Parameters for Frequency $\leq$ 30 GHz

	i=H_2	i=He	i=NH_3
γ_i	1.6937	0.6997	0.7523
Γ_i	0.8085	1.0	1.0
ζ_i	1.3263	0.1607	0.6162
Z_i	0.8199	-0.7269	1.3832
d		-0.0139	
D_{inv}		0.9619	

- Inversion Parameters for Frequency $>$ 30 GHz are the same as Devaraj et al. 2014 low pressure model.
- Rotational and Roto-Vibrational are the same as Devaraj et al. 2014.

Difference in nadir emission using different models for the microwave absorption of NH_3 (computed using JAMRT)

Frequency (GHz)	Nadir Brightness Temperature (K)		
	Hanley	Devaraj	Bellotti
0.6	932.81	895.27	903.47
1.25	538.2	525.91	527.23
2.6	346.92	346.70	347.17
5.2	266.50	264.70	266.09
10	210.89	208.57	210.20
22	137.83	137.79	138.01

NH_3 abundance: 166 ppm
H_2O abundance: 0.2%

Conclusion

A new model for ammonia opacity under jovian conditions has been developed which outperforms the two current models implemented in JAMRT while adhering to stricter physical principals.

New High-Temperature H_2O Vapor Measurements

Frequency (GHz)	Measured Absorption[1] (dB/km)	Modified Karpowicz Model (dB/km)
557	31312	26557
658	2258	585
752	23973	19840

Temperature:	773 K
Pressure:	1.013 bar
H_2O abundance:	77%

[1] Yuhui Song et al. "High-Temperature H_2O Vapor Measurement Using Terahertz Spectroscopy for Industrial Furnace Applications". In: *IEEE Transactions on Terahertz Science and Technology* 6.1 (2016), pp. 26–31.