The Search for Deuterium in Molecular Clouds and B Stars

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The deuterium/hydrogen ratio is an important variable in several cosmological models. Two projects were conducted to determine the D/H ratio. By taking optical spectra of slowly-rotating B stars, and comparing the intensity of the Hα and Dα Balmer lines, values or upper limits of the D/H ratio can be found. Data from observations of several B stars and the Orion Nebula were reduced using IRAF and compared to theoretical models. By analyzing radio spectra from deuterated molecules and correcting for chemical fractionation effects, another measurement of the D/H ratio can be obtained. We analyzed spectra from the nebulae Sgr A , using NRAO's Line reduction program, to find line strengths for these deuterated molecules. Preliminary analysis of the radio data showed a higher than expected deuterium abundance in the Galactic center.

Why Is Deuterium Important?

From 100 to 1000 seconds after the big bang, during the era of nucleosynthesis, hydrogen, helium, and some heavier isotopes, like deuterium, formed out of cooling matter. The amount of deuterium that survived was dependent on the baryonic density of the universe at that time: deuterium nuclei fused with hydrogen to form a helium isotope with only one neutron, so the greater the abundance of nucleons, the less deuterium would remain.

In an effort to determine whether or not deuterium has contemporary sources of production, observations at several places in the galaxy have been taken. If deuterium is purely primordial, astration should ensure a negative gradient in the deuterium abundance towards the relatively busy, dense galactic center, and if deuterium is formed in stellar processes, we should see the opposite distribution (Ostriker and Tinsley 1975).

Taken together with the predictions of current cosmological models, the hypothesis that deuterium is not manufactured in later stellar processes could prove useful. Determining the abundance of deuterium in the contemporary universe (and thus the baryon density) may produce evidence for either an open or closed universe model, and also aid in our understanding of the evolution of baryons (Pasachoff and Fowler 1973 and 1988).

Radio Data

We took radio spectra of the Sgr A and Sgr B2 molecular clouds with the NRAO 12 m millimeter-wave telescope at Kitt Peak, Arizona, on May 17-18, 1993 (Lubowich *et al.* 1994). Additional spectra were taken on June 29, 1993 by T. J. Balonek. We chose the positions within the Sgr A molecular cloud based on a prior low signal-to-noise detection of deuterated molecules by A. A. Penzias (1979) and on subsequent mapping of molecular abundances by Y. C. Minh, W. M. Irvine, and P. Friberg (1991).

We observed many molecular species, with frequencies ranging from 71 to 145 GHz, our prime target being the J=1 to J=0 transition of DCN (deuterated hydrocyanic acid) which occurred at 72.414 GHz. We also observed the DCN J=2 to J=1 transition, DNC, and a multitude of relevant comparison species — HNC, HCO+, $HC^{15}N$. We mapped DCN line strength in five positions surrounding the center of Sgr A. The mapping positions correspond to 1' offsets to the north, south, east, and west, and a 2' offset to the south. The other lines were observed at the center position only.

An estimate of the true D/H ratio can be made from the ratio of DCN to HCN only after applying theoretical fractionation corrections. Chemical fractionation, which refers to the preferences certain molecules have for certain isotopes, is strongly dependent on cloud kinetic temperature and electron density, which in turn depend on cloud density and cosmic ray ionization rate. Thus, by comparing many molecular species in clouds that are as similar as possible, we will be able to determine the galactic D/H gradient, without considering fractionation effects. If the D/H gradient is consistent with our necessary hypothesis that deuterium has no contemporary sources, then fractionation effects can be computed and used with these data to determine a true value for D/H.

In the case of deuterated molecules, fractionation works favorably for observers, enhancing abundances by a factor of 10 to 10^4 (Dalgarno and Lepp 1985; Opendak 1993) allowing DCN to be detected. HCN, however, is such a strong line that some self-shielding occurs, which could result in an erroneously high value of D/H. To alleviate this, we observed the J=1 to J=0 transition of the molecular isotope $H^{13}CN$, which is rare enough to prevent self-shielding from becoming a major problem. The conversion between DCN/$H^{13}CN$ and DCN/HCN is achieved by taking into account the fractional abundance of the isotopic species, which Penzias estimates to be 1/20 in the Sgr A molecular cloud.

We reduced all of the data using the NRAO spectral-line-analysis program **LINE** (for details, refer to *The Unipops Cookbook)*. Data from each filter bank were displayed and reduced separately. Bad channels were eliminated, and replaced with the average of the two neighboring channels. The average noise in regions without lines was then set to zero by subtracting a baseline from the spectrum. We chose the lowest order baseline (usually 0th order, sometimes 1st order) that produced a good fit, to avoid subtracting out weak spectral features. We then combined the corrected data of the same frequency. The root-mean-square (RMS) value, a measure of the noise, was computed in the regions used to fit the baseline.

Because of the increasing thickness of the atmosphere, scans taken at lower elevation were considerably noisier. In the spectra of the Sgr A center position at 72 GHz, the low elevation data were rejected because sufficient data with a much lower noise level had been obtained. When scans with similar noise levels were combined, the resultant noise appeared to decrease roughly as the square root of the number of scans combined, as expected. Data were rejected in one other instance, when one of the filter banks produced a line feature where no line had been before in some, but not all, of the 144 GHz scans. In this instance, only the affected portion of the scan was deleted.

When possible, the spectral features of the combined scans were fit with Gaussian curves. The fitting procedure returned values for the line center, the width at half maximum, and the peak intensity. For weaker lines, we integrated the signal over the same velocity ranges as exhibited in the strong lines. While the Gaussian approximation is adequate for strong lines, for weak lines, the integrated intensity values are much more accurate.

Preliminary analysis of the results reveal a much higher DCN line strength, and thus DCN/HCN ratio, than was anticipated. Our results improved on Penzias's 1-sigma detection of DCN in Sgr A. We measured peak intensities for the Sgr A center position that were approximately nine times greater than the noise level for the J=1 to J=0 transition, and three times above the noise level for the J=2 to J=1 transition. A more detailed analysis of our data is currently in progress.

Location	Molecule	Transition J=	Line Center (MHz)	Gaussian Intensity (K-km/s)	Integrated Intensity (K-km/s)	Width at Half Maximum (km/s)	RMS of Spectra (ΔTr^*)
Sgr A center	DCN	1-0	72415.8	1.99	1.82		
Sgr A center	DCN	2-1	144830.0	0.91	0.97	23.63	0.013
Sgr A North (1')	DCN	1-0	72411.9	0.62	0.50	59.09	0.013
Sgr A West (1')	DCN	1-0	72414.6	1.32	1.41	41.49	0.016
Sgr A East (1')	DCN	1-0	72419.5	1.41	0.83	44.00	0.019
Sgr A South (1')	DCN	1-0	72413.7	1.32	1.41	25.02	0.019
Sgr A South (2')	DCN	1-0	72414.8		0.37		
Sgr A Center	H^{13}CN	1-0 hyperfine	86336.4	19.38		20.36	0.023
Sgr A Center	H^{13}CN	1-0 hyperfine	86343.1	45.91		28.40	0.023
Sgr A Center	HCO$^+$	1-0	89184.7	76.88		25.73	0.023
Sgr A Center	DNC	1-0	76312.6	5.54	1.22	103.95	0.015
Sgr A Center	HNC	1-0 F=0-1	90660.5	46.03		20.03	0.023
Sgr A Center	HNC	1-0 F=1-1	90666.9	59.39		24.69	0.023

Optical Data

We re-reduced optical echelle spectra from slowly rotating early B stars which were reduced during last year's summer Keck exchange at Williams College, by W. Best, T. Ramond, and S. Sandys (Best, *et al.*, 1992). These stars (Tau Herculis, Iota Herculis, and 67 Ophiuchi) were chosen both because they rotated slowly, giving sharp spectral lines, and showed evidence of boron. Although boron is consumed in a star's core, these stars keep fragile metals like boron and deuterium fairly intact in their less violent upper atmospheres.

However, after reduction of the spectra Best, *et. al* discovered that these stars were also nonradial pulsators, stars that expand and contract in complex patterns, therefore producing erratic Doppler shifts in their spectra. Individual spectra thus could not be simply co-added. Using the

IRAF procedures **splot** and **imshift**, we accommodated for the shifts and produced sharper spectra than those of last year. The velocities of each star at the different times they were observed were also calculated (see graph).

Once we corrected the spectra to take into account the stars' nonradial pulsation, we fit our spectra to theoretical models provided by Dr. Monique Spite of l'Observatoire de Paris at Meudon, France; T. Ramond also worked with her. We show graphs of the spectrum of Tau Herculis and a blowup of the Dα region, plotted over three models for different deuterium abundances. The theoretical calculations show that the Dα line is surprisingly broad, spanning 1.5 angstroms. Thus, we expect to see a subtle depression in the spectrum over a wider range than the individual noise fluctuations; the S/N ratio in the spectra obtained during this observing run should be sufficient to resolve any deuterium present. However, some problems with our mathematical models persist, most notably an inaccuracy in the slope of the hydrogen line wings, where the Dα line should be. We thus need models with slightly different surface gravities and temperatures. Once these new models are available to fit our observations, we expect to determine if and how much deuterium is in the upper atmospheres of our program stars. We expect to be able to set an upper limit for D/H.

Another problem in observing these stars is that because of the Doppler shifts, the Dα line coincided with an atmospheric water line (the sharp spike in Figure 5). Although the Dα line is much larger than the telluric line, we undertook some preliminary work on finding other stars that lack this problem. One of our original program stars, Gamma Pegasi, may be better; we need observing time at a different time of year to observe it. A scheduled observing run in January 1994 should provide data from gamma Pegasi.

During January 1993, D. A. Lubowich, J. M. Pasachoff, S. Sandys, and A. Wong made echelle observations at Kitt Peak of the Orion Nebula and of the star Eta Leonis. Because of bad weather, there were not enough observations to reveal deuterium in either the emission spectra from Orion or the absorption spectra from Eta Leonis. Gamma Pegasi was unobservable. Just in case, and as a practice for subsequent reductions, we reduced the data using IRAF; as expected, the deuterium line did not show up in our spectra.

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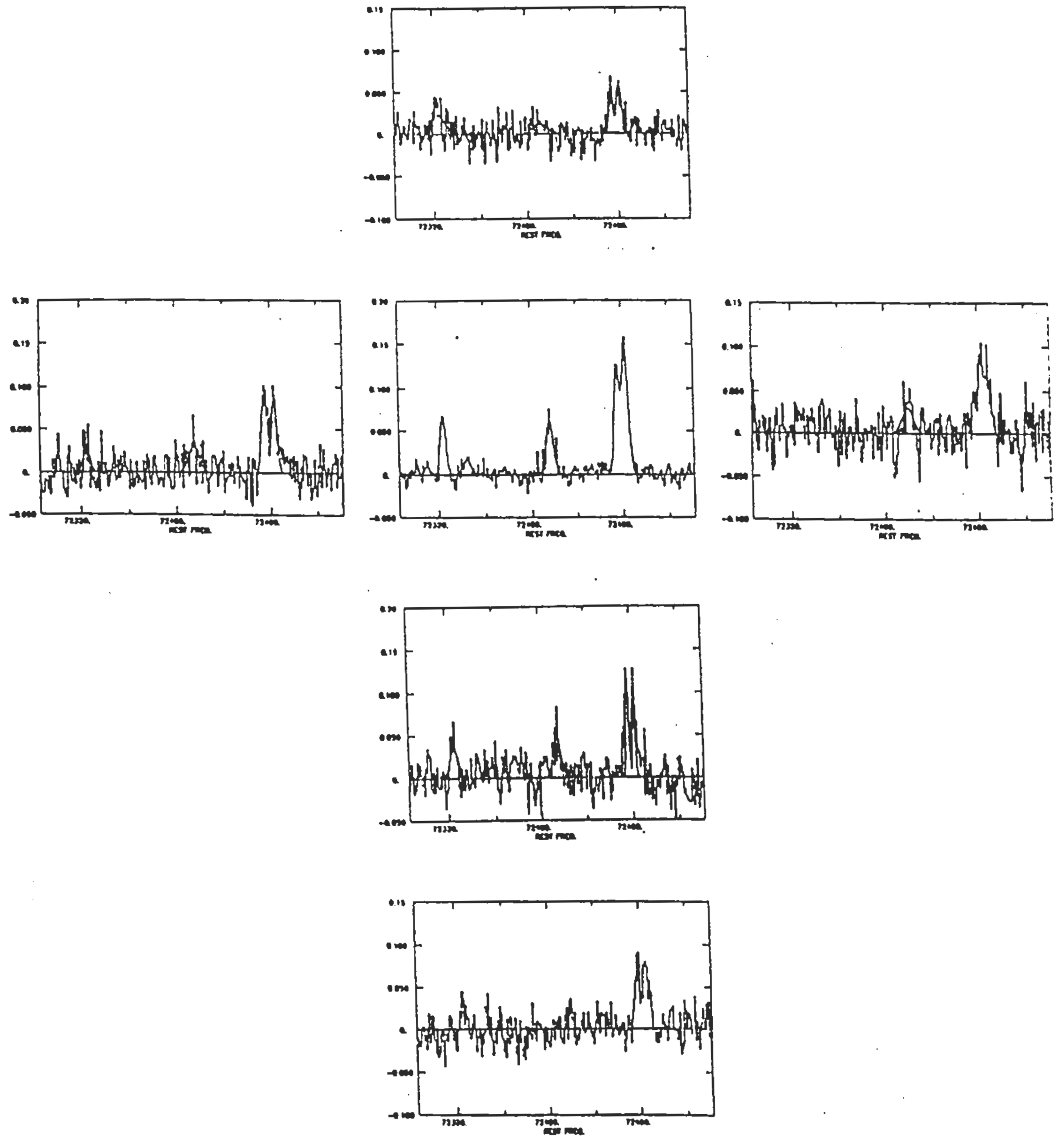

Figure 1. **Results of Mapping DCN**: The center scan is a product of 20 scans combined. The RMS of the center scan equals 0.007 K. The N, S, E, W positions correspond to 1' offsets from the center position of RA 17:42:42, DEC -28:58:00. The southernmost position represents a 2' offset from the center. All of the offset positions are the product of 6 scans combined. The RMS of the offset positions range between 0.013K and 0.019K.

gaussians. This scan, with RMS = 0.023, is the product of 6 scans combined.