

## 1,3-DIHYDROXYACETONE IN SAGITTARIUS B2(N-LMH): THE FIRST INTERSTELLAR KETOSE

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### ABSTRACT

We present here the results of an initial search for 1,3-dihydroxyacetone [or DHA,  $\text{CO}(\text{CH}_2\text{OH})_2$ ], the simplest ketose monosaccharide, toward the Sagittarius B2(N-LMH) hot core. Nine possible DHA emission lines have been observed with the Caltech Submillimeter Observatory, from which a rotational excitation temperature of  $220 \pm 65$  K and a beam-averaged column density of  $(4.9 \pm 2.2) \times 10^{15} \text{ cm}^{-2}$  are derived. If confirmed by additional observations, DHA would be among the most abundant complex molecules yet detected. DHA is not considered in any existing grain mantle or molecular cloud chemical model, highlighting the need for a more detailed investigation of the formation of prebiotic compounds in hot cores.

*Subject headings:* ISM: abundances — ISM: clouds — ISM: individual (Sagittarius B2(N-LMH)) — ISM: molecules — radio lines: ISM

*Online material:* color figure

### 1. INTRODUCTION

It is now widely believed that molecules important to the development of biological systems were delivered to the early Earth by planetesimals and their associated interplanetary dust particles (Oro 1961). Yet the degree of complexity reached by prebiotic organic chemistry before the formation of planetesimals and its impact on the evolution of planetary surfaces remains a mystery. Nearly 140 molecules, mostly organic, have been discovered in the interstellar medium (ISM), principally toward so-called hot molecular cores where the radiation and/or shocks from newly formed stars evaporate grain mantles and drive a complex gas-grain chemistry (Charnley 2001). Approximately 50 of these compounds have been seen in the comae of comets, and many biologically related monomers have also been detected in carbonaceous chondrites (Sephton 2002; Cooper et al. 2001). Observational searches for complex molecules in hot cores can therefore offer clues to the chemical links between these sources and meteorite, comet, or planet parent bodies.

Many of such spectral line searches have focused on the Sagittarius B2(N-LMH) source, which is found to have among the highest column densities of complex molecules ever detected. The discovery of the simplest  $\alpha$ -hydroxy aldehyde, glycolaldehyde ( $\text{CH}_2\text{OHCHO}$ ), toward this source (Hollis et al. 2000, 2004) opens the possibility for more complex organics being present in the ISM. Indeed, a suite of sugars and other polyhydroxylated compounds chemically related to glycolaldehyde has been found in aqueous extracts of the Murchison meteorite matrix (Cooper et al. 2001). Glycolaldehyde was found to be spatially extended in the Sgr B2(N-LMH) cloud relative to other complex organics (Hollis et al. 2001), a conclusion reinforced by the low-excitation temperature of the centimeter-wave transitions recently detected with the Green Bank Telescope (GBT; Hollis et al. 2004). Similar properties are exhibited by ethanol and acetaldehyde ( $\text{CH}_3\text{CH}_2\text{OH}$  and  $\text{CH}_3\text{CHO}$ , respectively; Martín-Pintado et al. 2001; Chengalur & Kanekar 2003) and suggest that these species are formed on grain mantles and liberated by shocks near the Galactic center (Hollis et al. 2004).

Glycolaldehyde is also much less abundant than its structural isomers acetic acid ( $\text{CH}_3\text{COOH}$ ; Snyder et al. 2002) and methyl formate ( $\text{HCOOCH}_3$ ; Hollis et al. 2000), especially in the warm, dense region that defines the Sgr B2(N-LMH) hot core, as might be expected since it is the least stable of the three isomers (methyl formate is the most stable). At present there are no hot core chemical models that can account for the formation of glycolaldehyde or any of the three-carbon (3C) and larger compounds seen in Murchison, and so the study of interstellar molecular complexity is largely guided by observational considerations. One such molecule is 1,3-dihydroxyacetone (DHA), or  $\text{CO}(\text{CH}_2\text{OH})_2$  (for a structure, see Fig. 1). DHA is a monosaccharide, or sugar, commonly used as the active ingredient in sunless tanning products. Monosaccharides are polyhydroxylated aldehydes (or aldoses, whose chemical formula is  $\text{H}-[\text{CHOH}]_k-\text{CHO}$ ) and ketones (or ketoses, whose general structure is given by  $\text{H}-[\text{CHOH}]_l-\text{CO}-[\text{CHOH}]_m-\text{H}$ ) with the general formula  $[\text{C}(\text{H}_2\text{O})]_n$ , where  $n \geq 3$ . DHA and glyceraldehyde ( $\text{CH}_2\text{OHCHOHCHO}$ ) are thus the simplest ketose and aldose monosaccharides, respectively. DHA is used in numerous biological pathways, including the production of ATP, and is synthesized via glycolysis.

As is true for the 2C organics, sugars are more energetic than esters and acids (hence their biological utility), while ketoses are more stable than aldoses. DHA would therefore be more likely to survive under hot core conditions than glyceraldehyde. Indeed, in the laboratory, glyceraldehyde is seen to isomerize to DHA (Lovas et al. 2003). Recent laboratory assignments of the rotational spectra of glyceraldehyde and DHA have provided the necessary basis for deep observational studies (Lovas et al. 2003; Widicus et al. 2004). The  $C_{2v}$  symmetry of DHA gives it somewhat stronger millimeter-wave emission features than glyceraldehyde. A glyceraldehyde *K*-band search with the GBT to an rms of  $\sim 5$  mK revealed no transitions (Hollis et al. 2004).

Here we present an initial survey of DHA transitions toward the Sgr B2(N-LMH) hot core. We choose this source because of its demonstrated molecular complexity and in order to place the abundance of DHA in chemical context, as the only reported searches for related species such as glycolaldehyde or glyc-

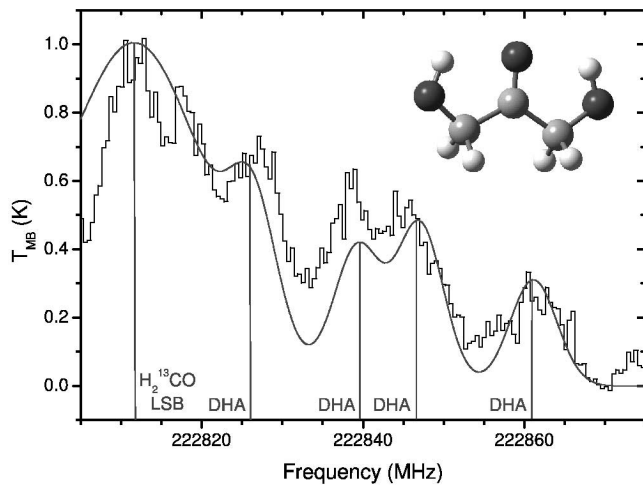


FIG. 1.—Simulated spectrum of 1,3-dihydroxyacetone (DHA) lines at 220 K compared to an observed Sgr B2(N-LMH) spectrum. The structure of DHA is shown in the inset. [See the electronic edition of the Journal for a color version of this figure.]

eraldehyde and other structurally similar complex organics such as ethylene glycol ( $\text{HOCH}_2\text{CH}_2\text{OH}$ ) and acetone [ $(\text{CH}_3)_2\text{CO}$ ] are toward Sgr B2(N-LMH). The observations are presented in § 2, while an analysis of the observed spectral lines is reported in § 3. The Letter concludes with a short discussion of the possible chemical implications of this work in § 4.

## 2. OBSERVATIONS

A search for DHA emission in the 1.3 mm atmospheric window was conducted with the Caltech Submillimeter Observatory (CSO). The parameters for the DHA lines used in this search, specifically the transition quantum numbers, rest frequencies, Einstein  $A$ -coefficients times the upper state degeneracy, and upper state energies, are listed in Table 1. All observed lines are transitions within the ground vibrational state. Many of these lines are actually asymmetry doublets or blends of multiple transitions between similar yet distinct quantum states that lie at nearly the same energy. These will appear in observational spec-

tra as a single blended line because of the  $\geq 10 \text{ km s}^{-1}$  line widths characteristic of Sgr B2. Only one frequency has been listed for asymmetry doublets occurring at the same frequency; for all others, the frequency of each individual component has been listed.

The survey was conducted using the CSO 230 GHz double-sideband (DSB) heterodyne receiver on the nights of 2003 July 13–23/September 14–21 and of 2004 June 30–July 7. Typical system temperatures ranged from 200 to 600 K, and the source position selected was  $\alpha(1950) = 17^{\text{h}}44^{\text{m}}10^{\text{s}}.1$ ,  $\delta(1950) = -28^{\circ}21'17''$ , which is coincident with the Sgr B2(N-LMH) hot core. The chopping secondary with a  $70''$  throw was used along with chopper-wheel calibration and the facility 1.5 GHz, 500 MHz, and 50 MHz acousto-optic spectrometer (AOS) back ends to minimize the spectral baseline fluctuations. The FWHM of the CSO at these frequencies is  $\sim 30''$ , and all data are placed on the  $T_{\text{MB}}$  temperature scale using a main-beam efficiency of 70% determined using observations of the planets. Line confusion was a perpetual difficulty that we faced during the observations due to the DSB setup of the CSO and the dense spectral nature of the Sgr B2(N-LMH) source. Line positions were therefore verified by observing at each local oscillator (LO) setting with several small frequency offsets. A  $v_{\text{LSR}}$  of  $62 \text{ km s}^{-1}$  was used for the 2003 July observations. Potential dihydroxyacetone lines were observed at  $64 \text{ km s}^{-1}$ , and so this  $v_{\text{LSR}}$  was then used for the remaining observations.

## 3. RESULTS

A total of nine possible DHA emission lines were detected with the CSO with a mean  $v_{\text{LSR}}$  of  $63.4 \pm 3.2 \text{ km s}^{-1}$ . The observational spectra from the 500 MHz AOS in the  $v_{\text{LSR}} = 0\text{--}100 \text{ km s}^{-1}$  window are shown in Figure 2. The  $v_{\text{LSR}}$  scales have been adjusted such that the LO frequency is centered at  $64 \text{ km s}^{-1}$ . Nine additional lines were either severely blended with other lines or completely obscured by stronger features in the signal or image sideband. No DHA lines were found to be absent from any clean 1.3 mm spectral windows observable at the CSO.

Least-squares Gaussian fits to each observed line are summarized in Table 1 and shown in Figure 2. The integrated in-

TABLE 1  
A SUMMARY OF DHA EMISSION LINES FROM SGR B2(N-LMH)

$\nu_0^a$ (MHz)	$J'_{K'_a, K'_c} - J''_{K''_a, K''_c}$	$Ag_u$ ( $10^2 \text{ s}^{-1}$ )	$E_u$ (K)	$T_{\text{MB}}^b$ (K)	$\Delta\nu^c$ ( $\text{km s}^{-1}$ )	$v_{\text{LSR}}^c$ ( $\text{km s}^{-1}$ )
219059.1 .....	$14_{1,3} - 13_{10,4}$	1.23	64.98	0.14	10.60(16)	62.91(17)
	$14_{1,4} - 13_{10,3}$	1.23	64.98			
222826.4 .....	$61_{3,58} - 60_{4,57}$	5.17	344.98	0.48	11.50(250)	64.50(21)
222839.4 .....	$61_{4,58} - 60_{3,57}$	5.71	344.98	0.39	7.74(224)	65.23(26)
222847.0 .....	$15_{11,4} - 14_{10,5}$	1.44	67.71	0.35	8.29(252)	60.74(40)
	$15_{11,5} - 14_{10,4}$	1.44	67.71			
222861.1 .....	$60_{5,56} - 59_{4,55}$	4.78	341.68	0.19	10.77(132)	63.24(42)
223293.9 .....	$63_{1,62} - 62_{2,61}$	6.78	349.60	0.40	17.36(64)	62.38(9)
	$63_{2,62} - 62_{1,61}$	6.78	349.60			
243591.0 .....	$67_{3,64} - 66_{4,63}$	8.53	412.61	0.24	13.12(51)	63.78(10)
243593.0 .....	$67_{4,64} - 66_{3,63}$	8.53	412.61			
254459.9 .....	$72_{1,71} - 71_{2,70}$	11.67	453.49	0.20	8.95(140)	65.86(19)
	$72_{2,71} - 71_{1,70}$	11.67	453.49			
261654.3 .....	$75_{0,75} - 74_{1,74}$	14.30	479.97	0.18	9.22(46)	62.31(12)
	$75_{1,75} - 74_{0,74}$	14.30	479.97			

<sup>a</sup>  $1 \sigma$  uncertainties are 0.1 MHz.

<sup>b</sup>  $1 \sigma$  uncertainties are  $< 10 \text{ mK}$ .

<sup>c</sup>  $1 \sigma$  uncertainties are listed in parentheses in units of last significant figure.

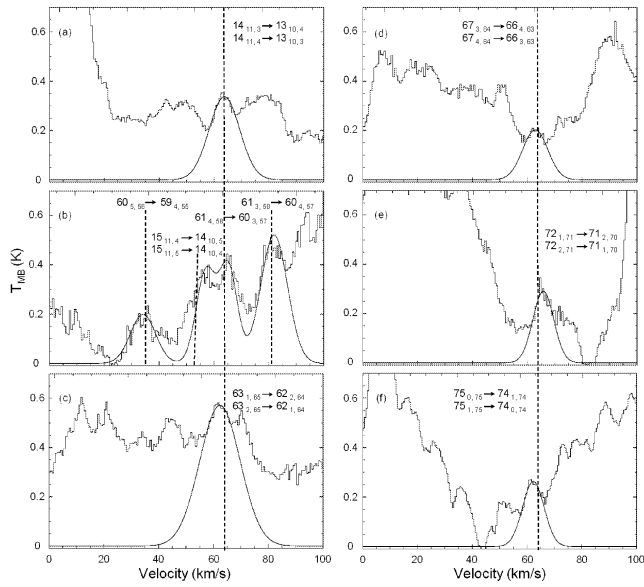


FIG. 2.—Possible DHA transitions observed toward Sgr B2(N-LMH) with the least-squares Gaussian fits to each line. Spectra are from the CSO 500 MHz AOS, and a linear baseline subtraction of the continuum has been performed. The vertical dotted line indicates  $v_{\text{LSR}} = 64 \text{ km s}^{-1}$ . (b) The positions of additional DHA lines relative to  $64 \text{ km s}^{-1}$  are indicated in the spectrum.

tensity was calculated using  $\int_{-\infty}^{\infty} T_b dv = 1.064 T_{\text{MB}} \Delta v$ , where  $T_{\text{MB}}$  is the peak line intensity corrected to the main-beam temperature scale ( $T_A^*/0.7$  for the CSO at 230 GHz) and  $\Delta v$  is the line width FWHM. No beam dilution corrections were applied because the spatial scale of the emission is unknown. Only single Gaussian fits are reported here since many of the potentially blended lines in Figure 2 are unassigned, and hence the relative contributions from individual features are poorly constrained.

A rotation-diagram approach was used to determine the rotational temperature and column density of DHA toward Sgr B2(N-LMH) in the limit of local thermal equilibrium and optically thin emission. The background radiation brightness has also been assumed to be negligible. Under these conditions the integrated intensity of a transition,  $\int_{-\infty}^{\infty} T_{\text{MB}} dv$ , is

$$\int_{-\infty}^{\infty} T_{\text{MB}} dv = \frac{hc^3}{8\pi k\nu^2} A g_u \frac{N_T}{Q(T_{\text{rot}})} e^{-E_u/kT_{\text{rot}}}, \quad (1)$$

where  $\nu$  is the transition frequency,  $N_T$  is the beam-averaged total column density (over  $\sim 30''$  here),  $A$  is the transition Einstein  $A$ -coefficient,  $g_u$  is the upper state degeneracy,  $Q(T_{\text{rot}})$  is

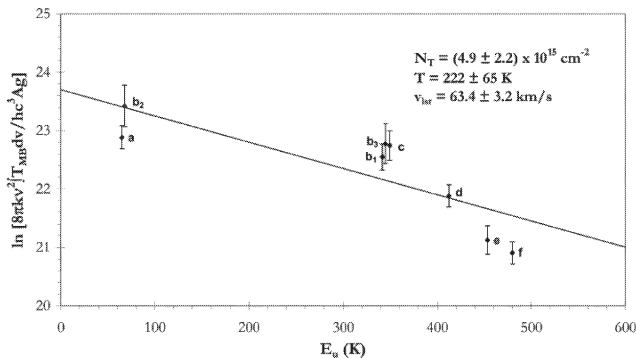


FIG. 3.—Rotation diagram for DHA toward Sgr B2(N-LMH). The labels correspond to the panels of Fig. 2.

the partition function,  $T_{\text{rot}}$  is the molecular rotational temperature, and  $E_u$  is the transition upper state energy (Nummelin et al. 1998b). Only the ground and first four DHA vibrational states are populated at  $T \lesssim 250 \text{ K}$ , and a full rotational analysis has been performed for these states (Widicus et al. 2004). The rotational constants determined for each vibrational state have therefore been used such that the partition function is approximated as

$$Q(T_{\text{rot}}) \approx \sum_{i=0}^4 e^{-E_i/kT_{\text{rot}}} \sqrt{\frac{\pi}{A_i B_i C_i}} \left( \frac{kT_{\text{rot}}}{h} \right)^3. \quad (2)$$

A plot of  $\ln [(8\pi k\nu^2)/(hc^3 A g_u) \int_{-\infty}^{\infty} T_b dv]$  versus  $E_u$  therefore gives a line with a slope inversely proportional to  $T_{\text{rot}}$  and with an intercept equal to  $\ln [N_T/Q(T_{\text{rot}})]$ . The rotation diagram for DHA is shown in Figure 3. A molecular rotational temperature of  $222 \pm 65 \text{ K}$  and a column density of  $(4.9 \pm 2.2) \times 10^{15} \text{ cm}^{-2}$  were derived, where the errors represent 95% confidence intervals.

Four lines corresponding to DHA transitions were observed in one window at the 222839.40 MHz LO setting (Fig. 2b); these data are shown in Figure 1 along with a  $T_{\text{rot}} = 220 \text{ K}$  simulated spectrum. The relative intensities, line-center frequencies, and line widths of the DHA lines were fixed, and the intensities scaled, to best match the observed spectrum. The additional strong line is due to  $\text{H}_2^{13}\text{CO}$  in the image sideband, and all parameters for this line were fixed to those determined by Nummelin et al. (1998a). The simulation shows that other unidentified spectral features may be present in the DSB spectrum and that the integrated intensity of the 222826.4 MHz DHA line is most affected by these features. It is therefore not included in the rotation-diagram analysis.

A spectral window overlapping in frequency with two strong dihydroxyacetone lines has also been observed in deep integrations with the Kitt Peak 12 m telescope (J. M. Hollis 2004, private communication). There are emission features at the appropriate frequencies for these DHA transitions, but one of the lines appears to be blended with an unidentified line. Their inclusion in the rotation-diagram analysis is quite difficult because of the lack of information regarding line widths for DHA emission features in this frequency range, and therefore these data have not been included in this study.

#### 4. DISCUSSION

These results are the first observational evidence for the presence of the 3C ketose 1,3-dihydroxyacetone in the ISM. The derived DHA excitation and velocity are in excellent agreement with other species detected in the Sgr B2(N-LMH) hot core, for which the most commonly quoted rotational temperature and  $v_{\text{LSR}}$  are 200 K and  $64 \text{ km s}^{-1}$ , respectively (see Liu et al. 2001 and references therein). The derived DHA column density of  $(4.9 \pm 2.2) \times 10^{15} \text{ cm}^{-2}$  does lead to interesting questions about the formation of and subsequent behavior of this molecule in the hot core, however. Emission from the high-excitation lines of methyl formate, acetic acid, ethyl cyanide ( $\text{CH}_3\text{CH}_2\text{CN}$ ), dimethyl ether ( $\text{CH}_3\text{OCH}_3$ ), and acetone [ $(\text{CH}_3)_2\text{CO}$ ] is known to be compact with respect to the CSO beam (see Snyder et al. 2002 and references therein). If similar filling factors are used for DHA, then it would be more abundant than any of these compounds except dimethyl ether. Both the chopping scheme and the higher frequencies of CSO observations render them insensitive to spatial distribution for extended, low-excitation emission as is seen from molecules such as acetaldehyde, ethanol,

and glycolaldehyde. Direct comparisons show that these molecules are also less abundant than DHA.

A further complication is the inconsistent treatment of the partition functions of complex molecules. Typically only the ground vibrational state is included in partition function calculations as laboratory characterizations of excited states are often incomplete. The inclusion of vibrational state terms can greatly affect the derived total column densities of complex species under hot core conditions. For a molecule like glycolaldehyde, the inclusion of torsional states increases the partition function by ~50% at 200 K, but they can be safely ignored below 50 K (Widicus Weaver et al. 2005). The exclusion of excited vibrational state terms in the DHA analysis would lower the column density by ~60%.

Nevertheless, DHA would be among the most abundant complex molecules in the Sgr B2(N-LMH) hot core should the present analysis be confirmed by further observations, and so an efficient formation route must exist. No quantitative chemical scheme for the production of species such as glycolaldehyde and DHA has been presented. Observations of complex molecules toward low-mass protostars where the dynamical timescales are short (Schöier et al. 2002; Cazaux et al. 2003) and careful studies of the potential reactions leading to HCOOCH<sub>3</sub> all seem to point toward a grain mantle synthesis (Horn et al. 2004). In this regard it is intriguing to note that, with appropriate rearrangements, all of these species can be formed from reactions involving the abundant grain mantle constituents CO, HCOOH, and CH<sub>3</sub>OH or their radical precursors.

Survivability in hot cores may be another important aspect of DHA chemistry. As a ketose, it is both thermodynamically more stable and less reactive than both glycolaldehyde and glyceraldehyde in hot gas. Isomerism in 3C and larger compounds is also quite extensive, and both dimethyl carbonate [(CH<sub>3</sub>O)<sub>2</sub>CO] and methyl glycolate (CH<sub>3</sub>OCOCH<sub>2</sub>OH) are even more stable than DHA. These isomers would likely be created by any surface chemistry leading to sugars. The microwave spectrum of methyl glycolate is known (Brochu & Buckley 1973), and the microwave spectrum of dimethyl carbonate as well as the (sub)millimeter spectra of both species have recently been obtained in our laboratory. Observational searches for these molecules are planned for the upcoming observing season, and the relative abundances of the 3C compounds should place stringent constraints on their possible formation routes.

The spectral characteristics of asymmetric rotors such as DHA make a definitive interstellar detection quite difficult. While some spectral windows contain multiple emission lines, most contain only one strong line due to the relatively large spacing between adjacent *K* levels within a given *J* state. It can be argued that many of the isolated features presented here could arise from other unidentified species or from the excited vibrational state lines of previously detected molecules. This argument is countered by the striking similarity between the observed and simulated spectra shown in Figure 1. This degree of coincidental overlap with other hot core species in both rest frequency and intensity is unlikely, but additional observations are clearly warranted.

Combined centimeter+millimeter observations are particularly powerful, and additional DHA observations with the GBT are planned for winter 2005. Other molecules observed in Sgr B2(N-LMH) show two-component behavior in which higher energy transitions give characteristic hot core temperatures but in which lower energy transitions yield much colder excitation temperatures. It is thought that these lower energy states are populated in an extended, potentially subthermal, source, possibly formed by shock-liberated grain mantle ices (Martín-Pintado et al. 2001; Hollis et al. 2004). DHA should demonstrate such behavior if it is produced by a grain surface mechanism, and so the GBT observations should offer considerable insight into the formation of this molecule. The determination of the spatial scale of DHA emission toward Sgr B2(N-LMH) is another important step in the characterization of this molecule, and further aperture synthesis observations to this end are underway.

We are grateful to J. M. Hollis, L. E. Snyder, S. Y. Liu, and A. R. Remijan for their advice and guidance during the completion of this project, especially in regards to the complex velocity fields of Sgr B2(N-LMH). We would also like to thank S. Bisschop, R. Braakman, A. Boogert, and A. Walsh for their assistance as backup observers at the CSO, and B. Drouin for his insight into molecular partition functions. We gratefully acknowledge the patience and generosity of the CSO TAC and would like to thank the CSO staff for their support during observations. Observations with the CSO are supported by NSF grant AST-0229008; additional support was provided by the NASA Exobiology and SARA programs, grants NAG5-8822 and NAG5-11423.

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ERRATUM: “1,3-DIHYDROXYACETONE IN SAGITTARIUS B2(N-LMH): THE FIRST INTERSTELLAR KETOSE”  
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The Einstein  $A$ -coefficients times the upper state degeneracy values ( $Ag_u$ ) in Table 1 were calculated incorrectly because of an inconsistency in the partition functions used to generate the spectral predictions presented in the laboratory work (S. L. Widicus, R. Braakman, D. R. Kent IV, & G. A. Blake, *J. Mol. Spectrosc.*, 224, 101 [2004]) and in the submillimeter and microwave spectral line catalog available at <http://spec.jpl.nasa.gov> (H. M. Pickett, R. L. Poynter, E. A. Cohen, M. L. Delitsky, J. C. Pearson, & H. S. P. Muller, *J. Quant. Spectrosc. Radiat. Transfer*, 60, 883 [1998]). We thank J. M. Hollis for bringing this discrepancy to our attention. The correct  $Ag_u$  values are reported in Table 1 below.

This correction increases the quantity  $\ln [(8\pi k\nu^2)/(hc^3Ag_u)] \int_{-\infty}^{\infty} T_b dv$  by roughly a factor of 3 and therefore shifts the points on the rotation diagram (Fig. 3) upward, leading to a revised DHA column density of  $(1.54 \pm 0.75) \times 10^{16} \text{ cm}^{-2}$ . This increase in the column density further strengthens the conclusion that, if confirmed, DHA would be among the most abundant complex molecules in the Sgr B2(N-LMH) hot core.

TABLE 1  
 A SUMMARY OF DHA EMISSION LINES FROM SGR B2(N-LMH)

$\nu_0^a$ (MHz)	$J'_{K'_a, K'_c} - J''_{K''_a, K''_c}$	$Ag_u$ ( $10^{-2} \text{ s}^{-1}$ )	$E_u$ (K)	$T_{\text{MB}}^b$ (K)	$\Delta\nu^c$ ( $\text{km s}^{-1}$ )	$v_{\text{LSR}}^c$ ( $\text{km s}^{-1}$ )
219059.1 .....	$14_{11,3} - 13_{10,4}$ $14_{11,4} - 13_{10,3}$	0.41 0.41	64.98 64.98	0.14	10.60(16)	62.91(17)
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223293.9 .....	$63_{1,62} - 62_{2,61}$ $63_{2,62} - 62_{1,61}$	2.24 2.24	349.60 349.60	0.40	17.36(64)	62.38(9)
243591.0 .....	$67_{3,64} - 66_{4,63}$	2.55	412.61	0.24	13.12(51)	63.78(10)
243593.0 .....	$67_{4,64} - 66_{3,63}$	2.55	412.61			
254459.9 .....	$72_{1,71} - 71_{2,70}$ $72_{2,71} - 71_{1,70}$	3.85 3.85	453.49 453.49	0.20	8.95(140)	65.86(19)
261654.3 .....	$75_{0,75} - 74_{1,74}$ $75_{1,75} - 74_{0,74}$	4.72 4.72	479.97 479.97	0.18	9.22(46)	62.31(12)

<sup>a</sup> 1  $\sigma$  uncertainties are 0.1 MHz.

<sup>b</sup> 1  $\sigma$  uncertainties are <10 mK.

<sup>c</sup> 1  $\sigma$  uncertainties are listed in parentheses in units of last significant figure.

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