Herschel/HIFI Discovery of a Far-Infrared DIB Analog†,‡

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Abstract. The *Herschel* Space Observatory carried out observations at far-infrared wavelengths, which significantly increased our knowledge of the interstellar medium and the star-formation process in the Milky Way and external galaxies, as well as our understanding of astrochemistry.

Absorption features, known, e.g., from observations at millimeter wavelengths, are more commonly observed in the far-infrared, in particular toward strong dust continuum sources. The lowest energy transitions are not only observed at LSR-velocities related to the source, but often also at velocities associated with diffuse molecular clouds along the line of sight toward the background source.

Unbiased spectral line surveys of the massive and very luminous Galactic Center sources Sagittarius B2(M) and (N) were carried out across the entire frequency range of the high-resolution Heterodyne Instrument for Far-Infrared Astronomy (HIFI). An absorption feature was detected toward both sources at about 617.531 GHz, corresponding to 20.599 cm^{-1}, 485.47 μm, or 2.5539 meV. This feature is unique in its appearance at all velocity components associated with diffuse foreground molecular clouds, together with its conspicuous absence at velocities related to the sources themselves. The carriers of at least a substantial part of the DIBs are thought to reside in the diffuse interstellar medium. Therefore, we consider this absorption feature to be a far-infrared DIB analog.

Subsequent dedicated observations confirmed that the line is present only in the foreground clouds on the line of sight toward other massive star-forming regions in the Galactic disk. There is indication that the feature has substructure, possibly of fine or hyperfine nature. Attempts to assign the feature to atomic or molecular species have been unsuccessful so far.

Keywords. Submillimeter: ISM, ISM: lines and bands, ISM: clouds, Line: identification

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† *Herschel* is an ESA space observatory with science instruments provided by European-led Principal Investigator consortia and with important participation from NASA.

‡ Note added in proof: M. Barlow *et al.* recently detected the same line toward a supernova remnant with the identification as the ground state rotational transition of ^{36}ArH$^+$ ("The Universe Explored by *Herschel*", Oct. 15−18, Noordwijk, the Netherlands). While the line is no longer unidentified, all other aspects of the discussion presented here remain valid. The correct assignment was confused by the fact that terrestrial Ar consists predominantly of ^{40}Ar, which, however, originates predominantly from the radioactive decay of ^{40}K. In addition, the initial CDMS entry of ^{36}ArH$^+$ was incorrect.

1. Introduction

The Herschel Space Observatory was launched on May 15 2009 to carry out spectroscopic and imaging observations at far-infrared wavelengths. The satellite is named after Sir William Herschel who discovered the infrared radiation. The mirror was 3.5 m in diameter and was the largest space-based single piece telescope dish and was equipped with three instruments (Pilbratt *et al.* 2010). The Heterodyne Instrument for Far-Infrared Astronomy (HIFI; de Graauw *et al.* 2010) was the most important instrument for frequency-resolved spectroscopic observations. It covered most of the $480-1910$ GHz (or $625-157$ μm) region in several sub-bands. It has a very high standard resolving power of $\sim 10^7$ (~ 1 MHz) and an optional high-resolution mode. SPIRE and PACS are imaging instruments and low-resolution spectrometers covering $670-57$ μm.
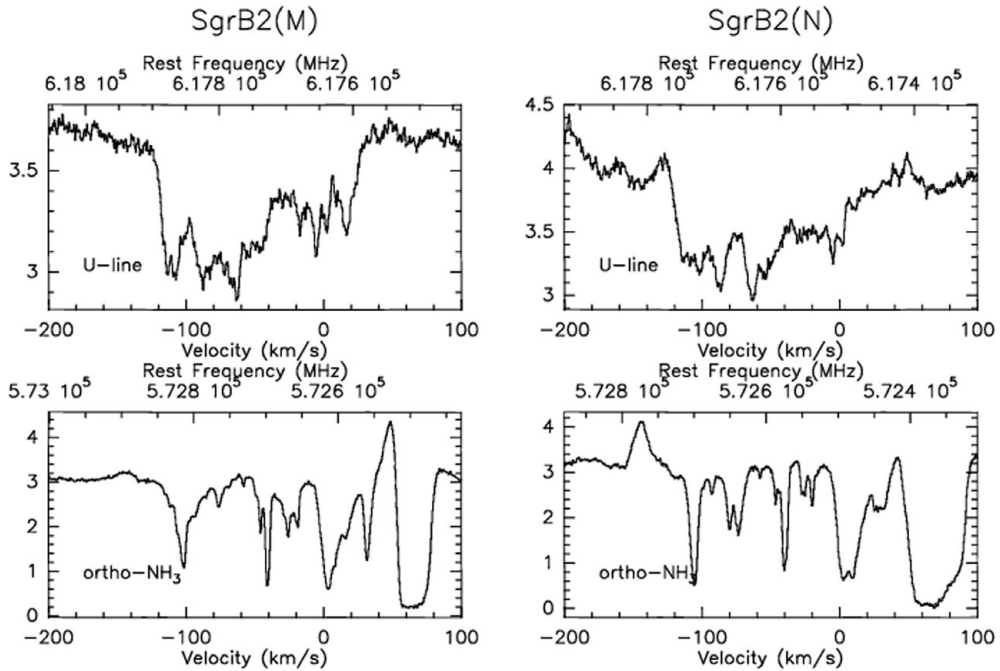
Prior to *Herschel*, the far-infrared region has been largely unexplored, even though there had been earlier missions, such as KAO, IRAS, ISO, SWAS, or Odin. This region can be accessed only to a limited extent from ground, even at elevated sites, because of the strong water and, to a lesser extent, O_2 absorptions.

The most important species studied with *Herschel* is water, including various isotopic variants, and in particular its low-energy rotational transitions. Atomic fine structure lines of C^+, a major cooling line of the ISM, or of N^+ or O were also frequent targets. Other, very important molecules are light hydrides, such as CH^+, CH, NH, NH_2, NH_3, OH, H_3O^+, HF, H_2S, and HCl. All of them had been detected in space before, but usually only to a limited extent, as the important rotational transitions occur in the HIFI frequency range, and in some cases even higher. The cationic hydrides H_2O^+ (Ossenkopf *et al.* 2010), H_2Cl^+ (Lis *et al.* 2010), and HCl^+ (De Luca *et al.* 2012) were detected with *Herschel* for the first time in the ISM. OH^+ (Wyrowski *et al.* 2010) and SH^+ (Menten *et al.* 2011) were detected with the Atacama Pathfinder EXperiment (APEX) from ground shortly before the launch of *Herschel*, and SH (Neufeld *et al.* 2012) was detected with the Stratospheric Observatory For Infrared Astronomy (SOFIA), because its ground state transition can not be observed with HIFI. OH^+, H_2O^+, and many other light hydrides were even seen in extragalactic sources. High-energy rotational transitions of molecules containing two non-hydrogen atoms were also important targets in dedicated observations. Examples include CO, which is usually seen as a good tracer of H_2 in dense parts of molecular clouds, SiO, a shock-tracer, HCN, HCO^+, and CCH.

Investigations into the molecular complexity of diverse types of sources such as star-forming regions, late-type stars, or external galaxies, through unbiased line surveys, were very important spectroscopic goals of the *Herschel* mission. Two such line surveys, toward the massive and very luminous Galactic Center sources Sagittarius B2(M) (Sgr B2(M) for short) and (N) revealed an unusual and unidentified absorption feature whose carrier is present at all velocities related to diffuse molecular clouds on the line of sight toward either source, but apparently completely absent at velocities associated with either source.

2. Observations of a U-line in absorption associated with the diffuse ISM only

The HEXOS (*Herschel*/HIFI Observations of Extraordinary Objects; Bergin *et al.* 2010) key program is concerned with unbiased molecular line surveys of star-forming regions in Orion and Sgr B2 covering the entire frequency range of the HIFI instrument. Two of the sources studied are Sgr B2(M) and (N). They are among the most massive and luminous star-forming regions in the Milky Way, located close to the Galactic Center. As both are strong continuum sources, especially at far-infrared wavelengths, atomic

SgrB2(M)

Rest Frequency (MHz)
6.18 10^5 6.178 10^5 6.176 10^5

U−line

Velocity (km/s)

Rest Frequency (MHz)
5.73 10^5 5.728 10^5 5.726 10^5

ortho−NH$_3$

Velocity (km/s)

SgrB2(N)

Rest Frequency (MHz)
6.178 10^5 6.176 10^5 6.174 10^5

U−line

Velocity (km/s)

Rest Frequency (MHz)
5.728 10^5 5.726 10^5 5.724 10^5

ortho−NH$_3$

Velocity (km/s)

Figure 1. Absorption features observed toward Sagittarius B2(M) (left) and (N) (right). The upper panels show absorption of an unidentified species, the lower show absorption of the ground state $J = 1 - 0$ transition of NH$_3$. Note: whereas NH$_3$ shows largely saturated absorption at velocities of around 70 km/s, which are due to the envelope of Sgr B2, there is no such absorption visible for the unidentified species. It only shows absorption in the diffuse spiral arm clouds between the sources and Earth which occur at velocities between about -110 and 40 km/s, also seen in the case of NH$_3$. The very small feature at highest frequencies, at a velocity of almost -120 km/s, is caused by a transition of methyleneimine.

and molecular lines are not only seen in emission, but also frequently in absorption (e.g. Neill *et al.* 2012 for Sgr B2(N)). Absorption features caused by low-lying rotational transitions show frequently not only absorption at velocities associated with the source, but also at velocities related to diffuse clouds on the sight-line toward the source, as can be seen for the ground state $J = 1 - 0$ transition of NH$_3$ in the lower panels of Fig. 1. The saturated absorption around 70 km/s is associated with the Sgr B2 complex. The weaker, but often still very pronounced absorption features between -110 km/s and about 40 km/s are caused by diffuse foreground clouds. The absorption features are fairly well separated, so that individual velocity components can be attributed to certain spiral arms of the Milky Way, as has been done for observations of SH$^+$, ^{13}CH$^+$, H^{13}CO$^+$, and c-C$_3$H$_2$ toward Sgr B2(M) (Menten *et al.* 2011). Ammonia is a tracer of the denser ISM, as are e.g. the related NH$_2$ and NH radicals. Therefore, its absorption at velocities associated with the two sources is very much stronger than that at velocities associated with diffuse clouds on the line of sight. The ground state transitions of species such as CH, HF, or H$_2$O trace H$_2$ well in the molecular as well as atomic diffuse medium. The cationic radicals OH$^+$ and H$_2$O$^+$, in contrast, are tracers of the mostly atomic diffuse ISM (Neufeld *et al.* 2010, Hollenbach *et al.* 2012). Such molecules display usually broader absorption features, and the absorption depths at velocities related to the source may be weaker than those at velocities related to diffuse clouds.

One absorption feature, detected in both line surveys of Sgr B2(M) and (N) near 617.5 GHz, was very different. As can be seen in the upper panel of Fig. 1, there appears to be no absorption present at velocities associated with either source, but absorption is present at all velocities associated with diffuse clouds along the sight-line toward the sources. No other absorption feature in either of the line surveys shows a similar behavior. Moreover, we do not know of any other source for which radio astronomical observations at other frequencies have produced an absorption with similar pattern. The absorption is rather broad toward both sources, thus it is difficult to judge if the U-line has some intrinsic sub-structure cause, e.g., by fine structure (FS) or hyperfine structure (HFS).

It was obvious to ask if this absorption feature is specific to Galactic Center sources, such as Sgr B2(M) and (N). Further observations of this U-line were, therefore, made within the framework of the PRISMAS (PRobing InterStellar Molecules with Absorption line Studies; e.g. Neufeld *et al.* 2010) key program. In particular, low-lying rotational transitions of light hydride species were observed toward strong continuum sources. The U-line could be targeted toward some of the sources, and it was detected weakly with reasonable to good signal-to-noise ratio toward four sources: W51, W49, W31C, and G34.3+0.1. The U-line was detected in all velocity components associated with diffuse clouds along the sight-line toward all sources, but again showed no absorption at velocities related to the source. Moreover, absorptions toward some of the sources suggest the U-line may consist of two, possibly three components which may be caused by FS or HFS.

3. Attempts to assign the carrier of the U-line

Considering that *Herschel* has observed spectroscopically for the most part rotational transitions of mainly fairly small molecular species and to a lesser extent FS transitions of relatively light atoms or rovibrational transitions of the C_3 molecule, and considering the low temperatures of the diffuse ISM, one expects the carrier of the U-line to be a fairly light atomic or molecular species, and the transition most likely a FS transition in the former case and a rotational transition in the latter. However, electronic or rovibrational transitions should not be excluded immediately.

FS splittings of atoms in their ground electronic state are larger than 620 GHz for the most part, including those of cations, exceptions are B and the ground state transition of C. FS transitions of atoms in electronically excited states may be an option, but only if the electronic states are metastable and presumably not too high in energy. The metastable ^2D splitting of O^+ is quite close, 593.89 (18) GHz (Sharpee *et al.* 2004), but not close enough. Other promising candidate transitions have not been found thus far.

Molecules in singlet electronic states with small HFS splitting are potential candidates. Molecules in doublet or higher states are only possible if the FS and HFS splitting is sufficiently small, or if the FS is so large that only the lowest spin-level is populated in the upper and lower rotational state.

Diatomic hydrides are frequently too light, as even the ground state rotational transition of HCl is too high in frequency, that of ArH^+ is slightly too low, and those of AlH and SiH^+ are far too low. In the case of molecules in a doublet or higher electronic state, even heavier molecules are required.

There are three ground state transitions in triatomic hydrides, because of the spin-statistics (*ortho/para*). Therefore, two have to fall out of the *Herschel*/HIFI frequency range. Moreover, the frequencies of H_2F^+ are too high, but those of SiH_2 are too low. Even larger hydrides are too heavy, unless they undergo large amplitude motions, such as NH_3 or H_3O^+. But the spectra of vaguely plausible candidates, such as H_5^+ or CH_5^+ are not known well enough.

Non-linear molecules of the type HAB, with A and B being light non-hydrogen atoms, are a distinct possibility. E.g., in the case of HNO, the *b*-type ground state transition occurs at 592.934 GHz. However, even for such a light molecule, $J = 1$ may be populated significantly at 2.725 K. Subthermal excitation may explain a potential non-detection of an associated $J = 1$ transition. Obviously, molecules with more atoms, such as HNCO, are unlikely because several rotational levels are populated. In none of the categories, plausible candidates have been found, therefore, we assume a molecular carrier in a metastable electronic state or a very exotic species.

4. The relation of the U-line to the DIBs

If we take into account that the Diffuse Interstellar Bands draw their name from their diffuse, i.e. fairly broad, appearance in the spectra recorded toward stars, one may ask how the present U-line relate to the DIBs. The U-line is broader than absorption features of species such as NH_3, which originate from the denser ISM, but this applies also to other absorption features of species present only in the more atomic diffuse ISM.

Even though the DIBs have been known for more than 100 years and more than 500 DIBs are currently known, comparatively little is known about their carriers (Snow 2013, these proceedings). Essentially all attempts to identify the carriers of certain DIBs have been rejected. There is, to our knowledge, only one uncontested assignment of a far-ultraviolet DIB and three less diffuse absorption features to CH (Watson 2001). However, this assignments is far from being widely recognized, mainly because of the rather unusual frequency region; most of the DIBs have been detected at visible frequencies (Snow 2013, these proceedings).

It is thought that a considerable amount of the carriers of the DIBs reside in the diffuse ISM and that most of them are molecular species (Sonnentrucker 2013, these proceedings). A possible breakthrough may have been achieved recently by the observations of DIBs toward the star Herschel 36 (Oka *et al.* 2013, these proceedings). The observation of CH^+ transitions involving $J = 1$ in the ground electronic state suggest a radiative temperature of the diffuse ISM in the direction of the star reaching almost 15 K, much higher than commonly observed. Some of the DIBs showed strong extended tails toward red, very different contours compared to the usual appearance. Molecular spectroscopic considerations lead to the conclusion that the carriers of these bands are most likely relatively small polar molecules with about 3 to 8 heavy atoms. Other DIBs not showing such a tail may be due to non-polar or larger molecules.

Thus, we believe that the identification of the carrier of our U-line may help to solve the DIB-conundrum. It is unlikely that this U-line is related spectroscopically to pairs of DIBs, certainly not if the U-line represents a rotational or rovibrational transition of a molecule. But the carrier of the U-line could be a carrier of one or more DIBs or could be chemically related to them. Radio astronomy has already contributed to the DIB puzzle, e.g. by rejecting the assignments of some DIBs to propadienylidene (l-C_3H_2; Liszt *et al.* 2012). Other examples of how radio astronomy may further solving the DIB puzzle were presented at this symposium (Liszt *et al.* 2013, these proceedings).

References

Bergin, E. A., Phillips, T. G., Comito, C., *et al.* 2010, *A&A*, 521, L20
de Graauw, T., Helmich, F. P., Phillips, T. G., *et al.* 2010, *A&A*, 518, L6
De Luca, M., Gupta, H., Neufeld, D., *et al.* 2012, *ApJ*, 751, L37
Hollenbach, D., Kaufman, M. J., Neufeld, D., *et al.* 2012, *ApJ*, 754, 105

Lis, D. C., Pearson, J. C., Neufeld, D. A., *et al.* 2010, *A&A*, 521, L9

Liszt, H., Sonnentrucker, P., Cordiner, M., & Gerin, M. 2012, *ApJ*, 753, L28

Menten, K. M., Wyrowski, F., Belloche, A., *et al.* 2011, *A&A*, 525, A77

Neill, J. L., Bergin, E. A., Lis, D. C., *et al.* 2012, *J. Mol. Spectrosc.*, 280, 150

Neufeld, D. A., Goicoechea, J. R., Sonnentrucker, P., *et al.* 2010, *A&A*, 521, L10

Neufeld, D. A., Falgarone, E., Gerin, M., *et al.* 2012, *A&A*, 542, L6

Ossenkopf, V., Müller, H. S. P., Lis, D. C., *et al.* 2010, *A&A*, 518, L111

Pilbratt, G. L., Riedinger, J. R., Passvogel, T., *et al.* 2010, *A&A*, 518, L1

Sharpee, B. D., Slanger, T. G., Huestis, D. L., & Cosby, P. C. 2004, *ApJ*, 606, 605

Watson, J. K. G. 2001, *ApJ*, 555, 472

Wyrowski, F., Menten, K. M., Güsten, R., & Belloche, A. 2010, *A&A*, 518, A26