Searching for Interstellar C\textsubscript{\textdegree}{}\textsuperscript{+} Using a New Method for High Signal-to-noise HST/STIS Spectroscopy

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Received 2017 April 7; revised 2017 June 2; accepted 2017 June 6; published 2017 June 23

Abstract

Due to recent advances in laboratory spectroscopy, the first optical detection of a very large molecule has been claimed in the diffuse interstellar medium (ISM): C\textsubscript{\textdegree}{}\textsuperscript{+} (ionized Buckminsterfullerene). Confirming the presence of this molecule would have significant implications regarding the carbon budget and chemical complexity of the ISM. Here we present results from a new method for ultra-high signal-to-noise ratio (S/N) spectroscopy of background stars in the near-infrared (at wavelengths of 0.9–1 \textmu{}m), using the Hubble Space Telescope (HST) Imaging Spectrograph (STIS) in a previously untested “STIS scan” mode. The use of HST provides the crucial benefit of eliminating the need for error-prone telluric-correction methods in the part of the spectrum where the C\textsubscript{\textdegree}{}\textsuperscript{+} bands lie and where the terrestrial water vapor contamination is severe. Our STIS spectrum of the heavily reddened B0 supergiant star BD+63 1964 reaches an unprecedented S/N for this instrument (~600–800), allowing the detection of the diffuse interstellar band (DIB) at 9577 \AA{} attributed to C\textsubscript{\textdegree}{}\textsuperscript{+}, as well as new DIBs in the near-IR. Unfortunately, the presence of overlapping stellar lines, and the unexpected weakness of the C\textsubscript{\textdegree}{}\textsuperscript{+} bands in this sightline, prevents conclusive detection of the weaker C\textsubscript{\textdegree}{}\textsuperscript{+} bands. A probable correlation between the 9577 \AA{} DIB strength and interstellar radiation field is identified, which suggests that more strongly irradiated interstellar sightlines will provide the optimal targets for future C\textsubscript{\textdegree}{}\textsuperscript{+} searches.

Key words: instrumentation: spectrographs – ISM: molecules – line: identification – techniques: spectroscopic

1. Introduction

The diffuse interstellar band (DIB) problem is the longest-standing puzzle in interstellar chemistry, seemingly impenetrable despite the dedicated efforts of astronomers and laboratory chemists since the early 20th century (Herbig 1995; Sarre 2006; Snow 2014). The DIBs manifest as broad spectroscopic absorption features in the optical to near-infrared (NIR) spectra of stars as their light passes through the diffuse interstellar medium (ISM), indicating the presence of a large quantity of (mostly carbonaceous) unidentified molecular material (e.g., Cordiner 2011). Foing & Ehrenfreund (1994) discovered two DIBs at 9577 \AA{} and 9632 \AA{} that they assigned to C\textsubscript{60} (ionized Buckminsterfullerene) based on a similarity with the absorption wavelengths that are seen in neon matrix spectroscopy (d’Hendecourt et al. 1992; Fulara et al. 1993). Recently obtained gas-phase spectra of C\textsubscript{60}–He\textsubscript{\textdegree} complexes (for n \leq 4; Campbell et al. 2015, 2016a; Kuhn et al. 2016) show that the match between the interstellar and laboratory wavelengths is accurate within the observational uncertainties (a fraction of an angstrom). The bare C\textsubscript{60} absorption wavelengths were confirmed in an independent laboratory study by Spieler et al. (2017) using C\textsubscript{60} cations embedded in He-droplets.

If confirmed, the detection of interstellar C\textsubscript{\textdegree}{}\textsuperscript{+} will constitute a major breakthrough in interstellar chemistry and may provide, for the first time, an insight into the true scale of the chemical complexity in the diffuse ISM. Measurements of the NIR electronic transitions of C\textsubscript{\textdegree}{}\textsuperscript{+} (in absorption) would also provide a unique complement to the discovery of mid-infrared C\textsubscript{60} and C\textsubscript{\textdegree}{}\textsuperscript{+} emission bands in circumstellar and interstellar environments (Cam et al. 2010; Sellgren et al. 2010; Berné et al. 2013).

Despite dedicated observational studies (Walker et al. 2015, 2016; Galazutdinov et al. 2017), the case for interstellar C\textsubscript{\textdegree}{}\textsuperscript{+} has not yet been proven beyond reasonable doubt. Based on the laboratory measurements, five absorption features are expected (at 9348.4, 9365.2, 9427.8, 9577.0, and 9632.1 \AA{}, with strength ratios 0.07:0.2:0.3:1.0:0.8; Campbell et al. 2017) that would also provide a unique correlation between the 9577 \AA{} DIB strength and interstellar radiation field is identified, which suggests that more strongly irradiated interstellar sightlines will provide the optimal targets for future C\textsubscript{\textdegree}{}\textsuperscript{+} searches.
transitions involve lower levels above the ground state (such as the split levels arising from Jahn–Teller distortion), a variable ratio could potentially occur. Although Walker et al. (2016) claimed interstellar detections of all five C$_{60}^+$ bands, the three weaker C$_{60}^+$ bands are problematic as they fall in a wavelength region heavily obscured by absorption due to water vapor in the Earth’s atmosphere (see Galazutdinov et al. 2000, 2017). Telluric-correction methods for such weak interstellar absorption features are error-prone as a result of incomplete telluric line cancelation, and from the possible presence of weak (unseen) stellar lines in the telluric standard spectrum. To rigorously confirm the identification of interstellar C$_{60}^+$ high signal-to-noise observations of all five absorption bands are required, preferably from outside Earth’s atmosphere.

In this Letter, we present the first ever ultra-high signal-to-noise ratio (S/N), high resolution stellar/interstellar spectra obtained using the Hubble Space Telescope (HST) imaging spectrograph, targeting four of the five C$_{60}^+$ features (λ9349, λ9365, λ9428, and λ9577) along a heavily reddened line of sight. Very high continuum signal-to-noise ratios (S/N > 500 per spectral channel) are commonly achieved using ground-based optical telescopes, but such sensitivity has not previously been obtained using (direct) HST spectroscopy at red and near-IR wavelengths due to severe CCD fringing. After successfully employing a previously untested “STIS scan” observing mode to target the star along the spectrograph slit (crossing hundreds of CCD rows to facilitate fringe cancelation), unprecedented S/Ns $\sim$ 600–800 per dispersion pixel have been obtained. These spectra have permitted the first search for weak interstellar absorption features in the NIR, unhindered by telluric absorption.

2. Observations and Data Reduction

To reliably detect the weaker C$_{60}^+$ DIBs, a high-S/N interstellar spectrum is required with minimal contamination from interfering stellar photospheric lines. The heavily reddened ($E_{B-V}$ = 1.01) B01 star BD+63 1964 was selected due to its extremely strong DIBs—the majority of DIBs are among the strongest for stars of comparable extinction (Tuarirsig et al. 2000)—as well as its early spectral type and relatively clean predicted spectrum in the vicinity of the λ9365 and λ9428 C$_{60}^+$ bands. The lightly reddened B0 I star 69 Cygni ($E_{B-V}$ = 0.14) was selected for comparison, to assist in the discrimination of stellar and interstellar features.

2.1. HST/STIS

Data were acquired over a single orbit for 69 Cyg and two orbits for BD+63 1964 using the G750M grating with a central wavelength of 9336 Å (covering the range 9050–9610 Å). This covers four of the five known C$_{60}^+$ bands; a change of grating tilt would be required to obtain the fifth band. We used the 52′′ × 0′′1 slit, and the plate scale was 0.005 per pixel. Following peakup and focusing maneuvers, a series of STIS-scan exposures was performed for each star, trailing the star along the slit at a constant rate with the shutter held open. For 69 Cyg, six exposures were obtained: two long scans spanning up to 1000 detector rows and four shorter scans spanning ~300 rows. The scan direction was alternated for successive exposures. For BD+63 1964 (observed in a separate visit after the optimal observing sequence had been established), eight identical forward scans were obtained spanning 700 detector rows each, toward the upper part of the CCD. A pair of flat-field exposures (contemporaneous fringe flats) was obtained in sequence following each pair of target star exposures, and 5–6 additional pairs of flats were obtained to fill in the remaining orbital time during occultation. Exposures of a Pt/Ne–Cr lamp were obtained during each orbit for wavelength calibration. Subsequent conversion from vacuum to air wavelengths was performed using the Morton (2000) formula.

The STIS CCD suffers from charge transfer inefficiency (CTI) during readout, as a result of long-term radiation damage. The raw frames were corrected for CTI using the procedure outlined by Anderson & Bedin (2010)14, which significantly reduces the severity of bad CCD columns. Standard dark current, bias, geometric distortion, and wavelength corrections were performed using the IRAF calstis package (Hodge et al. 1998). For BD+63 1964, the four trailed science exposures in each orbit were sufficiently well matched to allow statistical cosmic-ray rejection using ocrreject. This was not possible for 69 Cyg due to imperfect registration of the exposed rows between each frame, which may have occurred due to errors in the guide star tracking, as well as possible exposure timing errors.

Spectral extraction was performed by summing the counts along CCD columns. Bad pixels and residual cosmic rays were rejected based on their standard deviation (using a $3\sigma$ threshold), after normalizing the individual CCD rows by their median levels. Such row normalization was required due to variations in the illumination function along the slit, resulting from slight variations in the slit width and telescope scan rate. Scattered-light subtraction was performed with a low-order fit to the light under the two occulting bars (positioned 1/3 and 2/3 of the way along the slit). Extracted Pt/Ne–Cr lamp line widths were consistent with the nominal instrumental resolving power of 10,000 (30 km s$^{-1}$).

The STIS CCD suffers from severe fringing due to internal reflections at wavelengths greater than 700 nm, where the chip starts to become transparent to incoming light. Fringe amplitudes are variable with wavelength, with a maximum of ±20% near 900 nm (see, e.g., Figure 1). The aim of our fringe cancelation strategy was to match as closely as possible the illumination pattern of the science exposure to that of the flat field by STIS scanning. This approach has the major advantages of (1) reducing the impact of individual bad pixels and cosmic-ray hits, (2) allowing for orders of magnitude increases in the number of counts per science exposure, and (3) eliminating the need to change the slit mechanism during observations, resulting in a consistent optical setup for the science and flat-field exposures.

As shown in Figure 1, scanning the exposed star across hundreds of CCD rows results in significantly reduced fringe amplitudes (a five-fold reduction in the spectral rms in this case). Following correction using a contemporaneous fringe flat, we obtained apparently complete fringe cancelation down to the level of the statistical noise.

2.2. CFHT ESPaDOnS

For comparison with our STIS data, four 1000 s exposures of BD+63 1964 were obtained over two nights in 2016 December, using the ESPaDOnS échelle spectrograph of the

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14 See http://www.stsci.edu/hst/stis/software/analyzing/scripts/pixel_based_CTL.
Canada–France–Hawaii Telescope (CFHT). Observing conditions were good and the airmass was in the range of 1.41–1.49. The data were reduced by the automated Upena pipeline, which uses the Libre-ESpRIT data reduction software (Donati et al. 1997). The reduced spectra cover the range 370–1048 nm at a resolving power of ~80,000, and have a continuum signal-to-noise ratio of ~500 at 900 nm.

Due to the forest of atmospheric H2O absorption lines in our STIS range, the ESPaDOnS spectra need to be telluric-corrected. The conventional approach of division by a standard star is unreliable for the measurement of weak DIBs due to the likely presence of stellar features in the standard star spectrum, which would introduce artifacts upon division. We therefore adopted a transmission modeling approach, using synthetic atmospheric transmittances provided by the TAPAS website15 (Bertaux et al. 2014), adapted for Mauna Kea. A preliminary telluric correction was performed using the “rope length” method for weak to moderately strong lines (Raimond et al. 2012), excluding from the length the spectral intervals corresponding to the central parts of the strongest lines. The preliminary correction was then interpolated in the most heavily contaminated intervals to remove residual artifacts. Next, the observed data were fitted to the convolved product of this spectrum and the TAPAS synthetic transmittance, allowing for variable airmass, refined wavelength correction, and variable line-spread function. The observed data were divided by this new adjusted transmission spectrum to provide a new corrected spectrum. The second step was then iterated to convergence to produce the final corrected spectrum. Despite our best efforts, telluric residuals still remain at the locations of the most heavily saturated lines, which may be due to the time variability of the telluric spectrum, scattered-light residuals, or small asymmetries in the ESPaDOnS instrumental response function.

2.3. Comparison between STIS and ESPaDOnS Spectra

The main purpose of these ESPaDOnS spectra was to verify the reliability of our nonstandard STIS observation and reduction procedures. A comparison between the HST/STIS and the telluric-corrected CFHT/ESPaDOnS spectra is shown in Figure 2. Telluric-correction artifacts in panels (a) and (b) are severe, preventing a reliable comparison in the vicinity of the weaker C60 bands. However, in the less problematic range 9500–9600 Å (panel (c)), the agreement between the two instruments is excellent, which demonstrates the success of our STIS observation and data reduction strategy. Slight discrepancies may be due to differences in the instrumental resolving power, telluric-correction residuals, or uncertainties in the continuum level of the high-dispersion CFHT spectrum. Some uncertainty in the STIS scattered-light correction also remains, leading to uncertainty in the zero level. A more detailed characterization of the (2D) scattered-light properties for STIS scan exposures awaits further study.

3. Results

The combined scattered-light-subtracted exposures of BD +63 1964 and 69 Cyg reached total counts of 8 × 105 and 5.5 × 105, respectively (per dispersion pixel). The presence of weak stellar and interstellar features precludes an accurate measurement of the continuum rms, but in regions free of any obvious lines, S/N = 600–800 was found for BD +63 1964 and ~700 for 69 Cyg. To our knowledge, this is the highest S/N ever demonstrated with STIS for direct near-infrared spectroscopy at full grating resolution. The continuum-normalized spectra are shown in Figure 3.

Both stars are B0 supergiants and have nearly identical stellar spectra. We used the non-LTE model atmosphere code CMFGEN (Hillier & Miller 1998, 1999; Hillier 2011), which solves the radiative-transfer equation for a spherically symmetric wind in the comoving frame under the constraints of radiative and statistical equilibrium. An effective temperature of 27,000 K, macro-turbulent velocity of 120 km s−1, and projected rotational velocity of 85 km s−1 were derived for both of the stars. The modeled lines are identified in Figure 3. Four features stand out in the BD +63 1964 spectrum that are not present in 69 Cyg or in the stellar model, which are likely due to interstellar absorption. The first three of these (at 9088, 9302, and 9412 Å) are identified as new DIBs; Galazutdinov et al. (2000) also found a possible DIB near 9412 Å. The absorption feature at 9577 Å coincides with the laboratory C60 wavelength. 69 Cyg also shows evidence for weak absorptions at 9577 and 9412 Å.

The equivalent width (EW) of the 9577 band is 74 ± 3 mÅ. A Gaussian fit to its profile gives EW = 76 ± 3 mÅ, with a central wavelength of 9576.60 ± 0.03 Å, a central depth of 2.3%, and FWHM = 3.1 ± 0.1 Å. These line strength measurements may be considered accurate to within about ±10% due to uncertainties in the STIS scattered-light subtraction.

A close-up view of the four observed C60 band regions is shown in Figure 4. A spectral model for C60 is overlaid using the laboratory wavelengths and band strengths of Campbell et al. (2016a). We adopt Gaussian band shapes because a

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15 http://ether.ipsl.jussieu.fr/tapas/
Lorentzian profile provides a poor match for the observed $\lambda 9577$ band wings (Figure 4). The model has been Doppler shifted to match the interstellar K I velocity. As with most heavily reddened diffuse sightlines, the K I line toward BD+63 1964 (recorded in our ESPaDOnS data) shows a complex velocity structure, with three main components at
and ionization levels weak stellar OII line, and is broader and deeper than expected. The equivalent width ratio of the wavelength of 9577.4
uncertainties, our inferred (absorption. The strength of the 9428 feature is partially contaminated by a
additional
be due to a lower than normal degree of ionization in this
The extreme weakness of the 9577 band per unit E<sub>R-V</sub> may be due to a lower than normal degree of ionization in this
sightline. The well-known DIB at 6283 Å has a large EW/E<sub>R-V</sub> value in diffuse clouds that are strongly irradiated by UV (see above references), while the 5797 Å DIB tends to be favored in more neutral, less irradiated clouds. The λ5797/λ6283 EW ratio is thus considered to be a tracer of the radiation field strength in the line of sight. Data have been taken from compilations of optical DIB measurements by Xiang et al. (2017) and the λ9577 measurements of Galazutdinov et al. (2000) to study the relationship between EW(9577)/E<sub>R-V</sub> and the λ5797/λ6283 DIB strength ratio. Additional λ6283 and λ5797 measurements were obtained from archival data from the CFHT and Telescope Bernard Lyot. The results for nine sightlines are shown in Figure 5, including the present results for BD+63 1964. Even without HD 37022 (a highly irradiated sightline through the Orion Nebula with unusually high EW(9577)/E<sub>R-V</sub>, the trend is for increasing λ9577 strength in gas pervaded by stronger radiation fields. In a survey of DIBs and atomic lines toward BD+63 1964 by Ehrenfreund et al. (1997), a relatively high gas density and low level of ionization was inferred, and the extremely low λ5797/λ6283 ratio is suggestive of weakly irradiated gas. The trend for increasing EW(9577)/E<sub>R-V</sub> with radiation field strength is consistent with the assignment to C<sub>60</sub> or another species whose ionization stage becomes dominant in more irradiated diffuse clouds (see also Foing & Ehrenfreund 1997).

5. Conclusion
We performed the first successful test of the HST “STIS scan” spectroscopic observational mode. The resulting spectroscopic S/N (up to ~800) is, to our knowledge, by far the highest demonstrated with STIS for direct stellar measurements at full grating resolution. This technical demonstration opens up a new wavelength range for interstellar, stellar, and exoplanetary spectroscopy, with unprecedented sensitivity.

We obtained the first “clean” measurements of the spectral region covering the λ9348, λ9365, λ9428, and λ9577 C<sub>60</sub> bands without the confounding presence of telluric contamination or fringing artifacts. The λ9577 band exhibits a closely Gaussian shape with FWHM and peak wavelength consistent with the laboratory measurement of 9351 Å by Walker et al. 2016, as well as overlapping stellar He II absorption. The λ9365 feature is partially contaminated by a weak stellar O II line, and is broader and deeper than expected. The λ9428 feature is too weak for a reliable measurement.

4. Discussion
The strengths of different DIBs are known to vary among sightlines with differing physical and chemical properties, independent of the total amount of interstellar material (e.g., Krelowski & Walker 1987; Ehrenfreund & Jenniskens 1995; Cami et al. 1997; Elyajouri et al. 2017; Ensor et al. 2017). The EW per unit reddening (EW/E<sub>R-V</sub>) provides a measure of the relative strength of a given DIB. For BD+63 1964 we find EW(9577)/E<sub>R-V</sub> = 73 mÅ, which is among the smallest values known for this band. Unfortunately for our present study, this means that BD+63 1964 is one of the least favorable heavily reddened sightlines in which to search for C<sub>60</sub>, which explains to some degree our difficulties in establishing (or disproving) the presence of the weaker C<sub>60</sub> absorption bands.

The extreme weakness of the λ9577 band per unit E<sub>R-V</sub> may be due to a lower than normal degree of ionization in this

![Figure 5. Strength of the λ9577 C<sub>60</sub> band (per unit reddening) vs. the equivalent width ratio of the λ6283 and λ5797 DIBs (an indicator of radiation field strength) for a sample of Galactic sightlines, labeled by HD number.](image-url)
NASA through a grant from the Space Telescope Science Institute, which is operated by the Association of Universities for Research in Astronomy, Inc., under NASA contract NAS 5-26555. F.N. acknowledges Spanish grants FIS2012-39162-C06-01, ESP2013-47809-C3-1-R, and ESP2015-65597-C4-1-R. ESPaDOnS observations were obtained under program 16BD86 at the Canada–France–Hawaii Telescope, which is operated by the National Research Council of Canada, the Institut National des Sciences de l’Univers of the Centre National de la Recherche Scientifique of France, and the University of Hawaii.

Facilities: HST (STIS), CFHT(ESPaDOnS).

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