Investigating trace gases in the Martian atmosphere using the ExoMars Trace Gas Orbiter Part 1: Analysis of ESA PSA NOMAD SO Channel Data

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Introduction:

In 2016, the European Space Agency's (ESA) ExoMars Trace Gas Orbiter (TGO) was launched to investigate the nature of methane, on Mars, utilising the Nadir and Occultation for MArs Discovery (NOMAD), Vandaele et al. (2015) [1], and Atmospheric Chemistry Suite (ACS), Korablev et al. (2018) [2], instruments, both of which have the sensitivity to make the detection, Liuzzi et al. (2019) [3]. However, the arrival of the TGO and subsequent science mission has detected no CH_4, with upper limits of 0.05 ppbv, Korablev et al. (2019) [4], 0.06 ppbv Knutsen et al. (2021) [5], and 0.02 ppbv Montmessin et al. (2021) [6] derived.

In contrast, NASA's Curiosity Sample Analysis at Mars Tunable Laser Spectrometer instrument (SAM-TLS) Mahaffy et al. (2012) [7] has made multiple measurements of CH_4, including measuring an elevated CH_4 background of 7.2 ± 2.1 ppbv CH_4 over a 60-sol period in 2013, Webster et al. (2015) [8]. Subsequently, Webster et al. (2018) [9], using SAM-TLS determined a mean CH_4 abundance of 0.41 ± 0.16 ppbv, as well as a repeatable seasonal variation from 0.24-0.65 ppbv. Moreover, on the 20th June 2019 a 19.5 ± 0.18 ppbv CH_4 emission in Gale Crater was reported by SAM-TLS, Moores et al. (2019) [10]. Furthermore, the Planetary Fourier Spectrometer (PFS) onboard Mars Express detected 15.5 ± 2.5 ppbv of CH_4, above Gale Crater, one day after SAM-TLS independently detected a CH_4 spike of 5.78 ± 2.27 ppbv, Giuranna et al. (2019) [11]. Since then, PFS has detected no CH_4.

As part of a novel search for Martian trace-gases, such as CH_4, all publicly available ESA Planetary Science Archive (PSA) NOMAD Solar Occultation (SO) calibrated Level 3 (L3) data has been processed to calculate ≈ 79,000 maps of transmittance residuals (TR) against wavenumber and tangent height, covering all available NOMAD diffraction orders, from 21st April 2018 to 31st December 2019. These representations, provided as an open dataset may be useful in identifying new trace-gas species, highlighting which spectra are worthy of performing retrievals and/or contain systematic errors, as well as identifying missing absorption lines in forward models.

Method:

The following procedure provides the general method used for calculating the transmittance residuals, steps 1-5. Extending the method, in steps 6-9, enables the creation of diffraction order averages of NOMAD SO observations.

1. Use `PDS4 Tools` PDS SBN (2021) [15] to read all NOMAD SO L3 calibrated transmittance spectra `.xml/.tab` files for a particular diffraction order.
2. For each NOMAD solar occultation assign all values for transmittance, transmittance errors, wavenumbers, and starting tangent point altitude.
3. For a particular NOMAD SO bin, loop through all measurements of the occultation and perform a set of 5th degree polynomial fits using `numpy polyfit` to all spectra.
4. Subtract the appropriate polynomial fit, utilising `numpy poly1d` with the wavenumber grid of the observation, from the transmittance spectra, creating a set of residual spectra - note that these residuals are bin specific.
5. Repeat step 4. for all bins and create the bin averaged set of spectra, i.e. observations indexed 1-4, 5-8, etc. are averaged. Note that certain filters must be applied, as the total number of observations, *n* within a solar occultation does not necessarily satisfy *n* mod4 = 0.
6. A set of rectangular bivariate spline fits is performed on the transmittance minus polynomial baseline values, over a rectangular mesh of wavenumber and tangent heights, using the `scipy RectBivariateSpline` module. The order of the bivariate spline is taken as a 5th degree polynomial, in both wavenumber and tangent height directions.
7. Evaluate the bivariate spline using the `ev` method on a meshed grid.
8. Export the 2D arrays of transmittance residual values as a `.npy` files and repeat or all other solar occultations.
9. Iteratively open all `.npy` files and average the 2D arrays of transmittance residual values.

All code and data associated with this research will be made open source to the community on.

Results:

Extending from individual representations we will present diffraction order averages of NOMAD SO observations calculated for all publicly available ESA PSA NOMAD SO L3 data. Averaging spectra improves the signal-to-noise ratio of observations, Robert et al. (2016) [16], Liuzzi et al. (2019) [3] and has been applied in multiple studies searching for trace gases, such as CH_4, in the Martian atmosphere, such as Giuranna et al. (2019) [11], Formisano et al. (2004) [19] and Geminale et al. (2011) [22].

Figures 1-4 show the average transmittance residuals vs wavenumber and tangent height, for diffraction orders 133, 134, 135 and 136, orders of particular interest in the search for CH_4. Figures 1-4 are annotated with suggestions on the cause(s) of particular spectral lines from comparisons against TauREx [23] and Planetary Spectrum Generator (PSG) simulations, Villanueva et al. (2018) [16] and Villanueva et al. (2022) [17].

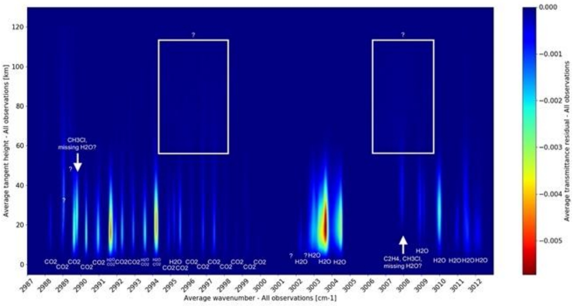

Figure 1: Diffraction Order 133. Plot of average TR, for 355 solar occultation observations. PSG [16][17] simulations suggest that if present H_2O, O_3, CO_2, CH_4, C_2H_4, C_2H_6, and CH_3Cl are potentially retrievable within 133. Robert et al. (2016) [18] suggests CH_4, C_2H_4, and C_2H_6 are potentially retrievable.

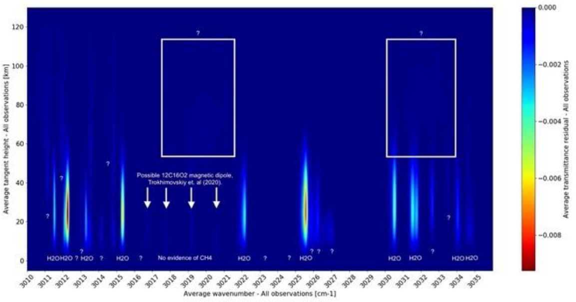

Figure 2: Diffraction Order 134. Plot of the average transmittance residual, for 2418 solar occultation observations.

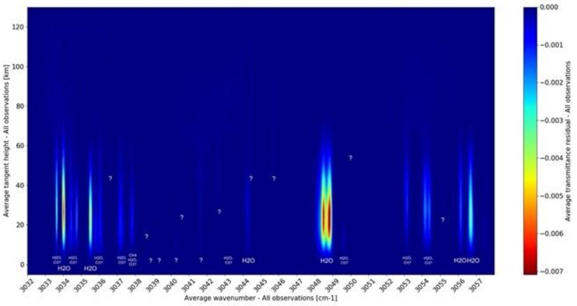

Figure 3: Diffraction Order 135. Plot of average TR, for 194 solar occultation observations. PSG [16][17] simulations suggest that if present H_2O, O_3, CO_2, CH_4, and C_2H_4 are potentially retrievable within 135. Robert et al. (2016) [18] suggests CH_4, and O_3 are potentially retrievable.

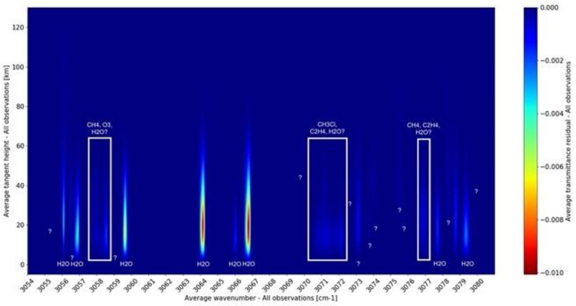

Figure 4: Diffraction Order 136. Plot of average TR, for 724 solar occultation observations. Robert et al. (2016) [18] suggests CH_4, and C_2H_4 are potentially retrievable. PSG simulations suggest that if present CH_4, CH_3Cl, C_2H_4, H_2O and O_3 are potentially retrievable within 136.

Figure 2 of diffraction order 134 from 3010-3036 cm^{-1} shows no clear evidence of CH_4, although evidence for the magnetic dipole of CO_2, between 3016-3021 cm^{-1}, Trokhimovskiy et al. (2020) [14] is. Figure 4 of diffraction order 136 from 3054-3080 cm^{-1} shows a feature between 3070-3075 cm^{-1} that appears to correspond to CH_3Cl and/or C_2H_4 in PSG [16][17] simulations. Alternatively, this could be an instrument issue, H_2O/CO_2 side order contributions, or an unknown line. Furthermore, from individual representations of diffraction order 129, evidence for HCl, Korablev et al. (2021) [12], Olsen et al. (2021) [13] and in diffraction order 134, evidence for the magnetic dipole of CO_2, Trokhimovskiy et al. (2020) [14], has been identified. Note that the applicability of averaging spectra should be considered for highly variable species such as H_2O.

Conclusions:

A full spectral assessment of all publicly available NOMAD SO channel transmittance data from 21st April 2018 to 31st December 2019 has been performed. Suggestions on the causes of particular lines are given, however, the source of many lines in NOMAD SO channel transmittance residuals are challenging to establish. The cause of many lines should be investigated by future research.

This research has found no clear evidence for the abundances of CH_4 on Mars as reported by Formisano et al. (2004) [19], Krasnopolsky et al. [20], Mumma et al. (2009) [21], Webster et al. (2015) [5] and Webster et al. (2018) [9]. This research instead supports the levels of CH_4 reported by Korablev et al. (2019) [4] and Knutsen et al. (2021) [5]. Furthermore, from individual transmittance residual representations evidence for HCl, Korablev et al. (2021) [12], Olsen et al. (2021) [13] and the magnetic dipole of CO_2, Trokhimovskiy et al. (2020) [14], has been identified.

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