

Impact of Spectroscopy on CH₄ Total Column Retrievals from Sentinel-5P/TROPOMI in the Short-Wave Infrared

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Introduction

- ▶ Methane (CH₄) strongly affects the global climate
- ▶ Short-Wave IR spectra to infer molecular concentrations
- ▶ Accurate modeling of molecular absorption mandatory

BIRRA — Beer InfraRed Retrieval Algorithm

Nonlinear least squares (NLS): $\min_{\mathbf{x}} \|\mathbf{y} - \mathbf{F}(\mathbf{x})\|^2$

$$\mathbf{F}(\mathbf{x}) = r(\nu)/\pi \cos \theta I_{\text{sun}}(\nu) \exp \left[- \sum_m \alpha_m \tau_m(\nu) \right] \otimes S(\nu, \gamma, \dots) + b$$

τ_m molec optical depth; S ISRF; θ SZA; b baseline

$$\mathbf{x} \in (r, \mathbf{b}, \alpha, \gamma, \delta, \dots).$$

- ▶ BIRRA infers information from absorption features [2, 3]
- ▶ State vector \mathbf{x} contains geophysical parameters
- ▶ Py4CATS line-by-line forward model based on GARLIC [6]
- ▶ BIRRA was originally developed for SCIAMACHY nadir CO and CH₄

SEOM-IAS — Improved Atmospheric Spectroscopy

- ▶ Spectroscopic database for TROPOMI around 2.3 μm [1]
- ▶ New line positions, intensities, broadening parameters
- ▶ Additional 'beyond Voigt' line parameters
- ▶ Speed-dependent Rautian profile + line-mixing (SDRM)

gas	data	# lines	S [cm ⁻¹ /molec cm ²]	$\gamma_{\text{air}}^{(0)}$ [cm ⁻¹]	n	$\gamma_{\text{air}}^{(2)}$ [cm ⁻¹]	ν_{vc} [cm ⁻¹]
CH ₄	SEOM	6205	$6.7 \cdot 10^{-27} - 5.5 \cdot 10^{-21}$	0.019–0.182	0.19–1.82	0.008405(610)	0.00911(65)
	H16	8375	$1.0 \cdot 10^{-29} - 5.5 \cdot 10^{-21}$	0.034–0.077	0.67–0.77		
	G15	7213	$9.5 \cdot 10^{-28} - 5.4 \cdot 10^{-21}$	0.034–0.077	0.46–0.97		
H ₂ O	SEOM	1177	$1.4 \cdot 10^{-30} - 2.2 \cdot 10^{-23}$	0.004–0.141	0.31–1.02	0.007197(35)	0.01083(12)
	H16	1197	$1.0 \cdot 10^{-32} - 2.2 \cdot 10^{-23}$	0.004–0.109	0.32–0.73		
	G15	1101	$8.4 \cdot 10^{-30} - 2.2 \cdot 10^{-23}$	0.004–0.096	0.32–0.69		
CO	SEOM	110	$1.0 \cdot 10^{-31} - 3.5 \cdot 10^{-21}$	0.042–0.081	0.67–0.79	0.00607(10)	0.0047(10)
	H16	110	$1.0 \cdot 10^{-31} - 3.5 \cdot 10^{-21}$	0.042–0.081	0.67–0.79		
	G15	160	$1.1 \cdot 10^{-36} - 3.6 \cdot 10^{-21}$	0.040–0.079	0.69		

Table: Spectroscopic line data for the 2311–2352 nm interval. The last two columns show the mean of the 'beyond Voigt' air-broadening speed-dependence and Dicke narrowing parameters. The number of non-zero values is indicated in the parentheses [4].

Level 1→2 Processing

Input data required for the retrieval

- ▶ S5P radiance and irradiance data
- ▶ BDPM and ISRF's
- ▶ **Spectroscopic line data:** SEOM-IAS, HITRAN, GEISA
- ▶ Atmospheric data on p , T and specific humidity
- ▶ A priori information on molecular concentration profiles
- ▶ Terrain elevation from the ETOPO global relief model
- ▶ Cloud-mask from VIIRS aboard Suomi-NPP
- ▶ ...

Impact on CH₄ Spectrum

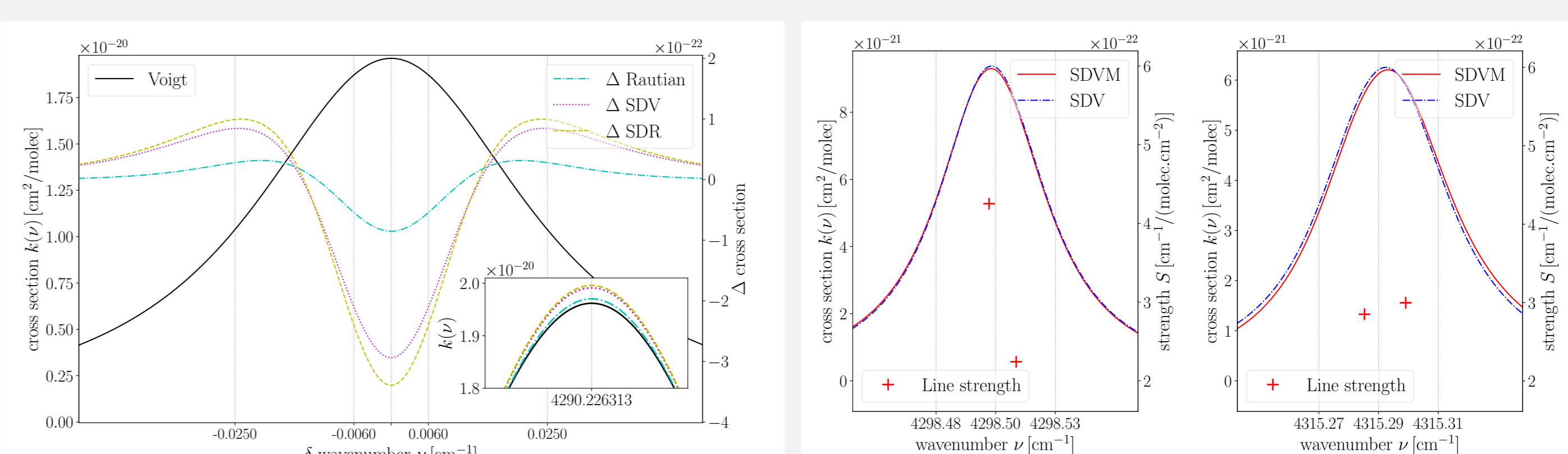


Fig. 1: (Left) CH₄ absorption cross sections for various line profiles at 330 hPa and 243 K computed with SEOM-IAS line data.

(Center&Right) The effect of line-mixing on molecular cross sections. Note the dependence on relative line strengths of neighboring lines [5].

Impact on CH₄ Retrieval

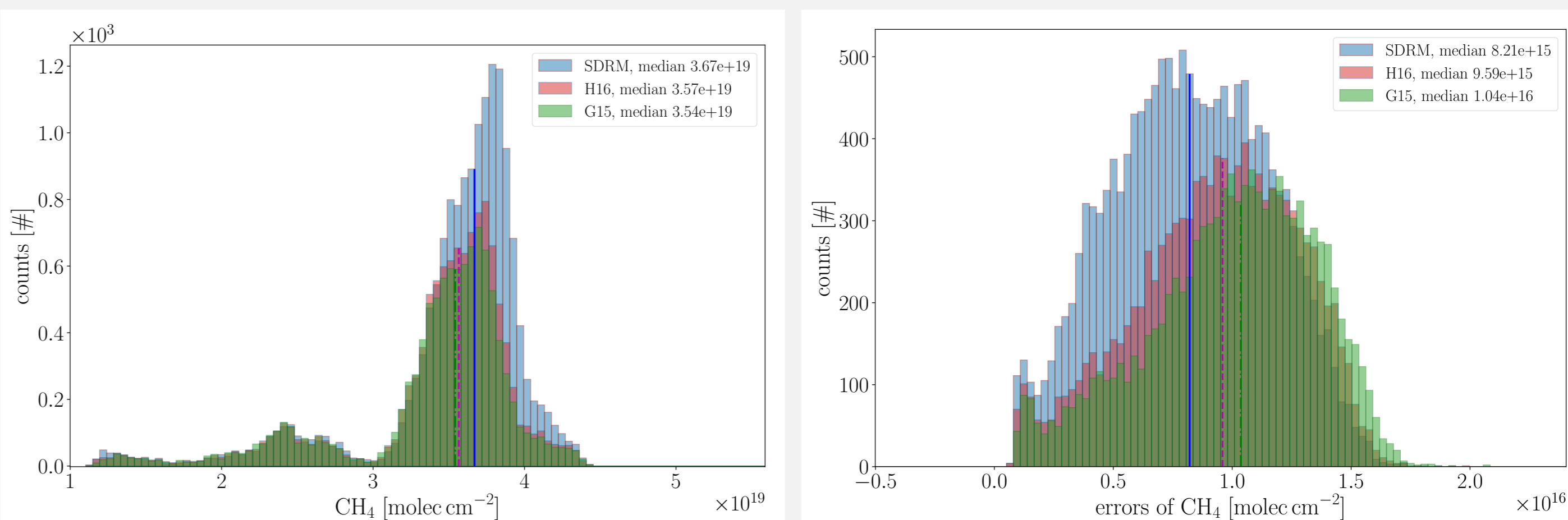


Fig. 2: CH₄ columns (left) over Amazonia in orbit 9553 along with errors (right) for different spectroscopic line lists and models [4].

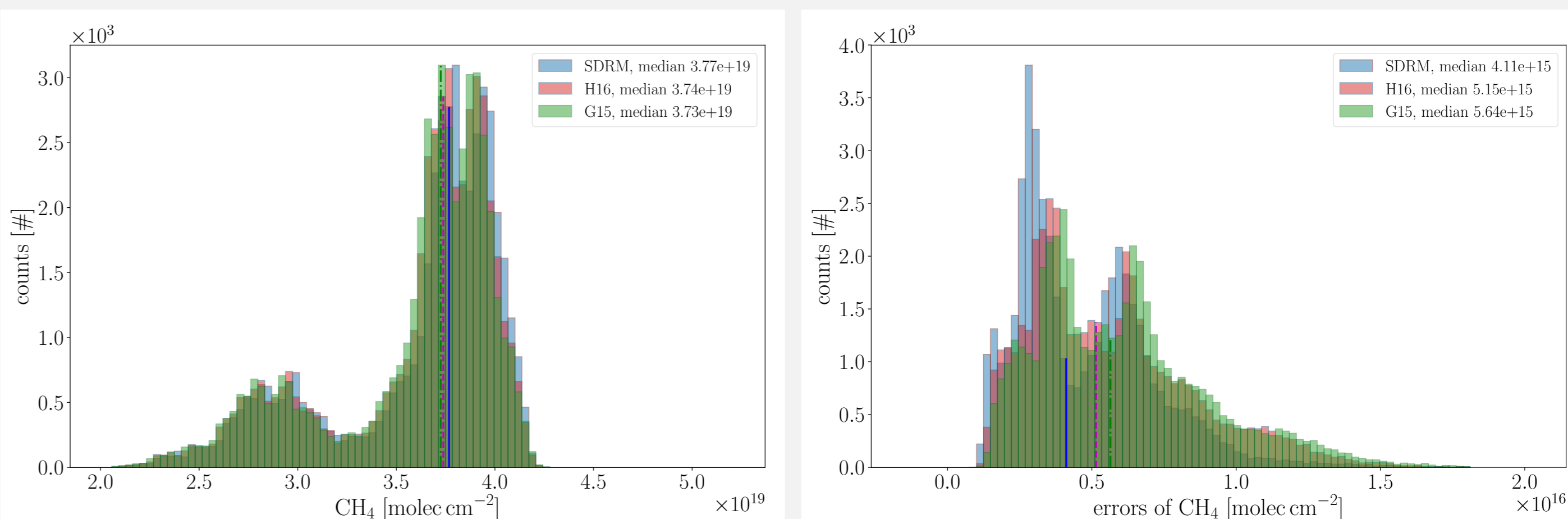


Fig. 3: CH₄ retrieved in orbit 7861 over the Sahara region [4].

Beyond SEOM-IAS/SDRM

	median		mean		variance	
	HTM	SDRM	HTM	SDRM	HTM	SDRM
α_{CH_4}	1.0475	1.0485	1.0467	1.0478	0.0157	0.0158
$\alpha_{\text{H}_2\text{O}}$	1.3450	1.3555	1.3929	1.3945	0.4495	0.4487
α_{CO}	0.9566	0.9572	0.9338	0.9344	0.0463	0.0461

Table: Retrieved scaling factors for the Hartmann-Tran (HTM) and SDRM line profiles from TROPOMI measurements in orbit 2923. The partial correlation parameter was manually set in the HTM profile [5].

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