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## Supplement of

## Mapping the $CO_2$ total column retrieval performance from shortwave infrared measurements: synthetic impacts of the spectral resolution, signal-to-noise ratio, and spectral band selection

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## S1. Overview

This supplement provides the exact list of resolving power values (Table S1) and average albedo values for the three surface models considered in this work (Table S2). Figures S1 and S2 illustrate the Jacobian matrices for concepts observing spectra and NanoCarb, respectively. This supplement provides results for all observational situations (Figures S3– 5, S7–10 and S12-17), different a posteriori correlation matrices (Figures S18 – S21), a version of Fig. 5 in linear scale for the horizontal axis (S11), and Figure S6 comparing OCO-2 performance results and the ones we can obtain synthetically.

## S2. Contents of this file

Tables S1, S2 and Figures S1 to S21.

200	289	378	467	556	644	733	822	911
1000	2000	3000	4000	5000	6000	7000	8000	9000
10000	12222	14444	16667	18889	21111	23333	25556	27778
30000								

Table S1. Exact list of resolving power values used in this work.

	SOL	VEG	DES
O <sub>2</sub> 0.76 μm band	0.10	0.45	0.50
CO <sub>2</sub> 1.6 µm band	0.22	0.29	0.57
CO <sub>2</sub> 2.05 μm band	0.18	0.09	0.58
O <sub>2</sub> 1.27 μm band	0.21	0.47	0.57

Table S2. Albedo values for the three surface models used in this work, averaged over MicroCarb bands.

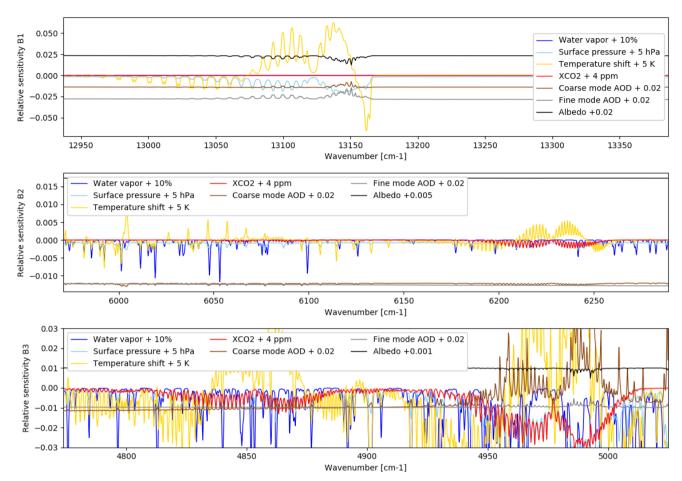


Figure S1. Relative measurement sensitivities at  $\lambda/\Delta\lambda = 10000$  for water vapor, surface pressure, temperature profile shift,  $X_{CO_2}$ , coarse and fine aerosol mode optical depths and band-wise albedo baseline for all CO<sub>2</sub>M spectral bands, for a vegetation-like albedo and a Solar Zenith Angle of 50°

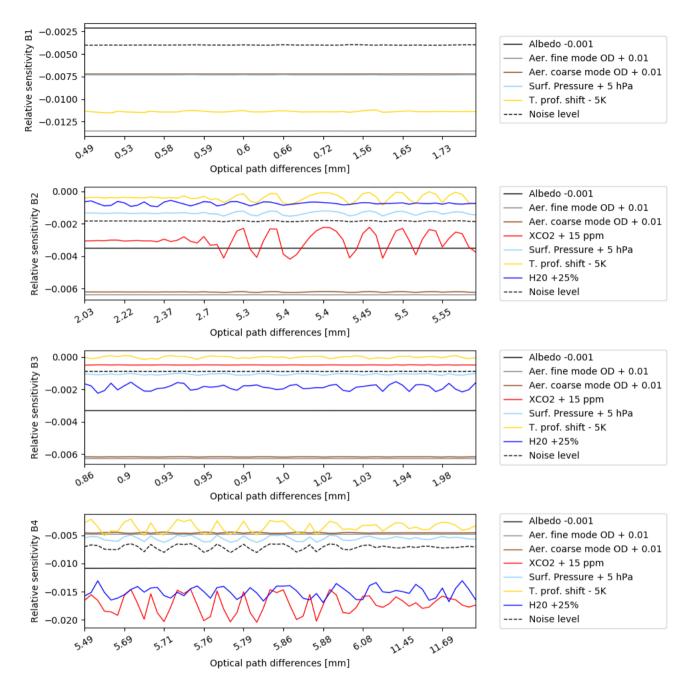
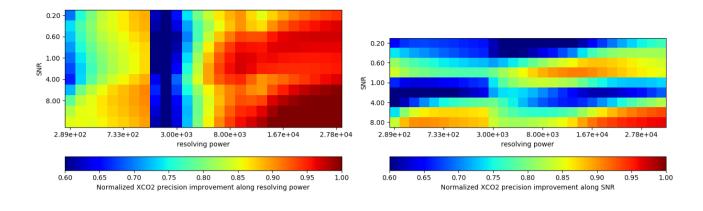


Figure S2. Relative NanoCarb measurement sensitivities for all NanoCarb bands, for water vapor, surface pressure, temperature profile shift,  $X_{CO_2}$ , coarse and fine aerosol mode optical depths and band-wise albedo baseline for a vegetation-like albedo and a Solar Zenith Angle of 50°.



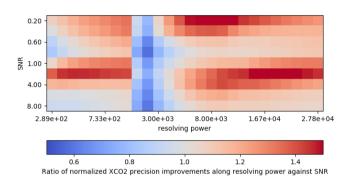


Figure S3. For VEG-50°, Normalized  $X_{CO_2}$  precision (noted  $\sigma_{XCO_2}$ ) improvements  $G(x_i|y_j) = [\sigma_{XCO_2}(x_{i-1}|y_j)/\sigma_{XCO_2}(x_{i+1}|y_j)]/[x_{i+1}/x_{i-1}]$ , with  $x_{i-1} < x_i < x_{i+1}$  for local improvements in resolving power (top left, with x being resolving power and y being SNR) and SNR (top right, with x being SNR and y being resolving power). The ratio between normalized  $X_{CO_2}$  precision improvements obtained along the resolving power dimension against the ones obtained along the SNR dimension is also shown (bottom right). Overall (except between  $\lambda/\Delta\lambda \sim 1000 - 4000$ ), we note that local improvements in resolving power provide more improvements in  $X_{CO_2}$  precision than improvements in SNR.

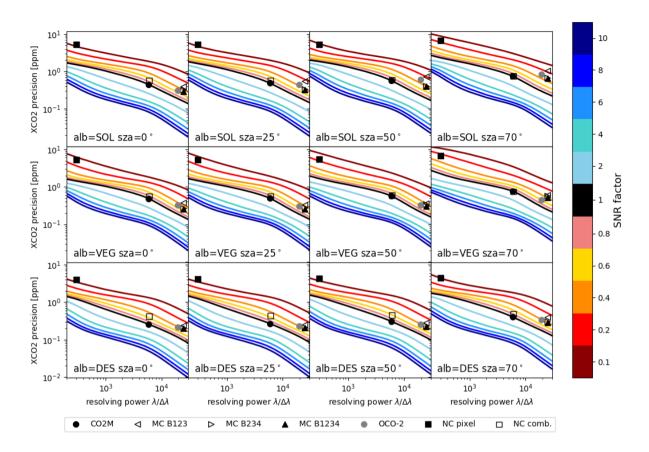


Figure S4.  $X_{CO_2}$  precision, or random error, for the fictitious CVAR instrument for resolving power  $\lambda/\Delta\lambda$  evolving from 200 to 30000 (horizontal axis), and for SNR evolving from 0.1 to 10 times CO<sub>2</sub>M reference SNR (colour scale), for SOL, VEG and DES albedo models (rows), and SZA values ranging from 0° to 70° (columns). Symbols give the same quantities for NanoCarb (NC, squares), MicroCarb (MC, triangles), CO<sub>2</sub>M (circle) and OCO-2 (grey circle). It should be noted that NanoCarb does not have a spectral resolution per se, the resolving powers used to plot its performance have been solely chosen for the sake of comparing NanoCarb and CVAR performance.

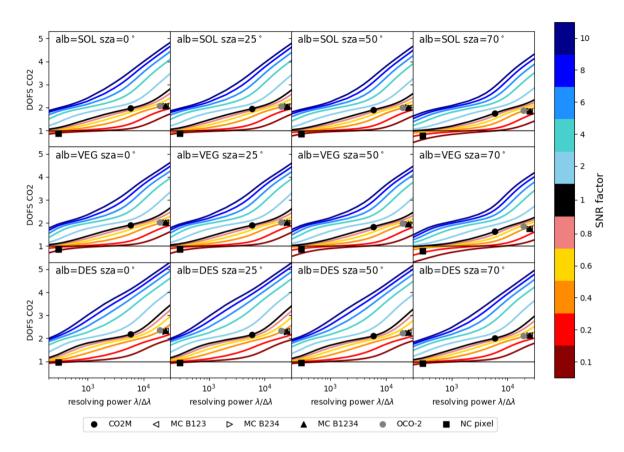


Figure S5. CO<sub>2</sub> degrees of freedom for the fictitious CVAR instrument for resolving power  $\lambda/\Delta\lambda$  evolving from 200 to 30000 (horizontal axis), and for SNR evolving from 0.1 to 10 times CO<sub>2</sub>M reference SNR (colour scale), for SOL, VEG and DES albedo models (rows), and SZA values ranging from 0° to 70° (columns). Symbols give the same quantities for NanoCarb (NC, squares), MicroCarb (MC, triangles), CO<sub>2</sub>M (circle) and OCO-2 (grey circle). It should be noted that NanoCarb does not have a spectral resolution per se, the resolving powers used to plot its performance have been solely chosen for the sake of comparing NanoCarb and CVAR performance.

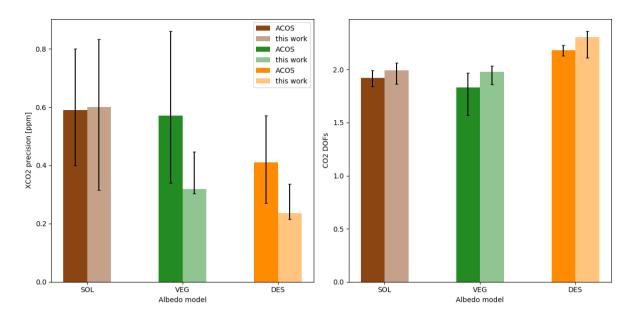


Figure S6.  $X_{CO_2}$  uncertainty (or precision) due to noise and CO<sub>2</sub>-related Degrees of Freedom (DOFs) from ACOS v8 L2 data (full colors) and from our synthetic study (light colors). For each albedo model considered in this study, we explored the year 2016 ACOS v8 L2 data downloaded for the work performed in Dogniaux et al. (2021). We averaged the precision field 'xco2\_uncert\_noise' (in L2StdND oco2 files) and DOFs results for soundings that match our albedo models within ±0.05. The error-bars range from the 10th to the 90th percentile of each distribution. Our synthetic OCO-2 results have been linearly interpolated to match the average OCO-2 Solar Zenith Angle in the considered ACOS data for each albedo model. The error bar range from the minimum to the maximum values obtained in our synthetic survey.

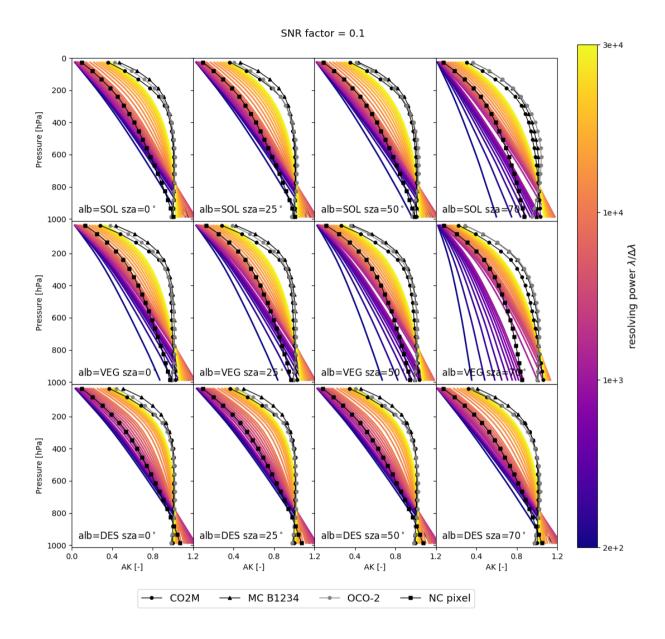


Figure S7. Vertical sensitivities (AKs) as a function of resolving power  $\lambda/\Delta\lambda$  for an SNR scaling factor of 0.1, for SOL, VEG and DES albedo models (rows), and SZA values ranging from 0° to 70° (columns). Lines with symbols give vertical sensitivities for CO<sub>2</sub>M (black circles), MicroCarb (black triangles), NanoCarb (black squares) and OCO-2 (grey circles).

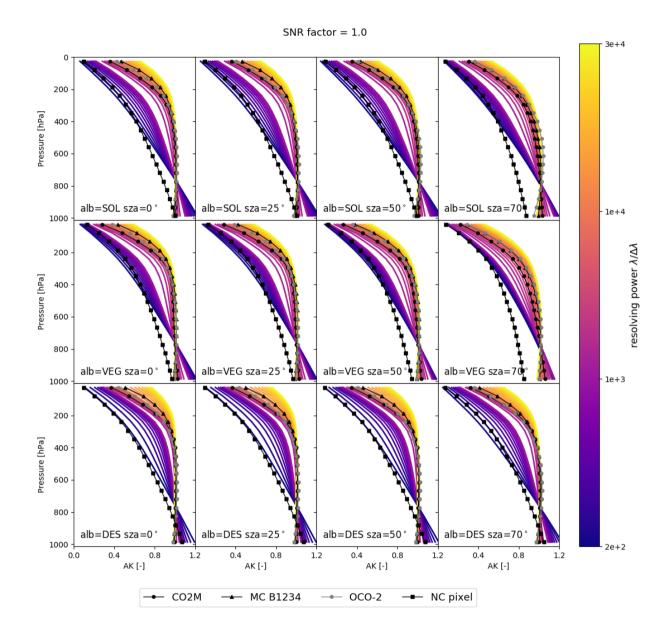


Figure S8. Vertical sensitivities (AKs) as a function of resolving power  $\lambda/\Delta\lambda$  for an SNR scaling factor of 1, for SOL, VEG and DES albedo models (rows), and SZA values ranging from  $0^{\circ}$  to  $70^{\circ}$  (columns). Lines with symbols give vertical sensitivities for CO<sub>2</sub>M (black circles), MicroCarb (black triangles), NanoCarb (black squares) and OCO-2 (grey circles).

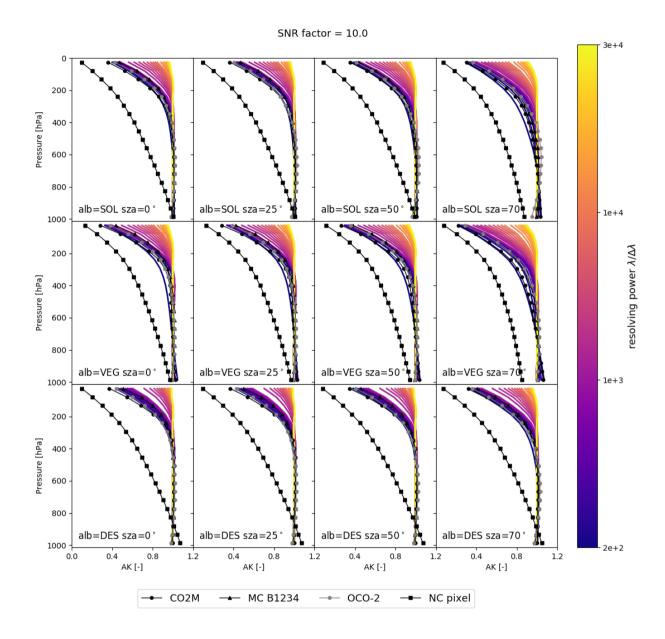


Figure S9. Vertical sensitivities (AKs) as a function of resolving power  $\lambda/\Delta\lambda$  for an SNR scaling factor of 10, for SOL, VEG and DES albedo models (rows), and SZA values ranging from 0° to 70° (columns). Lines with symbols give vertical sensitivities for CO<sub>2</sub>M (black circles), MicroCarb (black triangles), NanoCarb (black squares) and OCO-2 (grey circles).

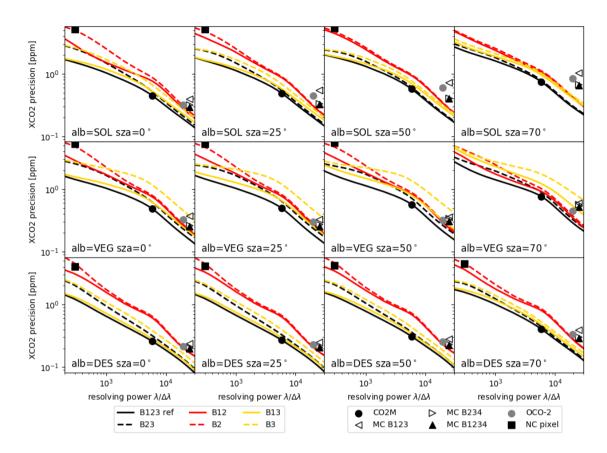


Figure S10.  $X_{CO_2}$  precision, or random error, for the fictitious CVAR instrument for resolving power  $\lambda/\Delta\lambda$  evolving from 200 to 30000 (horizontal axis), and for different spectral band selections: with and without  $O_2$  0.76  $\mu$ m band (B1, full and dashedlines, respectively), with both  $CO_2$  1.6 and 2.05  $\mu$ m bands (B23, black), with only the 1.6  $\mu$ m band (B2, red) and with only the 2.05  $\mu$ m band (B3, yellow), for SOL, VEG and DES albedo models (rows), and SZA values ranging from 0° to 70° (columns). Symbols give the same quantities for NanoCarb (NC, squares), MicroCarb (MC, triangles),  $CO_2M$  (circle) and OCO-2 (grey circle). It should be noted that NanoCarb does not have a spectral resolution per se, the resolving powers used to plot its performance have been solely chosen for the sake of comparing NanoCarb and CVAR performance.

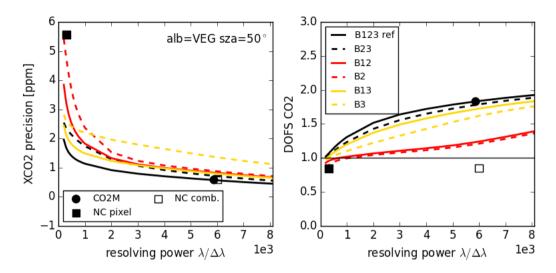


Figure S11. Same as Fig. 5, but in linear scale for the horizontal axis. It should be noted that NanoCarb does not have a spectral resolution per se, the resolving powers used to plot its performance have been solely chosen for the sake of comparing NanoCarb and CVAR performance.

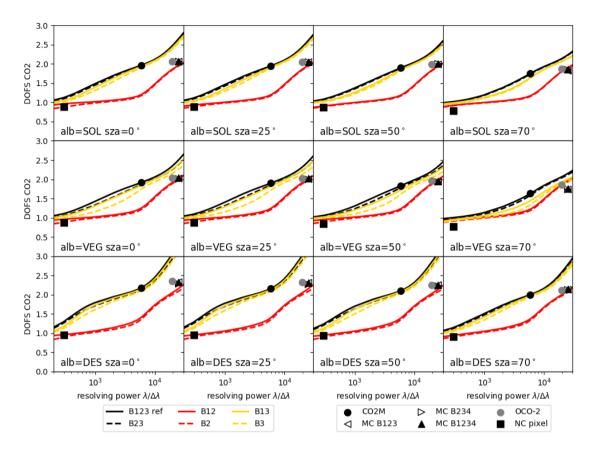


Figure S12. CO<sub>2</sub> degrees of freedom for the fictitious CVAR instrument, for resolving power λ/Δλ evolving from 200 to 30000 (horizontal axis), and for different spectral band selections: with and without O<sub>2</sub> 0.76 μm band (B1, full and dashed-lines, respectively), with both CO<sub>2</sub> 1.6 and 2.05 μm bands (B23, black), with only the 1.6 μm band (B2, red) and with only the 2.05 μm band (B3, yellow), for SOL, VEG and DES albedo models (rows), and SZA values ranging from 0° to 70° (columns). Symbols give the same quantities for NanoCarb (NC, squares), MicroCarb (MC, triangles), CO<sub>2</sub>M (circle) and OCO-2 (grey circle). It should be noted that NanoCarb does not have a spectral resolution per se, the resolving powers used to plot its performance have been solely chosen for the sake of comparing NanoCarb and CVAR performance.

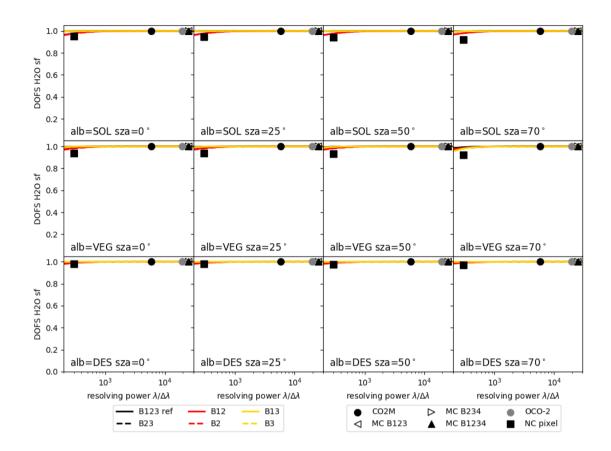


Figure S13. H<sub>2</sub>O scaling factor degrees of freedom for the fictitious CVAR instrument, for resolving power λ/Δλ evolving from 200 to 30000 (horizontal axis), and for different spectral band selections: with and without O<sub>2</sub> 0.76 μm band (B1, full and dashed-lines, respectively), with both CO<sub>2</sub> 1.6 and 2.05 μm bands (B23, black), with only the 1.6 μm band (B2, red) and with only the 2.05 μm band (B3, yellow), for SOL, VEG and DES albedo models (rows), and SZA values ranging from 0° to 70° (columns). Symbols give the same quantities for NanoCarb (NC, squares), MicroCarb (MC, triangles), CO<sub>2</sub>M (circle) and OCO-2 (grey circle). It should be noted that NanoCarb does not have a spectral resolution per se, the resolving powers used to plot its performance have been solely chosen for the sake of comparing NanoCarb and CVAR performance.

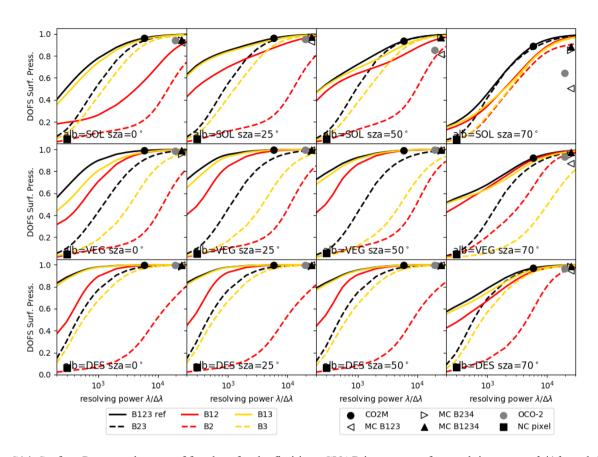


Figure S14. Surface Pressure degrees of freedom for the fictitious CVAR instrument, for resolving power  $\lambda/\Delta\lambda$  evolving from 200 to 30000 (horizontal axis), and for different spectral band selections: with and without  $O_2$  0.76  $\mu$ m band (B1, full and dashed-lines, respectively), with both  $CO_2$  1.6 and 2.05  $\mu$ m bands (B23, black), with only the 1.6  $\mu$ m band (B2, red) and with only the 2.05  $\mu$ m band (B3, yellow), for SOL, VEG and DES albedo models (rows), and SZA values ranging from  $0^{\circ}$  to  $70^{\circ}$  (columns). Symbols give the same quantities for NanoCarb (NC, squares), MicroCarb (MC, triangles),  $CO_2M$  (circle) and OCO-2 (grey circle). It should be noted that NanoCarb does not have a spectral resolution per se, the resolving powers used to plot its performance have been solely chosen for the sake of comparing NanoCarb and CVAR performance.

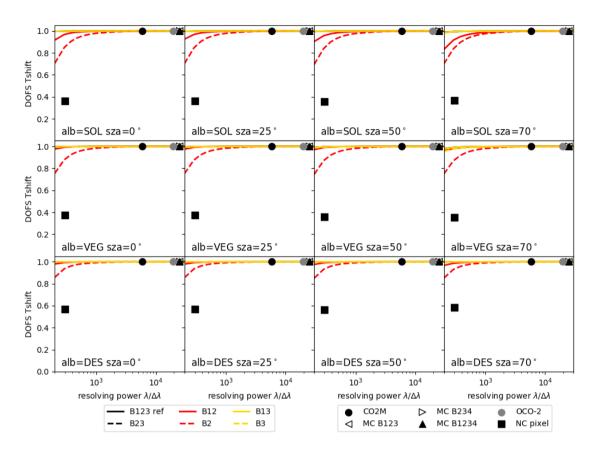


Figure S15. Temperature profile shift degrees of freedom for the fictitious CVAR instrument, for resolving power  $\lambda/\Delta\lambda$  evolving from 200 to 30000 (horizontal axis), and for different spectral band selections: with and without O<sub>2</sub> 0.76 µm band (B1, full and dashed-lines, respectively), with both CO<sub>2</sub> 1.6 and 2.05 µm bands (B23, black), with only the 1.6 µm band (B2, red) and with only the 2.05 µm band (B3, yellow), for SOL, VEG and DES albedo models (rows), and SZA values ranging from 0° to 70° (columns). Symbols give the same quantities for NanoCarb (NC, squares), MicroCarb (MC, triangles), CO<sub>2</sub>M (circle) and OCO-2 (grey circle). It should be noted that NanoCarb does not have a spectral resolution per se, the resolving powers used to plot its performance have been solely chosen for the sake of comparing NanoCarb and CVAR performance.

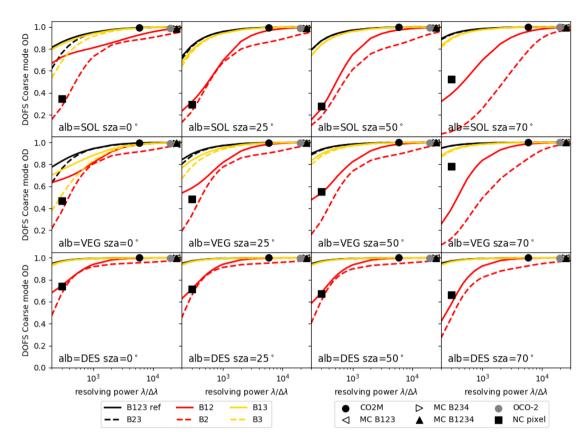


Figure S16. Coarse mode aerosol optical depth degrees of freedom for the fictitious CVAR instrument, for resolving power  $\lambda/\Delta\lambda$  evolving from 200 to 30000 (horizontal axis), and for different spectral band selections: with and without O<sub>2</sub> 0.76  $\mu$ m band (B1, full and dashed-lines, respectively), with both CO<sub>2</sub> 1.6 and 2.05  $\mu$ m bands (B23, black), with only the 1.6  $\mu$ m band (B2, red) and with only the 2.05  $\mu$ m band (B3, yellow), for SOL, VEG and DES albedo models (rows), and SZA values ranging from 0° to 70° (columns). Symbols give the same quantities for NanoCarb (NC, squares), MicroCarb (MC, triangles), CO<sub>2</sub>M (circle) and OCO-2 (grey circle). It should be noted that NanoCarb does not have a spectral resolution per se, the resolving powers used to plot its performance have been solely chosen for the sake of comparing NanoCarb and CVAR performance.

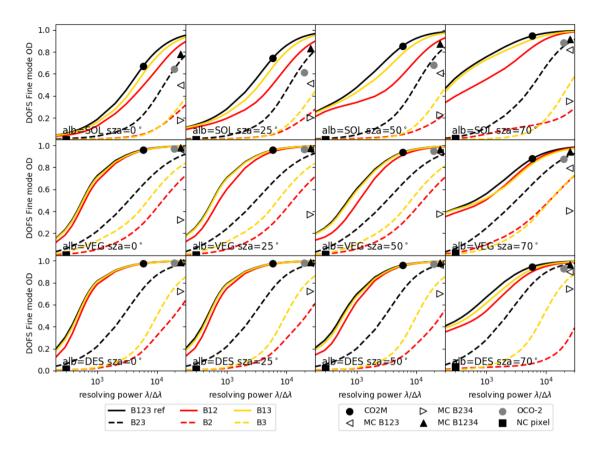


Figure S17. Fine mode aerosol optical depth degrees of freedom for the fictitious CVAR instrument, for resolving power λ/Δλ evolving from 200 to 30000 (horizontal axis), and for different spectral band selections: with and without O<sub>2</sub> 0.76 μm band (B1, full and dashed-lines, respectively), with both CO<sub>2</sub> 1.6 and 2.05 μm bands (B23, black), with only the 1.6 μm band (B2, red) and with only the 2.05 μm band (B3, yellow), for SOL, VEG and DES albedo models (rows), and SZA values ranging from 0° to 70° (columns). Symbols give the same quantities for NanoCarb (NC, squares), MicroCarb (MC, triangles), CO<sub>2</sub>M
(circle) and OCO-2 (grey circle). It should be noted that NanoCarb does not have a spectral resolution per se, the resolving powers used to plot its performance have been solely chosen for the sake of comparing NanoCarb and CVAR performance.

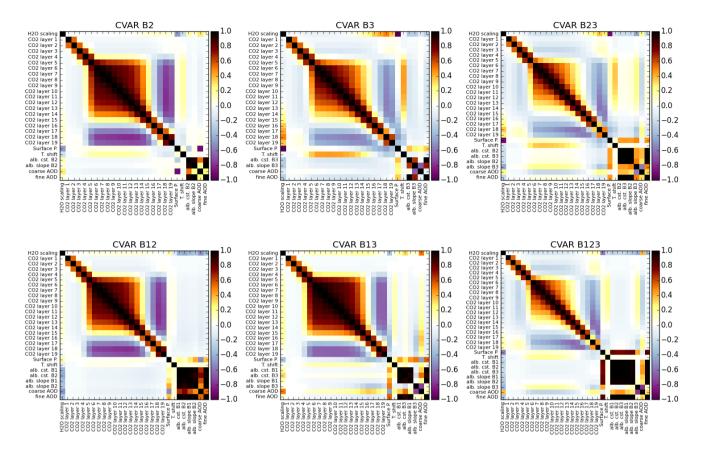


Figure S18. A posteriori correlation matrices for CVAR with a resolving power of 6000 for different spectral band combinations: without and with O<sub>2</sub> 0.76 μm band (B1, top and bottom rows, respectively), with only the 1.6 μm band (B2/B13, left), with only the 2.05 μm band (B3/B13, center), with both CO<sub>2</sub> 1.6 and 2.05 μm bands (B23/B123, right), for the VEG-50° situation.

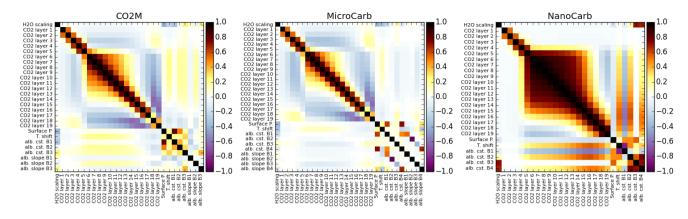


Figure S19. A posteriori correlation matrices for CO<sub>2</sub>M (left), MicroCarb (center) and NanoCarb (right), for the VEG-50° situation, when aerosol optical depth parameters are removed from the state vector.

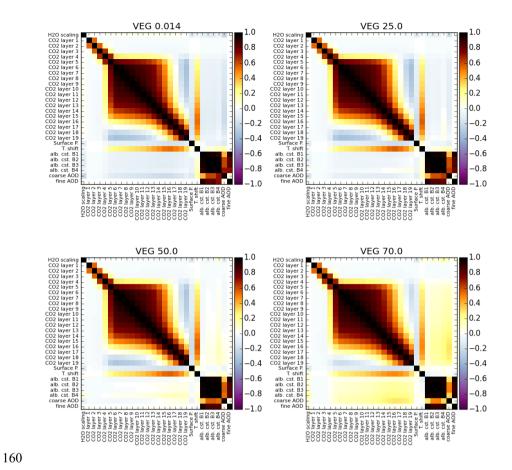


Figure S20. A posteriori correlation matrices for NanoCarb and different SZA values, for the VEG situations.

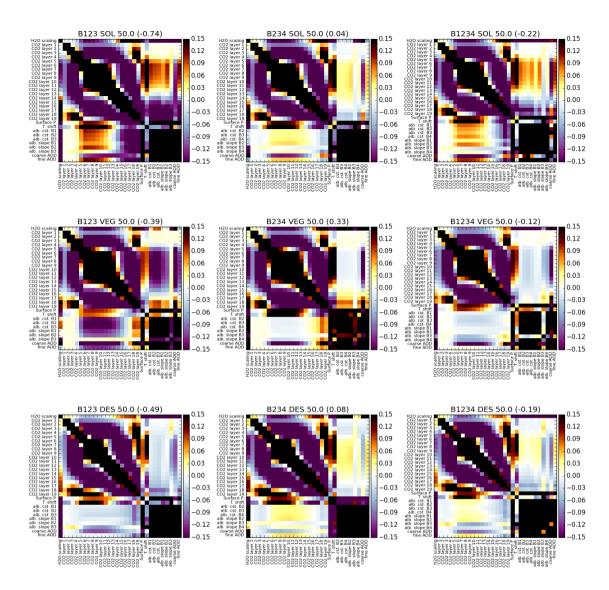


Figure S21. A posteriori correlation matrices for MicroCarb in three different band combination: B123 (left), B234 (center) and B1234 (left), for three different albedo models SOL (top), VEG (center) and DES (bottom), and for a SZA equal to  $50^{\circ}$ . The panel titles give in parenthesis the a posteriori Pearson correlation coefficient between  $X_{CO_2}$  and fine mode aerosol optical depth.