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A new laser-based and ultra-portable gas sensor for indoor and outdoor formaldehyde (HCHO) monitoring

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Table S1. Frequencies and line intensities of HITRAN lines used by HAPP fits

Wavenumber / cm^{-1}	Molecular species	Spectral line intensity (296 K) / cm^{-1} / molecule · cm^{-2}
2831.2598	CH_4	2.863e-22
2831.2701	CH_4	2.308e-25
2831.2737	HCHO	2.101e-20
2831.2780	CH_4	2.471e-22
2831.2802	CH_4	3.408e-25
2831.3160	CH_4	3.394e-23
2831.3259	HCHO	2.900e-21
2831.3366	CH_4	2.603e-25
2831.3501	CH_4	3.240e-25
2831.3550	HCHO	1.420e-20
2831.3657	CH_4	3.587e-25
2831.4055	HDO	1.812e-28
2831.4097	HDO	1.812e-28
2831.4209	**CH_4**	**1.553e-23**
2831.5393	**HCHO**	**5.622e-21**
2831.5534	CH_4	8.870e-25
2831.5576	**HCHO**	**5.543e-21**
2831.5616	**CH_4**	**1.549e-23**
2831.5801	HDO	4.140e-28
2831.6413	**HCHO**	**5.839e-20**
2831.6879	HCHO	1.499e-21
2831.6892	HCHO	1.499e-21
2831.6961	CH_4	6.671e-25
2831.6989	**HCHO**	**1.410e-20**
2831.8134	**HCHO**	**6.509e-21**
2831.8214	CH_4	3.671e-24
2831.8413	**HDO**	**3.014e-24**
2831.8516	CH_4	1.983e-24
2831.8906	HDO	9.812e-28
2831.8948	H_2O	1.595e-28
2831.9199	**CH_4**	**1.622e-21**
2831.9569	HDO	2.713e-27

Spectral lines from the same molecular species are fitted together rather than independently. Lines bolded in blue were used in experiments that utilized ultra-zero air, and it was discovered that all the lines listed produced a more superior fit than only the lines bolded in blue when sampling ambient air. Spectral frequencies and line intensities were accessed using HITRAN on the Web (http://hitran.iao.ru/) (Rothman et al., 2013).

Table S2. 1σ standard deviation for Aeris sensor at various integration times. All values are in pptv and were obtained by either (1) bubbling ultra-zero air (1000 sccm) though water (HDO mode) or (2) adding chemically-pure 99.5% CH_4 (< 1 sccm) to 5000 sccm ultra-zero air (CH_4 mode).

Integration time / s	ART fit HDO mode / pptv HCHO	HAPP fit HDO mode / pptv HCHO	Average of the two HDO modes / pptv HCHO	HAPP fit CH_4 mode / pptv HCHO
30	1200	1000	700	1350
60	1000	800	660	1100
120	730	600	530	720
300	430	380	330	460
900	230	190	180	320
1800	160	140	120	280
3600	140	100	100	230
7200	160	110	110	140
20000	170	160	160	200

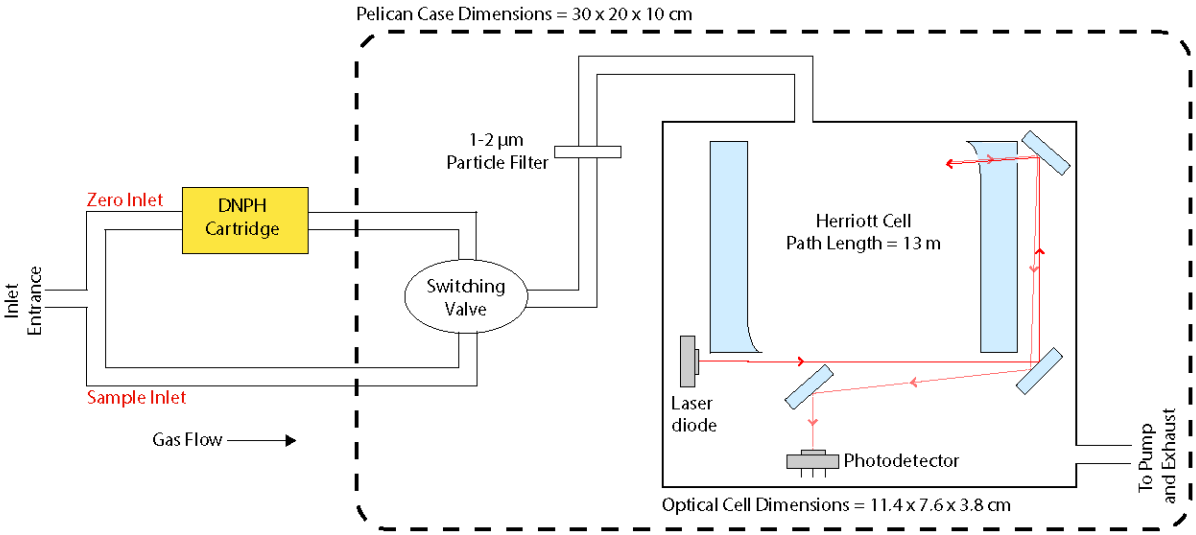

Figure S1. Schematic diagram of the Aeris sensor. Air flows through the inlet entrance, and the switching valve either allows air to pass directly into the instrument via the sample inlet or is first scrubbed of HCHO via the zero inlet. Before entering the Herriott cell, all dust is removed from the air flow with a 1-2 µm particle filter. The patented folded Herriott cell (US Patent #10,222,595) has a path length of 13 m and dimensions of 11.4 x 7.6 x 3.8 cm (Paul, 2019). The laser diode, photodetector, filters, and mirror coatings are proprietary information.

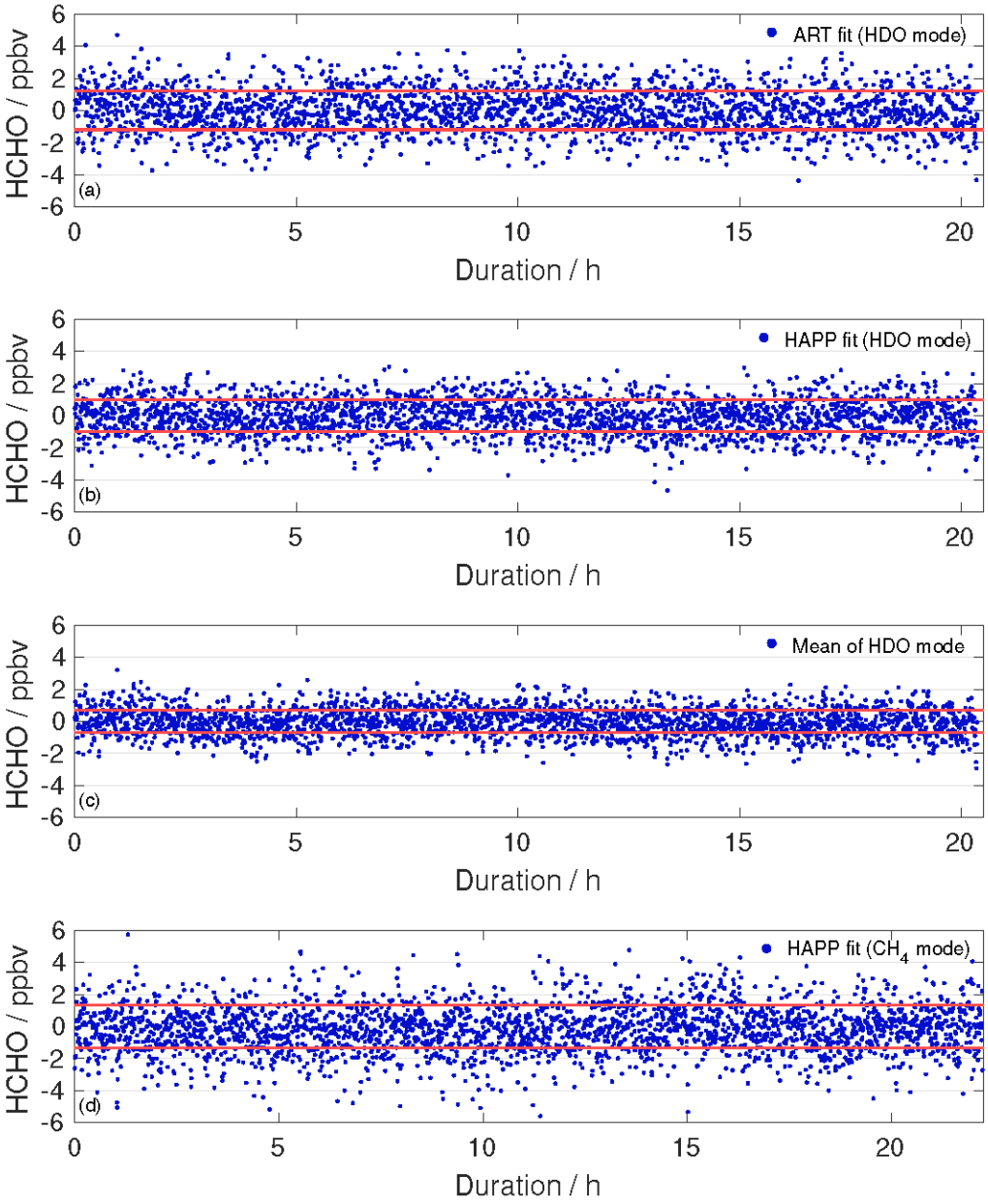

Figure S2. Raw time series data used to derive the Allan-Werle deviation curves in Figure 3. All points shown have an integration time of 30 s and were obtained by flowing ultra zero air through the Aeris sensor for a minimum of 20 h. Red lines indicate ±1σ standard deviation from the mean of the data. Raw data for (a) ART fit (HDO mode), (b) HAPP fit (HDO mode), (c) mean of HDO fits, and (d) HAPP fit (CH_4 mode).

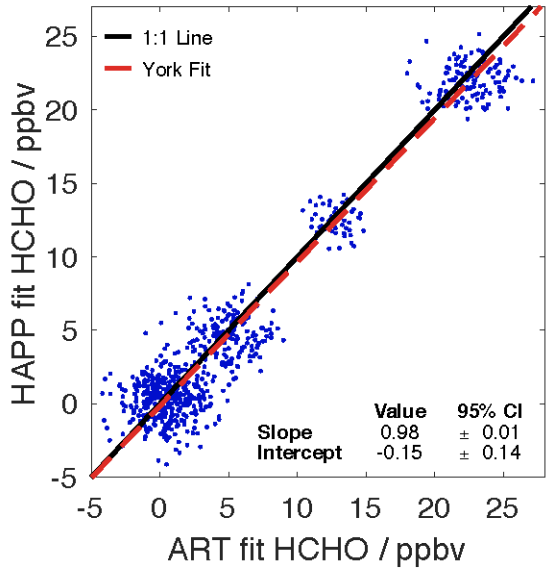

Figure S3. Correlation plot between the Aeris Real-time (ART) fit and the Harvard Aeris-Post Processing (HAPP) fit (R^2 = 0.941).

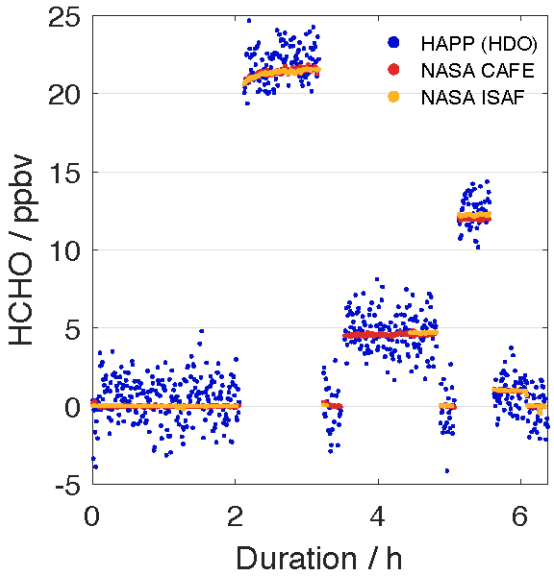

Figure S4. Time series showing the HCHO mixing ratios from the Aeris sensor (HAPP HDO fit) and NASA ISAF and CAFE during a multi–hour stepped intercomparison performed at NASA Goddard in November 2017. All data are reported with an integration time of 30 s.

Paul, J. B.: Compact Folded Optical Multipass System, US Patent #10,222,595. 2019.

Rothman, L. S., Gordon, I. E., Babikov, Y., Barbe, A., Benner, D. C., Bernath, P. F., Birk, M., Bizzocchi, L., Boudon, V., Brown, L. R., Campargue, A., Chance, K., Cohen, E. A., Coudert, L. H., Devi, V. M., Drouin, B. J., Fayt, A., Flaud, J.-M., Gamache, R. R., Harrison, J. J., Hartmann, J.-M., Hill, C., Hodges, J. T., Jacquemart, D., Jolly, A., Lamouroux, J., Le Roy, R. J., Li, G., Long, D. A., Lyulin, O. M., Mackie, C. J., Massie, S. T., Mikhailenko, S., Müller, H. S. P., Naumenko, O. V., Nikitin, A. V., Orphal, J., Perevalov, V., Perrin, A., Polovtseva, E. R., Richard, C., Smith, M. A. H., Starikova, E., Sung, K., Tashkun, S., Tennyson, J., Toon, G. C., Tyuterev, V. G. and Wagner, G.: The HITRAN2012 molecular spectroscopic database, J. Quant. Spectrosc. Radiat. Transf., 130, 4–50, doi:10.1016/J.JQSRT.2013.07.002, 2013.