Supporting Information

Development of an Inexpensive RGB Color Sensor for the Detection of Hydrogen Cyanide Gas

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Abstract:

The supporting information includes the RGB sensor and electronic configuration; gas-flow system configuration for low and high flow tests; LED responsivity spectrum; electrochemical detector response to hydrogen cyanide; explanation of early termination of hydrogen cyanide test; and RGB numerical values when the sensor was exposed to hydrogen cyanide at various relative humidity and times.

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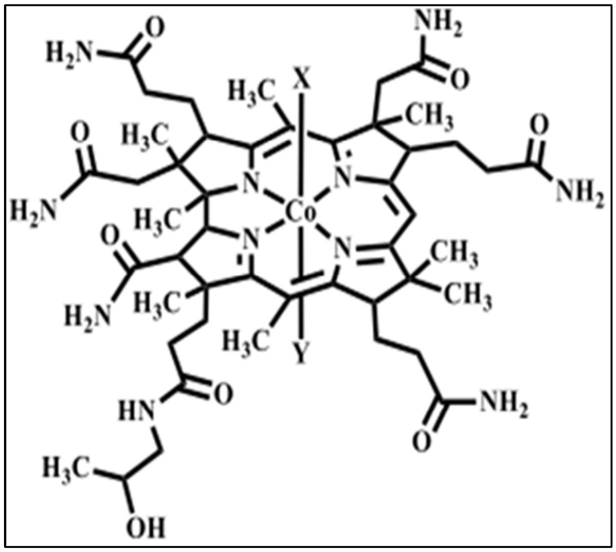

Figure S1—Structure of cobinamide (Cbi). The X and Y ligands can be neutral (e.g., water (H_2O), ammonia (NH_3), nitric oxide (NO), or anionic groups (e.g., OH^-, CN^-, SCN^-).

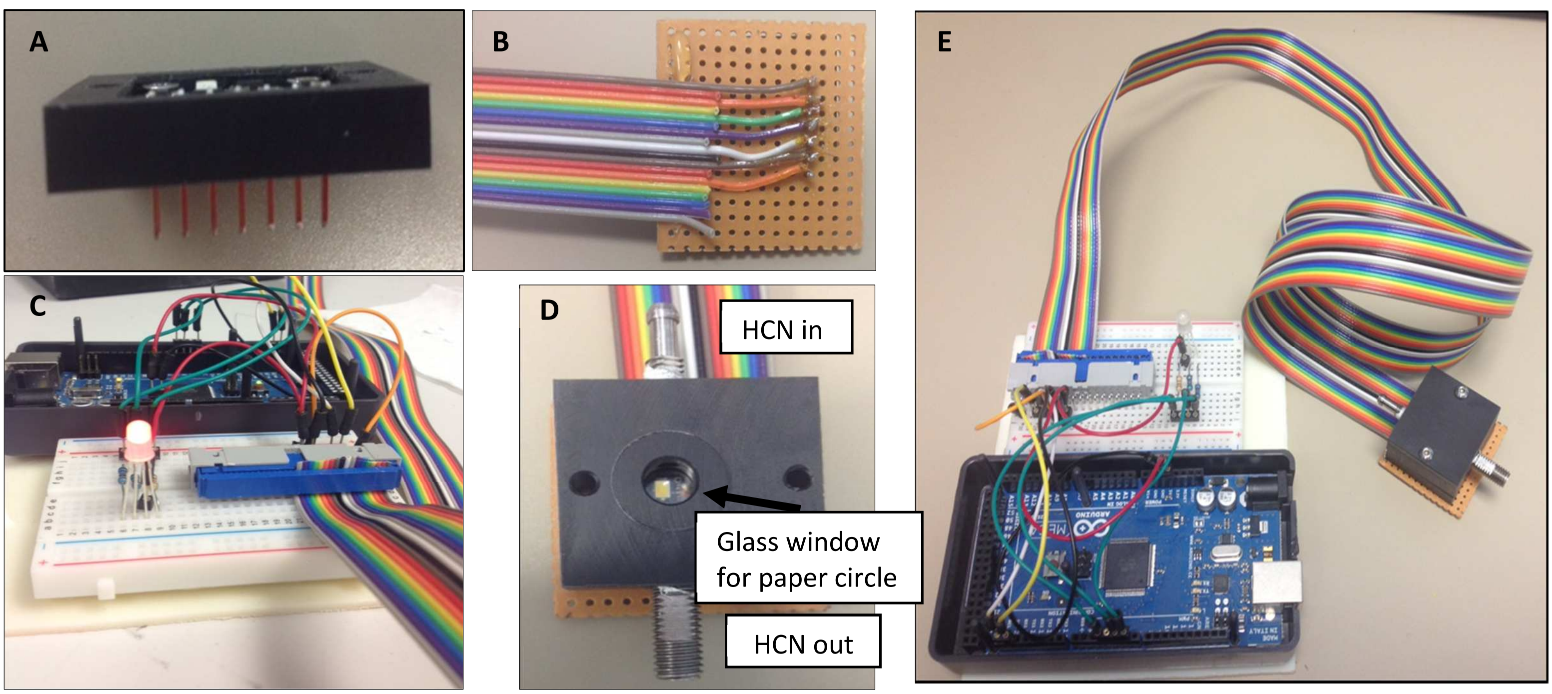

Figure S2—(A). Side view of RGB color sensor test holder with header pins. (B). Bottom view of color sensor test holder with soldered ribbon wires. (C.) Breadboard used to connect RGB color sensor to microcontroller. (D). Top view of glass center piece for placement of the paper circle. (E). Complete prototype of RGB color sensor including breadboard, microcontroller, and RGB color sensor enclosed in test holder.

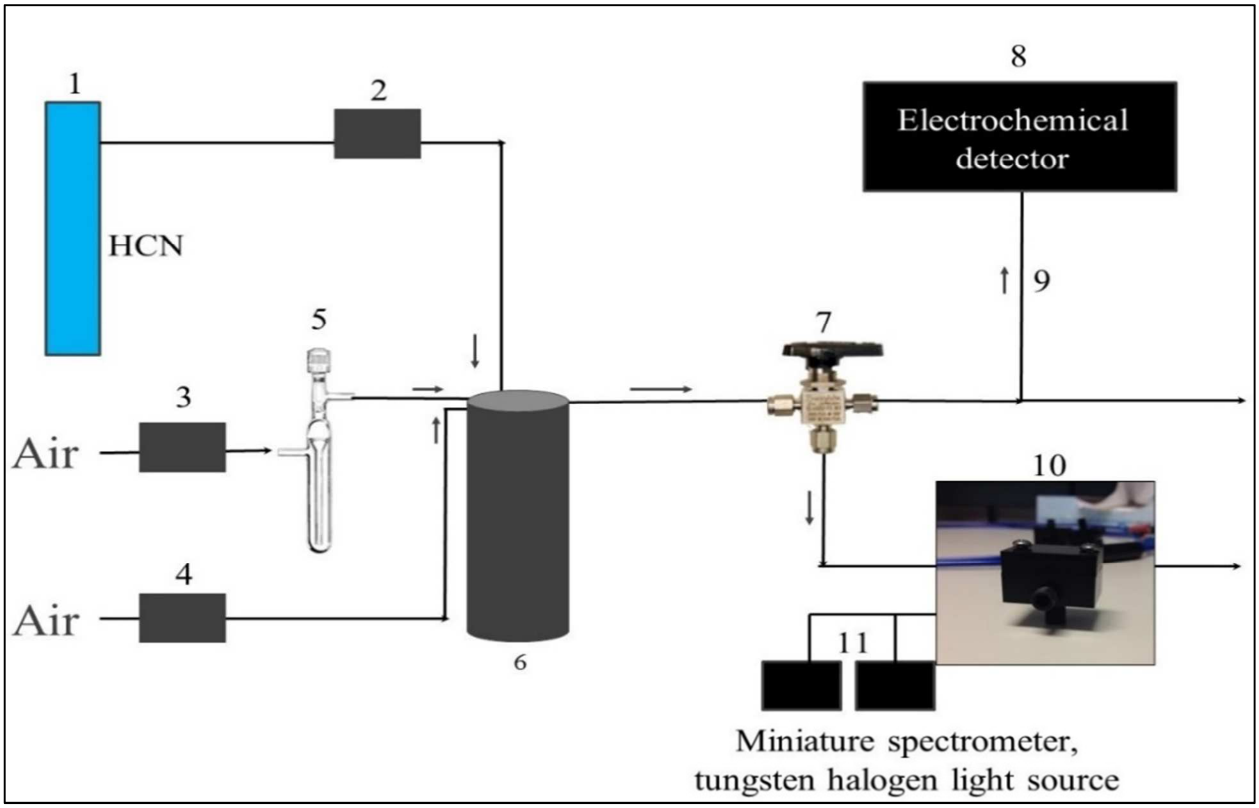

Figure S3—Experimental setup. Certified HCN (495 ± 2% ppm). 2. MFC 1 (0.000–1.000 ± 0.8% LPM). 3. MFC 2 (0.00–10.00 ± 0.8% LPM). 4. MFC 3 (0.00–10.00 ± 0.8% LPM). 5. Water bubbler for %RH control. 6. 1 L gas mixing vessel. 7. 3-way valve. 8. Interscan® HCN electrochemical detector (0.0–50.0 ppm, ± 2%. 9. Interscan® draws air at 0.5 LPM. 10. Sensor holder. 11. Ocean Optics® miniature USB spectrometer and light source (referred throughout as "diffuse reflectance configuration").

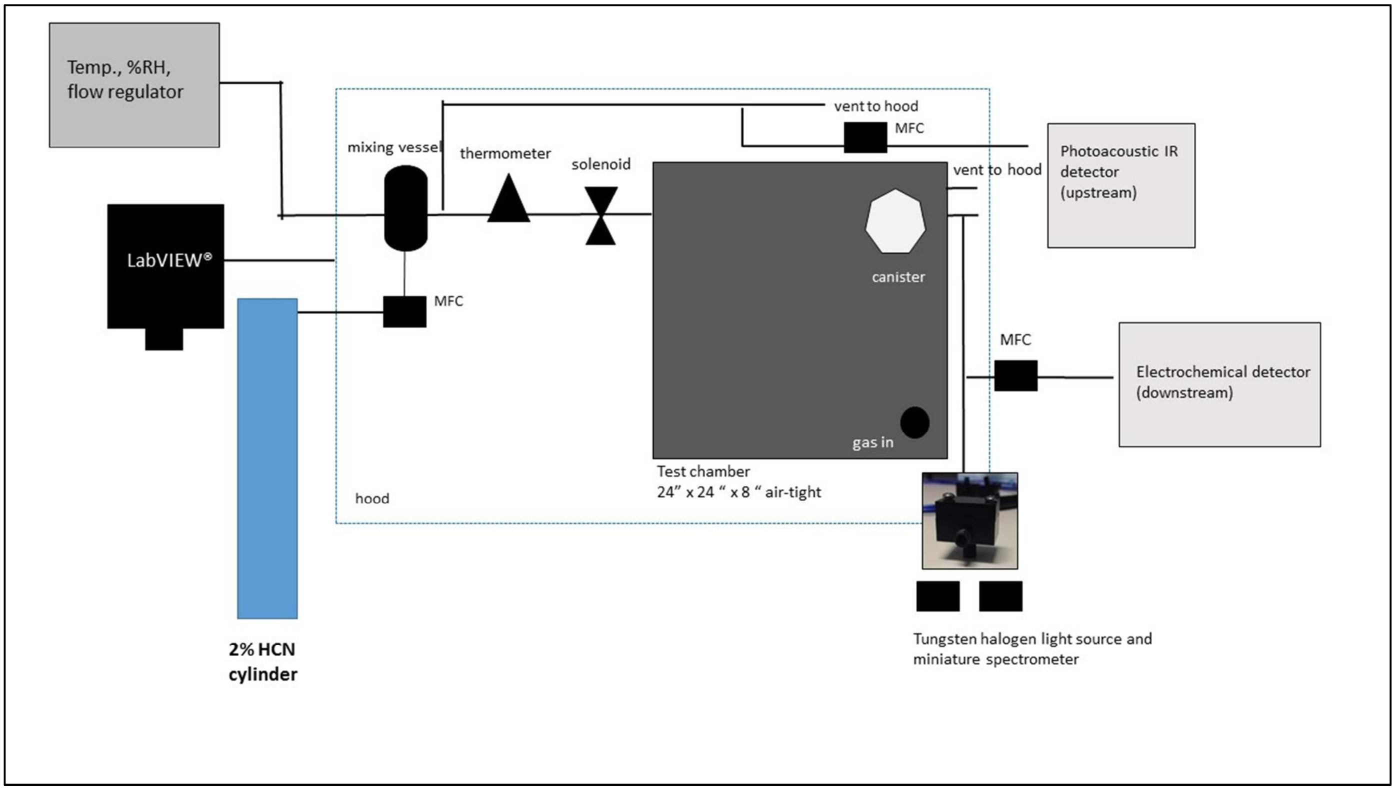

Figure S4—HCN experimental flow setup for breakthrough experiments

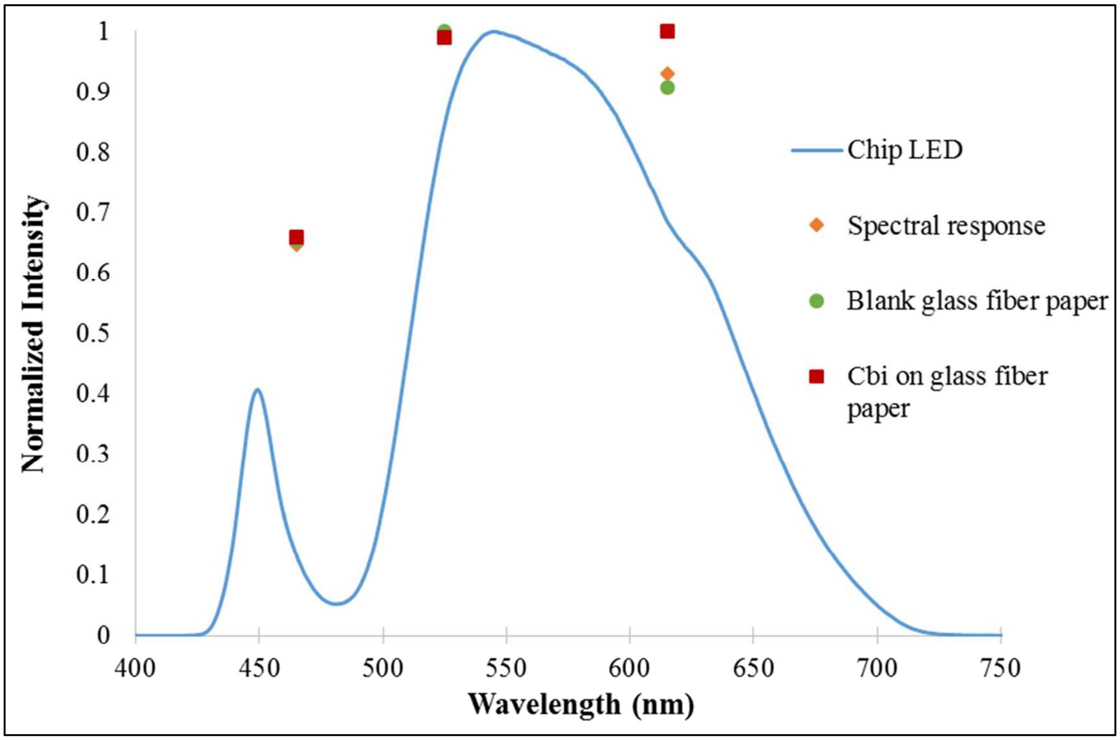

Figure S5—Normalized response of the white on-chip LED spectrum (blue line) using the diffuse reflectance configuration. Spectral response of the photodiodes using a mirror to reflect on-chip LED to photodiodes (diamond) and the responses of blank paper/Cbi on paper as a function of maximum wavelength/color (circle and square respectively) as detected by the RGB color sensor. Data in Tables S1 and S2.

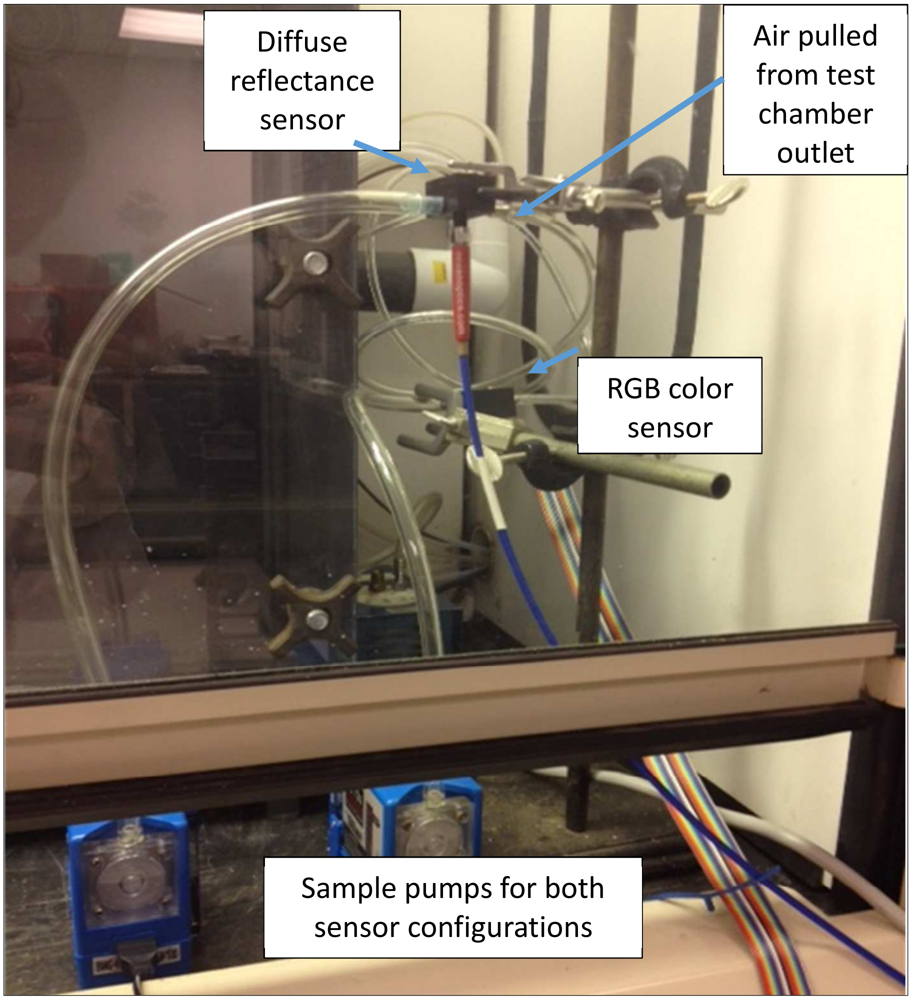

Figure S6—Experimental setup showing placement of the diffuse reflectance sensor and RGB color sensor in the hood and outside of the respirator test chamber.

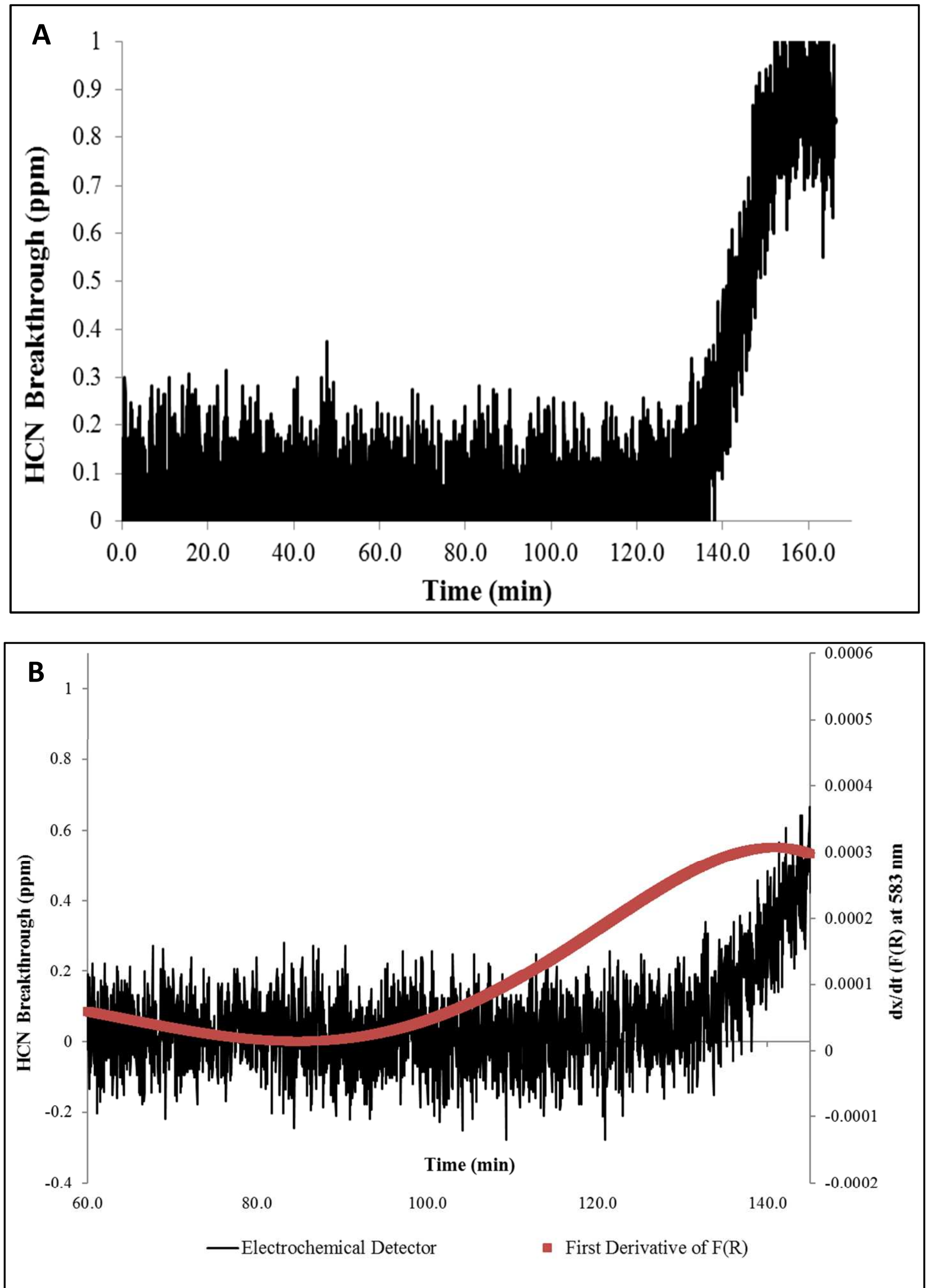

Figure S7—(A). Raw HCN breakthrough data of electrochemical detector. (B). First derivative of the Cbi F(R) spectrum (red) and raw electrochemical detector data (black).

Explanation for early termination of HCN breakthrough experiment: The test was ended prematurely because the 2%, 25.5 ft^3 HCN cylinder ran empty. A slow decrease in concentration began ~ 140 minutes into the test until the challenge gas concentration reached ~10 ppm HCN around 160 minutes. Breakthrough continued to occur through the CBRN canister so the testing was continued to show proof-of-concept of Cbi detection of HCN breakthrough. CBRN canisters are large and densely packed with ASZM-TEDA activated carbon, and are primarily used for first responders and military personnel where unknown, toxic contaminants and concentrations are likely. NIOSH certifies CBRN canisters based on the minimum service-life per manufacturers' request (15, 30, 45, 60, 90, or 120 minutes).[1] This is in part due to the lengthy time for complete breakthrough of these CBRN canisters. NIOSH typically certifies CBRN canisters under designation "Capacity 1" with a test time of 15 minutes. Therefore, tests running to complete breakthrough are not regularly performed, and the time to breakthrough was unknown prior to beginning these experiments. The large carbon bed of the CBRN canisters and lengthy breakthrough times make these tests not economically feasible to run as many replicate measurements as desired to breakthrough. Additionally, gas companies will not prepare concentrations of HCN in cylinders greater than 2% for transiting safety purposes. Comprehensive conclusions cannot be made with the limited amount of breakthrough data for HCN, however both the rapid and slow breakthrough test times show good correlation between the Cbi paper sensor (both using the RGB color sensor and diffuse reflectance configurations) and the electrochemical sensor upon HCN breakthrough.

Table S1—RGB values of blank glass fiber paper and 200.0 µM Cbi on glass fiber paper

Blank Glass Fiber Paper	**R**	**G**	**B**
Average (D.V.)	47110.2	51829.1	33808.5
95 % CI	818.2	898.4	575
% RSD	2.6	2.6	2.6
200.0 µM Cbi on Glass Fiber Paper	**R**	**G**	**B**
Average (D.V.)	41531.2	41118.2	27373.5
95 % CI	888.7	611.6	403.1
%RSD	5.7	4	3.9

Table S2—Normalized values for the spectral sensitivity of the RGB color sensor photodiodes, and response to paper as a function of wavelength maximum/color.

Wavelength Max.	**Spectral sensitivity using mirror (n=6)**	**Blank glass fiber (n=12)**	**Cbi on paper (n=30)**
465 nm (B)	0.65	0.65	0.66
525 nm (G)	1	1	0.99
615 nm (R)	0.93	0.91	1

Table S3—ΔC for $CN(H_2O)Cbi$ on paper at 0.0 ppm HCN over 60 minutes

Sample number	**R**	**G**	**B**	**ΔC**
1				
t = 0 min	42834	41729	28150	
t= 60 min	42961	41912	28169	**223.6**
2				
t = 0 min	40180	40708	27028	
t= 60 min	40260	40890	27100	**211.4**
3				
t = 0 min	40904	41746	27744	
t= 60 min	41050	41832	27759	**170.1**
4				
t = 0 min	40487	40374	27180	
t= 60 min	40519	40581	27150	**211.6**
5				
t = 0 min	41261	41504	27634	
t= 60 min	41322	41681	27599	**190.5**
6				
t = 0 min	38770	39427	26332	
t= 60 min	38829	39580	26302	**166.7**
			Average ΔC	195.6
			S.D.	23.7
			95 % CI	24.8

Table S4—Comparison of ΔC as a function of HCN concentrations and %RH

	Time (min)	Average ΔC 25% RH (n=3)	95% CI	Average ΔC 50% RH (n=3)	95% CI	Average ΔC 85% RH (n=3)	95% CI
Blank							
	1	17.2	28.03	15.7	29.8	14.2	11.9
	15	117.3	165.5	103.1	122.4	127	51.9
1.0 ppm							
	1	239.7	138	733.6	746.8	215.2	165.7
	15	1790.1	335.6	3277.6	45.4	4047.6	613.9
3.0 ppm							
	1	983.6	249.1	1983.9	162.4	2876.5	128.8
	15	2214.4	299.1	3218.5	20.4	3772.5	247.1
5.0 ppm							
	1	1124.4	455.3	2778	1784.2	3358	563.9
	15	2148.2	418.2	3645.4	1687.9	3957.6	921.5
10.0 ppm							
	1	1437.1	236.6	2737.6	242.4	4158	123.5
	15	2519.4	402.8	3539.7	552.3	4214.5	68.5

Reference

1. NIOSH, Determination of CBRN Acid Gases (Hydrogen Cyanide) Service Life Test, Air-Purifying Respirators Standard Test Procedure (STP). NPPTL., Ed. Pittsburgh, 2005.