Supporting Information

Room-to-Room Variability of Airborne PCBs in Schools and the Application of Air Sampling for Targeted Source Evaluation

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Methods and Materials

PUF Extraction

We used accelerated solvent extraction with acetone and hexane (1:1 v/v) to extract PCBs from PUF samples (Tisch Environmental, Cleves, OH, Part # TE-1014). During the ASE preparation, 50 ng of surrogate standards PCB 14 (3,5-dichlorobiphenyl), deuterated PCB 65 (2,3,5,6-tetrachlorobiphenyl -2′,3′,4′,5′,6′-d5), and PCB 166 (2,3,4,4’,5,6-hexachlorobiphenyl) were added to the PUF to allow for correction due to analytical losses and variability. Recoveries of PCB 14 were used to correct the masses of the mono-, di-, and trichlorinated congeners, d-PCB 65 for the tetra- and pentachlorinated congeners, and PCB 166 for the hexa-, hepta-, octa-, nona-, and decachlorinated congeners. Turbulent evaporation with nitrogen (Biotage TurboVap II Concentration Evaporator Workstation) was used to concentrate the extracts. Extracts were cleaned by passing them through sulfuric acid silica gel columns. Samples were then concentrated again, transferred to 2 mL glass autosampler vials, and spiked with 25 ng of internal standard d-PCB 30 (2,4,6-trichlorobiphenyl-2′,3′,4′,5′,6′-d5, C/D/N Isotopes, Pointe-Claire, QC, Canada) and 30 ng of internal standard PCB 204 (2,2′,3,4,4′,5,6,6′-octachlorobiphenyl, Cambridge Isotope Laboratories, Inc.).

Instrument Parameters

The GC was equipped with a Supelco SPB-Octyl capillary column (Poly(50% n-octyl/50% methyl siloxane, 30 m × 0.25 mm ID, 0.25 μm film thicknesses)) with UHP helium as the carrier gas (0.8 mL/min) and UHP nitrogen as the collision gas (1.5 mL/min). The GC operated in solvent vent injection mode at the following injection conditions: initial temperature 45 °C, initial time 0.06 min, ramp 600 °C/min to inlet temperature 325 °C at 4.4 psi. The GC oven temperature program was 45 °C for 2 min, 45 to 75 °C at 100 °C/min and hold for 5 min, 75 to 150 °C at 15 °C/min and hold for 1 min, 150 to 280 at 2.5 °C/min and final hold 5 min (total run time 70.86 min). The triple quadrupole MS electron ionization source was set to 260 °C. The MS-MS operated with the precursor-product transitions in **Table S1**.

The limit of quantification (LOQ) calculated from field blanks (n=3) for each PCB congener or group of co-eluting congeners is in **Table S2**.

Table S1. PCB precursor and product masses of unlabeled and deuterated calibration standards used in multiple reaction monitoring (MRM) mode on the triple quadrupole mass spectrometer[a]

Cl homolog	Precursor Mass	Product Mass
mono	188	152
di	222	152
tri	258	186
tetra	291.9	222
penta	325.9	255.9

hexa	359.8	289.9
hepta	393.8	323.9
octa	429.7	359.8
nona	463.7	393.8
deca	497.7	427.9
D5 tri	261	191
D5 tetra	296.9	277

[a] Unlabeled standards were from AccuStandard, New Haven, CT, USA. Labeled standards were from C/D/N Isotopes, Pointe-Claire, QC, Canada.

Table S2. Limit of quantification (LOQ) for each PCB congener or group of co-eluting congeners in units of nanograms per sample.[a]

PCB	LOQ	PCB	LOQ	PCB	LOQ	PCB	LOQ
1	0.01362	51	0.01939	106	0.000634	161	0.001098
2	0.0090	52	0.13024	107	0	162	0
3	0.02330	54	0.01332	108+124	0.002005	164	0
4	0.01408	55	0.004135	110	0.04368	165	0
5	0.009455	56	0.002099	111	0.000207	167	0
6	0.01690	57	0.000505	112	0.004438	169	0.000697
7	0.01031	58	0.001274	114	0.002736	170	0.001841
8	0.03618	59+62+75	0.02111	115	0.02936	171+173	0.001087
9	0.01049	60	0.001877	117	0.2380	172	0.008322
10	0.01123	61+70+74+76	0.05191	118	0.01122	174	0.002729
11	0	63	0.01078	120	0.000679	175	0.001903
12+13	0	64	0.01398	121	0.001832	176	0.004274
15	0	66	0.005476	122	0.001264	177	0.001376
16	0.01026	67	0.002319	123	0	178	0
17	0.01235	68	0.04684	126	2.731	179	0.00287
18+30	0.03145	72	0.08488	127	0	180+193	0.01018
19	0.005245	73	0.01391	129+138+163	0.02673	181	0.002802
20+28	0.02489	77	0.000546	130	0	182	0.004314
21+33	0.02489	78	0.000281	131	0	183	0.002484
22	0.01678	79	0.002586	132	0.01570	184	0.008796
23	0.002083	80	0.000342	133	0.00267	185	0.000844
24	0.01444	81	0.000599	134	0.003046	186	0
25	0.006013	82	0.01058	135+151	0.01091	187	0.01083
26+29	0.008147	83	0.008363	136	0.004205	188	0.002924
27	0.008567	84	0.02595	137	0.000239	189	0.000415
31	0.02702	85+116	0.1289	139+140	0.004051	190	0.001737
32	0.01027	86+97+109+119	0.01805	141	0.001639	191	0.001911
34	0.002575	87+125	0.04770	142	0	192	0.002033
35	0	88	0	143	0.001187	194	0.003387
36	0.0000402	89	0.000108	144	0.006287	195	0.001792
37	0	90+101+113	0.09897	145	0	196	0.001777
38	0.000311	91	0.005508	146	0.002835	197	0
39	0.000541	92	0.01063	147+149	0.06501	198+199	0.00481
40+71	0.02343	93+100	0.004218	148	0.002136	200	0
41	0.00392	94	0	150	0.000298	201	0.001487
42	0.004858	95	0.08511	152	0.002876	202	0.02519
43	0.01746	96	0.006738	153+168	0.02172	203	0.004443
44+47+65	0.05624	98	0.003914	154	0	205	0.002632
45	0.01252	99	0.01776	155	0.001067	206	0.00703
46	0.10062	102	0.000589	156+157	0	207	0.001742
48	0.01916	103	0	158	0.000373	208	0.004975
49+69	0.02958	104	0.003324	159	0	209	0.05214
50+53	0.05529	105	0.000402	160	0		

[a] The LOQ was calculated as the upper limit of the 99% confidence interval of the mass in the blanks (average + 3*standard deviation).

Determining Sample Volume

The variable K_{PUF} is calculated by the empirical equation (Shoeib[2]):

$$\log K_{PUF} = 0.6366 \log K_{OA} - 3.1774 \qquad \text{(eq S1)}$$

where K_{OA} is calculated by (Herkert[3]):

$$\log K_{OA(T)} = \log K_{OA(25°C)} - \frac{\Delta U_{OA}}{2.303 \times R}\left(\frac{1}{T} - \frac{1}{298.15}\right) \quad \text{(eq S2)}$$

where T is temperature (K), ΔU_{OA} is the internal energy of octanol-air transfer (J mol^{-1}), R is the gas constant (J mol^{-1} K^{-1}). The final concentration in air, C_{air}, is:

$$C_{air} = \frac{M_{PCB}}{V_{eff}} \text{ (eq S3)}$$

where M_{PCB} is the concentration of a PCB (ng).

Windspeed Measurements

The predicted average windspeed used in the Monte Carlo simulation was compared to physical measurements of the unoccupied Practice Gym (**Figure S1**).

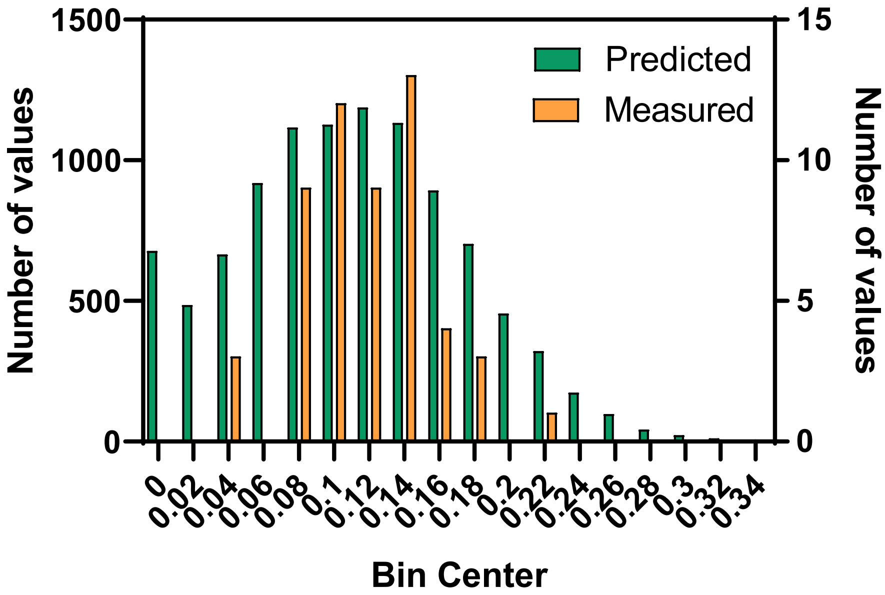


Figure S1. Histogram displaying the distribution of windspeeds found in the WS_{on} parameter used in the Monte Carlo simulation (Predicted, left axis) and in the Practice Gym (Measured, right axis).

Determining Vaporized Aroclor Profiles

Vaporized Aroclor profiles were determined by multiplying the liquid Aroclor profiles by each congener's vapor pressure and were normalized to the sum of all the congeners.[4] Vapor pressures were found from Fischer et al.[5] To test the validity of this method, the vapor pressure normalized profiles of PCBs in paint colorants were compared to the emission profiles of those same colorants using cos θ.[6] The vaporized colorant profiles matched the emission profiles of the colorants better than the concentrations of PCBs in the colorants without vapor pressure normalization.

Table S3. Comparison of the emission profiles of paint colorants to concentration profiles with and without vapor pressure normalization.

Cos θ Between:	D Colorant Concentration	D Colorant with Vapor Pressure Normalization
D (Green) Colorant Emissions	0.035	0.93
Cos θ Between:	DD Colorant Concentration	DD Colorant with Vapor Pressure Normalization
DD (Maroon) Colorant Emissions	0.91	0.99

Results

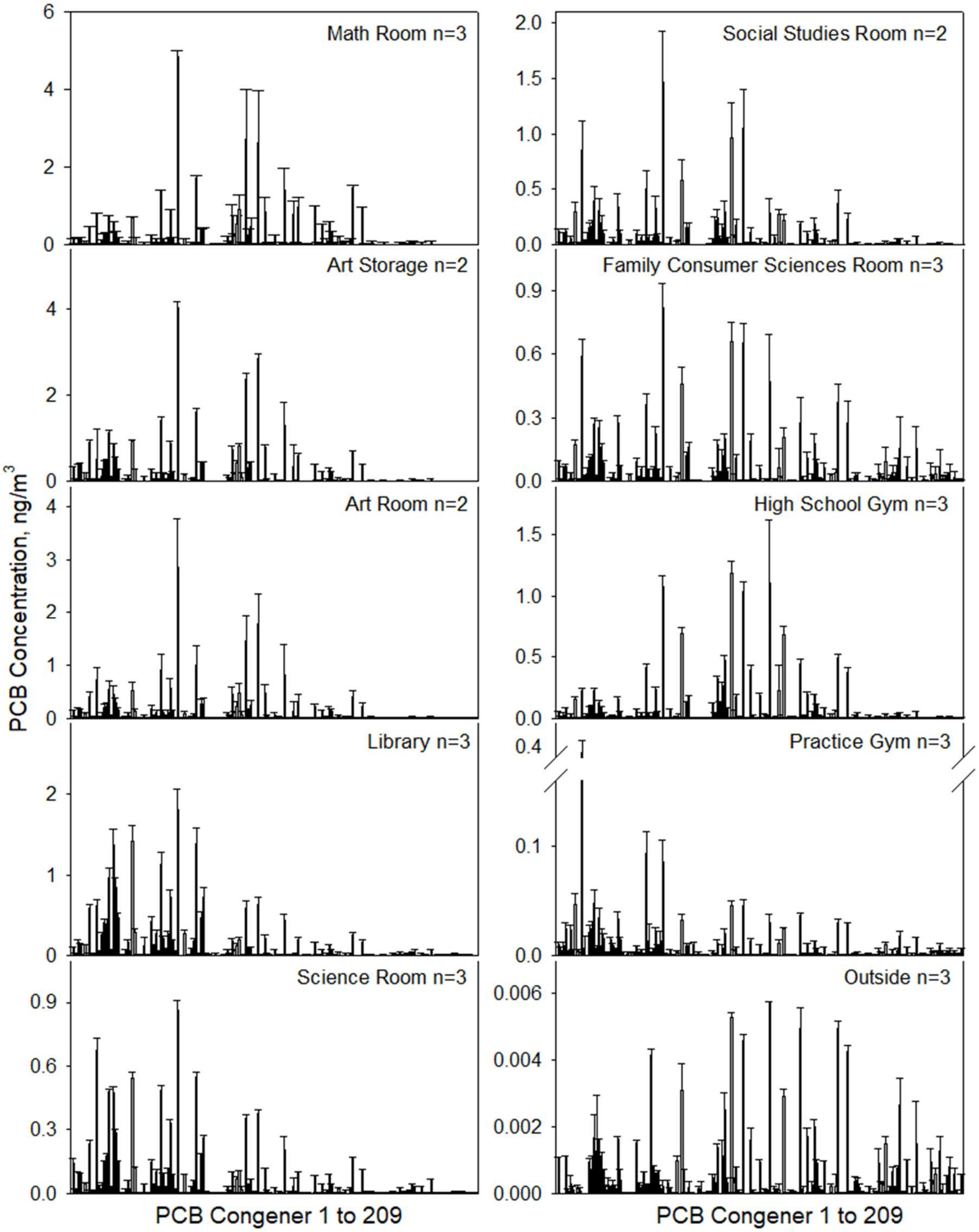


Figure S2. PCB Concentration of 209 congeners in each sampling location. The error bars represent standard deviation for all n=3 and the range (minimum and maximum) for all n=2.

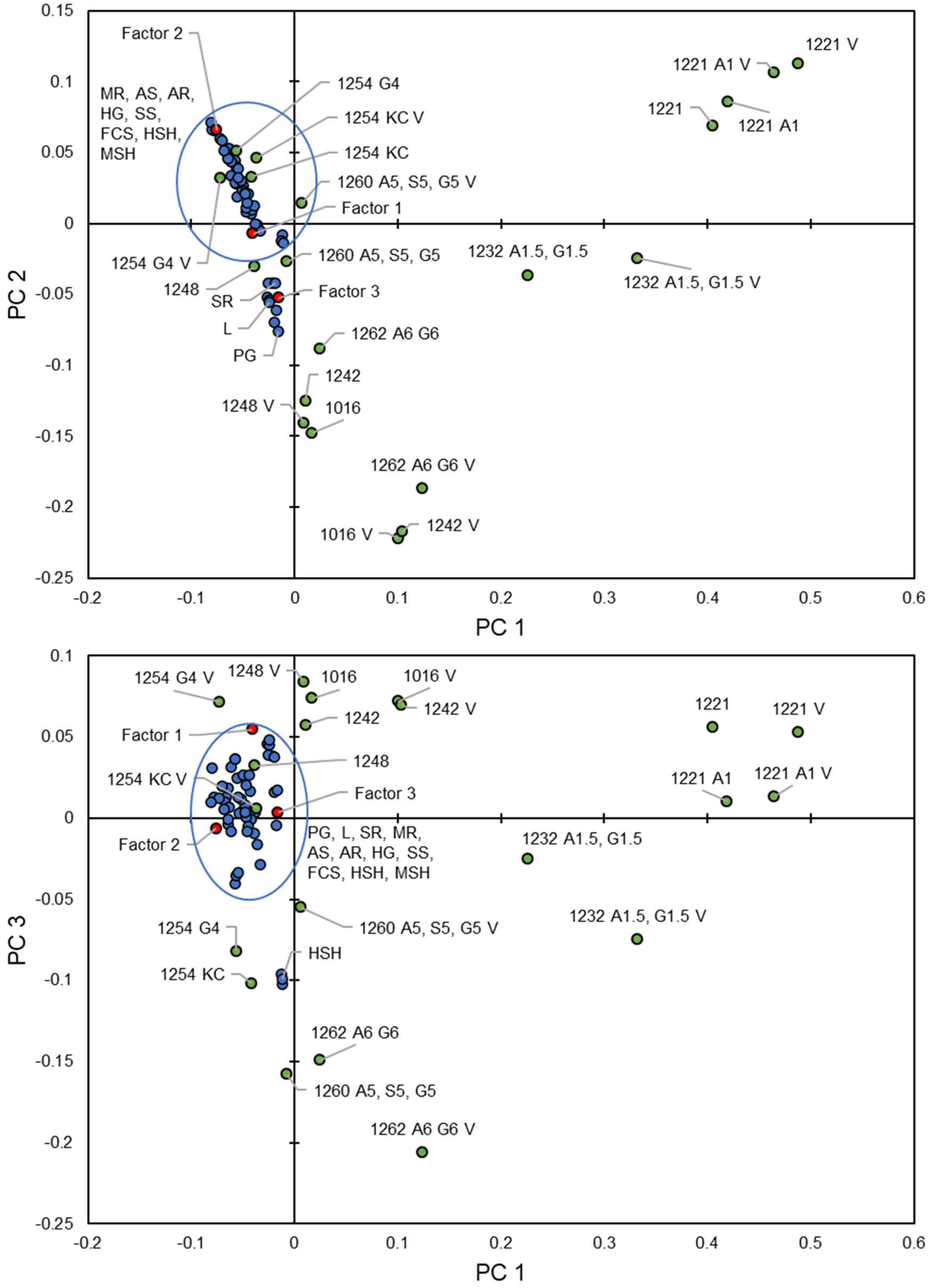
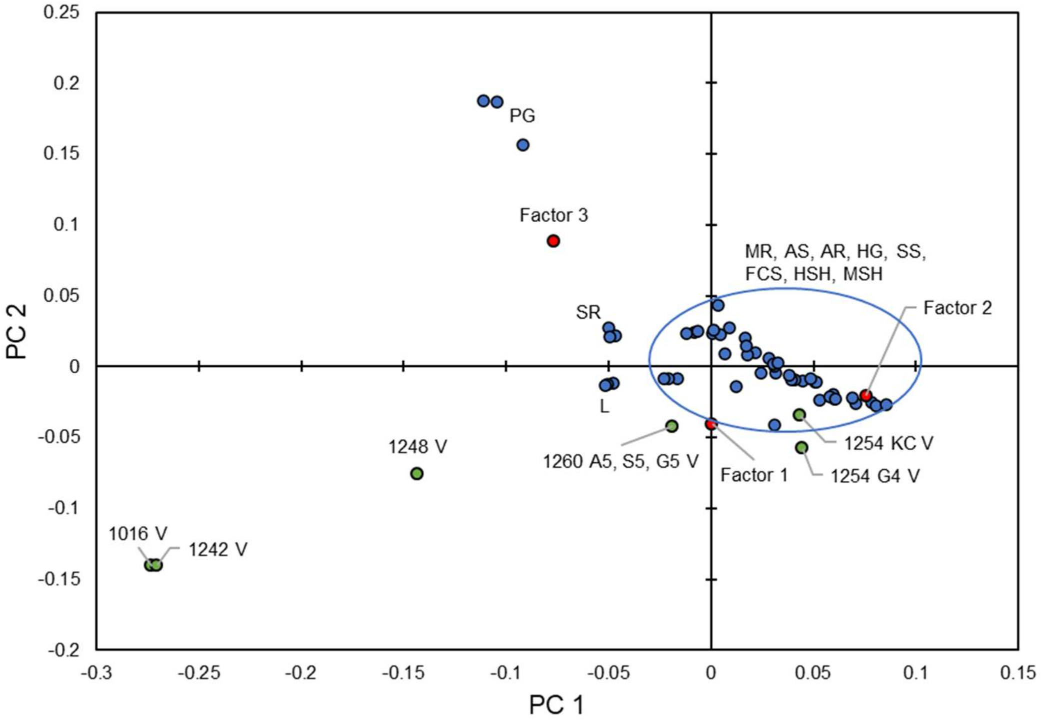
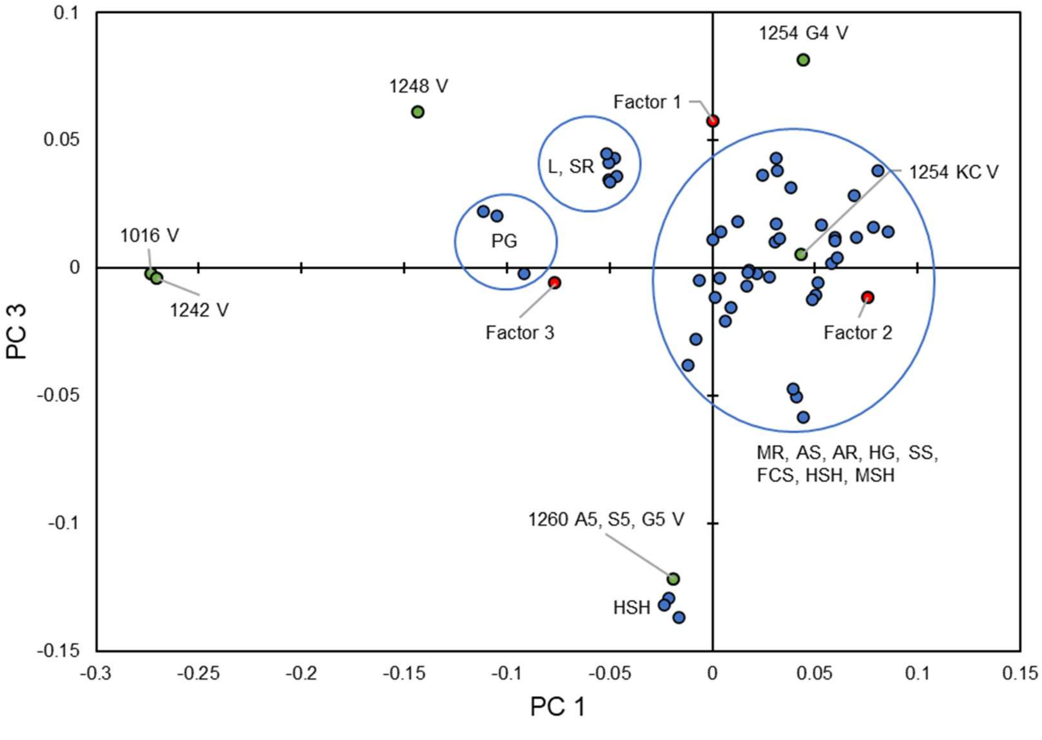


Figure S3. Groupings of PCBs for Principal Component (PC) 2 vs. PC1 (top) and PC3 vs PC1 (bottom). Green markers are Aroclors, red markers are the Factors, and the blue markers are the school air samples. Triplicate samples are shown but some data points overlap. The larger, blue circles indicate samples that are grouped together.


PC 2
PC 1
0.25
0.2
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
-0.2
-0.3
-0.25
-0.2
-0.15
-0.1
-0.05
0
0.05
0.1
0.15
PG
Factor 3
MR, AS, AR, HG, SS,
FCS, HSH, MSH
Factor 2
SR
L
1254 KC V
1248 V
1260 A5, S5, G5 V
Factor 1
1254 G4 V
1016 V
1242 V


PC 3
PC 1
0.1
0.05
0
-0.05
-0.1
-0.15
-0.3
-0.25
-0.2
-0.15
-0.1
-0.05
0
0.05
0.1
0.15
1254 G4 V
1248 V
Factor 1
L, SR
1254 KC V
PG
1016 V
1242 V
Factor 3
Factor 2
MR, AS, AR, HG, SS,
FCS, HSH, MSH
1260 A5, S5, G5 V
HSH

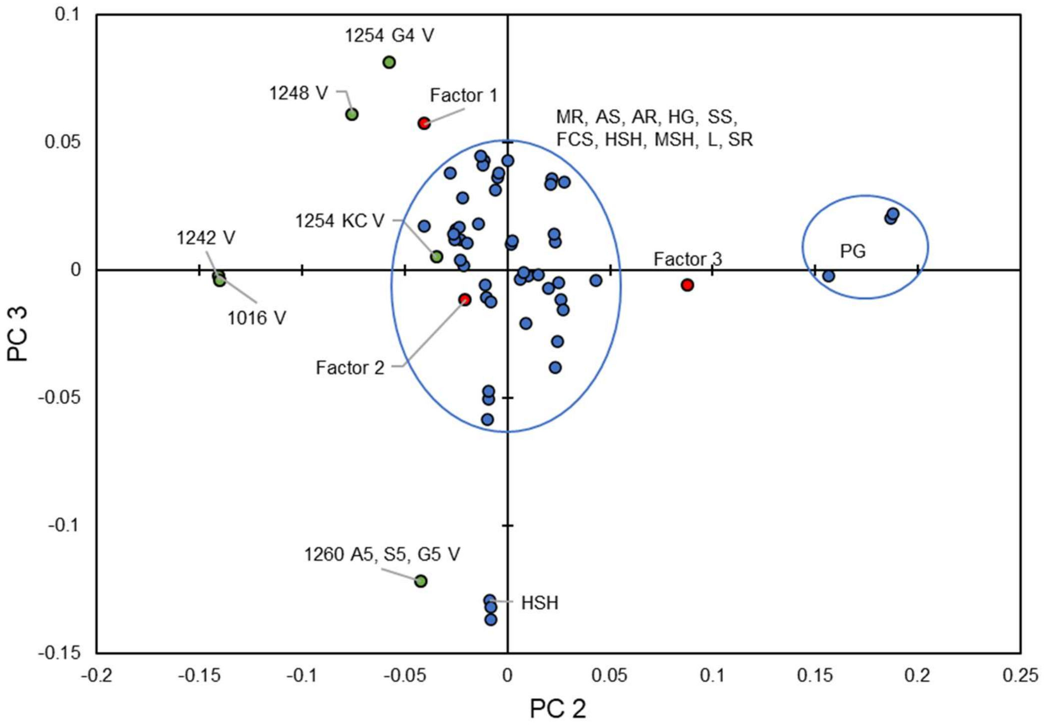


Figure S4. Groupings of PCBs for Principal Component (PC) 2 vs PC1 (top), PC 3 vs PC1 (middle), and PC3 vs PC2 (bottom). Green markers are Aroclors, red markers are the Factors, and the blue markers are the school air samples. Triplicate samples are shown but some data points overlap. Aroclors that did not fit the data well in **Figure S3** have been removed. PC 1 described 42.1% of the data, PC 2 described 24.3% of the data, and PC 3 described 15.9% of the data. Combined these 3 principal components described 82.3% of the data. The larger, blue circles indicate samples that are grouped together.

Literature Cited

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