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Supplement of

An investigation on hygroscopic properties of 15 black carbon (BC)-containing particles from different carbon sources: roles of organic and inorganic components

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Table S1. Bulk elemental compositions determined by elemental analysis and surface elemental compositions determined by X-ray photoelectron spectroscopy (XPS) of different BCPs.

BCPs	Bulk elemental compositions[a]						Surface elemental compositions[b]				
	C (wt%)	O (wt%)	H (wt%)	N (wt%)	S (wt%)	Ash (wt%)	C (wt%)	O (wt%)	N (wt%)	Si (wt%)	S (wt%)
Amaranth	32.08	21.92	2.56	2.63	0.781	40.03	75.21	18.98	4.28	1.05	0.47
Grass	58.8	23.18	3.92	2.285	0.156	11.66	76.02	19.53	2.67	1.42	0.37
Peanuts	49.31	18.35	3.81	1.485	0.874	26.17	71.44	22.52	3.4	2.25	0.4
Pea	64.065	22.19	4.13	1.35	0.454	7.809	74.75	20.56	2.62	1.75	0.32
Rice	54.87	17.4	3.35	0.76	0.315	23.31	73.39	20.37	1.57	4.67	ND[c]
Wheat	50.895	18.85	3.22	0.97	0.405	25.66	69.69	22.86	2.82	4.63	ND[c]
Millet	41.66	20.23	3.09	1.91	0.468	32.64	61.1	29.02	3.84	5.52	0.51
Corn	53.02	16	2.7	1.305	0.39	26.59	76.72	17.88	1.97	3.42	ND[c]
Sorghum	64.35	20.04	4.03	0.835	0.334	10.41	73.28	22.85	1.58	1.96	0.32
Bamboo	68.535	19.86	3.54	0.44	0.168	7.456	76.28	19.39	1.11	2.88	0.34
Red pine	69.985	25.52	3.8	0.22	0.077	0.395	82.9	16.43	ND[c]	0.66	ND[c]
Poplar	71.795	23.63	3.78	0.425	0.129	0.245	86.57	12.59	ND[c]	0.84	ND[c]
Diesel engine soot	36.94	20.05	2.64	3.31	1.652	35.41	78.95	18.72	1.07	1.26	ND[c]
Weifu diesel soot	76.455	18.51	2.19	0.385	0.979	1.482	78.07	21.15	ND[c]	0.78	ND[c]
Household soot	37.075	22.07	2.89	3.655	1.734	32.58	76.09	19.3	2.97	1.05	0.6

[a]Determined by EA. [b]Determined by XPS. [c]Not detected.

Table S2. Elemental composition, ash content, atomic ratio, and polarity index of alkali-extracted organic carbon (OC_{AE}) from three representative BCPs by elemental analysis.

Samples	Compositions (wt%)							
	C	O	H	N	S	H/C	(O+N)/C	Ash
Grass OC_{AE}	28.16	27.14	3.02	1.41	0.49	0.11	1.01	39.78
Wheat OC_{AE}	18.61	21.98	2.71	0.46	0.91	0.15	1.21	55.33
Household soot OC_{AE}	56.56	31.31	5.03	6.14	0.96	0.09	0.66	ND[a]

[a]Not detected.

Table S3. Ratio of the peak intensities of D band (1350 cm^{-1}) to G band (1582 cm^{-1}) of Raman spectra for different BCPs.

BCPs	I_D/I_G[a]
Amaranth	1.01
Grass	0.88
Peanuts	0.89
Pea	0.85
Rice	1.09
Wheat	0.98
Millet	0.86
Corn	0.94
Sorghum	0.9
Bamboo	1.09
Red pine	0.59
Poplar	0.57
Diesel engine soot	1.04
Weifu diesel soot	1.12
Household soot	0.77

Table S4. Porosity properties of different BCPs.

BCPs	V_{mic}[a] (m^3 g^{-1})	V_{mes}[b] (m^3 g^{-1})
Amaranth	0.001	0.003
Grass	0.003	0.005
Peanuts	0.001	0.001
Pea	0.003	0.002
Rice	0.013	0.01
Wheat	0.005	0.005
Millet	0.004	0.019
Corn	0.015	0.013
Sorghum	0.001	0
Bamboo	0.025	0.004
Red pine	0.03	0.002
Poplar	0.048	0.023
Diesel engine soot	0.008	0.013
Weifu diesel soot	0.068	0.416
Household soot	0.003	0.009

[a]Micropore volume, calculated using the Horvath-Kawazoe method.

[b]Mesopore volume, determined by subtraction of micropore volume from total pore volume which is shown in Table 1.

Table S5. Salinities of water extracts of different BCPs (BCPs to water ratio: 1/10, w/w).

BCPs	Salinity (‰)
Amaranth	0.180
Grass	0.080
Peanuts	0.070
Pea	0.060
Rice	0.010
Wheat	0.097
Millet	0.133
Corn	0.030
Sorghum	0.080
Bamboo	0.010
Red pine	0.000
Poplar	0.010
Diesel engine soot	0.060
Weifu diesel soot	0.057
Household soot	0.217

Table S6. Mineral compositions of different BCPs measured by X-ray fluorescence spectroscopy (XRF).

BCPs	Mineral compositions (%)																	
	SO_3	CaO	P_2O_5	Al_2O_3	ZnO	SiO_2	Fe_2O_3	Cl	K_2O	MgO	Na_2O	MnO	CuO	PbO	NiO	TiO_2	Cr_2O_3	BaO	Sr
Amaranth	0.500	1.070	0.240	0.480	0.002	1.730	0.210	0.170	2.140	1.060	0.130	0.006	0.001	ND[a]	ND[a]	0.022	ND[a]	0.007	0.002
Grass	0.092	0.290	0.360	0.037	0.001	1.500	0.014	0.140	2.380	ND[a]	ND[a]	0.004	ND[a]	ND[a]	ND[a]	ND[a]	0.001	ND[a]	ND[a]
Peanuts	0.120	0.510	0.320	0.310	0.002	1.920	0.073	0.038	1.260	0.360	0.058	0.015	ND[a]	ND[a]	ND[a]	0.011	ND[a]	ND[a]	ND[a]
Pea	0.120	0.480	0.120	0.016	N.D.	0.120	0.007	0.008	0.770	0.340	0.021	N.D.	ND[a]	ND[a]	ND[a]	ND[a]	ND[a]	ND[a]	ND[a]
Rice	0.024	0.050	0.030	0.016	0.001	2.630	0.005	0.006	0.220	0.023	ND[a]	0.006	ND[a]	ND[a]	ND[a]	ND[a]	ND[a]	ND[a]	ND[a]
Wheat	0.160	0.230	0.110	0.085	ND[a]	4.020	0.039	0.490	1.720	0.100	0.036	0.009	ND[a]	ND[a]	ND[a]	0.005	ND[a]	ND[a]	ND[a]
Millet	0.210	0.360	0.340	0.040	0.007	5.750	0.028	0.160	2.290	0.790	ND[a]	0.007	ND[a]	ND[a]	0.002	ND[a]	ND[a]	0.011	ND[a]
Corn	0.160	0.360	0.150	0.110	N.D.	3.740	0.038	0.260	1.200	0.190	0.027	0.022	ND[a]	0.004	ND[a]	0.007	ND[a]	ND[a]	ND[a]
Sorghum	0.190	0.710	0.059	0.047	0.002	0.500	0.025	0.300	1.820	0.320	0.037	0.002	ND[a]	ND[a]	ND[a]	ND[a]	ND[a]	ND[a]	ND[a]
Bamboo	0.120	0.110	0.180	0.260	0.003	1.280	0.029	0.130	1.630	0.110	ND[a]	0.016	ND[a]	ND[a]	ND[a]	0.003	ND[a]	ND[a]	ND[a]
Red pine	0.010	0.110	0.008	0.006	N.D.	0.026	0.002	0.002	0.072	0.230	ND[a]	0.005	ND[a]	ND[a]	ND[a]	ND[a]	ND[a]	ND[a]	ND[a]
Poplar	0.150	0.980	0.280	0.019	0.003	0.220	0.010	0.046	1.040	0.025	ND[a]	0.004	ND[a]	ND[a]	ND[a]	ND[a]	ND[a]	ND[a]	ND[a]
Diesel engine soot	2.890	1.090	0.200	0.180	N.D.	0.900	3.090	0.100	0.067	0.100	0.054	0.013	ND[a]	ND[a]	0.013	0.019	0.010	0.013	ND[a]
Weifu soot	0.250	0.230	0.094	0.036	0.019	0.016	0.014	0.006	0.002	0.170	ND[a]	0.001	0.002	0.003	0.001	ND[a]	0.002	ND[a]	ND[a]
Household soot	1.530	1.730	0.130	0.740	0.005	2.550	0.230	2.070	0.960	0.240	0.055	0.037	ND[a]	ND[a]	ND[a]	0.051	ND[a]	0.012	0.002

[a]Not detected.

Table S7. Ionic constituents of different BCPs measured by ion chromatography.

BCPs	Ionic contents (mg g^{-1})											
	Na^{+}	NH_4^{+}	K^{+}	Mg^{2+}	Ca^{2+}	Cl^{-}	COO^{-}	$C_2O_4^{2-}$	SO_4^{2-}	NO_3^{-}	PO_4^{3-}	F^{-}
Amaranth	1.6	0.77	9.52	7.64	0.86	13.46	ND[a]	ND[a]	14.9	0.17	1.94	0.09
Grass	1.71	2.37	6.4	0.72	2.57	8.43	0.79	0.54	2.27	0.22	2.7	0.1
Peanuts	0.4	0.36	5.79	0.41	0.43	0.69	0.04	2.07	3.72	0.05	0.67	0.34
Pea	2.03	2.26	4.74	0.78	1.43	0.28	0.06	2.69	5.56	0.1	0.45	0.15
Rice	0.57	2.69	0.13	0.11	0.26	0.06	0.01	1.06	0.63	0.01	0.16	0.01
Wheat	0.79	1.58	7.5	0.19	0.47	3.92	0.03	ND[a]	6.95	0.16	0.73	ND[a]
Millet	2.42	2.62	10.55	1.77	1.61	1.22	0.18	15.37	7.98	0.07	1.63	0.14
Corn	0.19	1.93	2.13	0.28	0.51	4.42	0.05	0.87	3.38	0.02	0.91	0.03
Sorghum	0.74	0.57	5.94	0.63	1	1.72	0.06	0.76	4.63	0.11	0.22	0.29
Bamboo	0.25	2.67	0.11	0.11	0.24	0.04	0.03	0.85	0.87	0.02	0.25	0.01
Red pine	0.15	1.28	0.15	0.05	0.13	0.05	0.02	N.D.	0.14	0.06	0.08	0.003
Poplar	0.1	0.55	0.42	0.17	0.38	0.28	0.01	0.07	0.38	0.01	0.24	0.5
Diesel engine soot	1.72	4.88	0.35	0.97	3.74	0.31	0.13	1.76	30.06	0.15	0.39	0.6
Weifu soot	1.15	0.13	0.07	0.29	3.65	0.19	ND[a]	ND[a]	23.51	0.2	5.41	0.42
Household soot	1.2	19.71	2.69	1.7	4.85	47.51	ND[a]	ND[a]	26.63	0.96	ND[a]	0.36

[a]Not detected.

Table S8. Accuracy (R^2 and P) values for regression on equilibrium water uptake against compositional and pore property parameters at different relative humidity (RH) levels.

Composition	23% RH		33% RH		43% RH		47% RH		75% RH		84% RH		94% RH	
	R^2	P	R^2	P	R^2	P	R^2	P	R^2	P	R^2	P	R^2	P
OC_{TGA}	0.32	0.028	0.36	0.0187	0.4	0.0113	0.47	0.0048	0.7	0.0001	0.82	$<$0.0001	0.52	0.0002
OC_{AE}	0.12	0.207	0.14	0.1652	0.17	0.1311	0.22	0.08	0.41	0.0097	0.64	0.0004	0.8	0.0001
EC	0.21	0.083	0.21	0.087	0.22	0.0798	0.25	0.06	0.39	0.0122	0.51	0.003	0.54	0.0019
Dissolved minerals	0.1	0.2471	0.11	0.23	0.12	0.2111	0.39	0.15	0.27	0.0468	0.45	0.0064	0.86	0.0001
NH_4^+	0.1	0.2548	0.13	0.19	0.16	0.1444	0.21	0.09	0.42	0.0092	0.6	0.0007	0.54	0.0034
Cl^-	0.04	0.4635	0.06	0.39	0.07	0.3305	0.11	0.23	0.24	0.0619	0.43	0.0076	0.7	0.0001
$C_2O_4^{2-}$	0.06	0.1938	0.05	0.2088	0.05	0.2120	0.05	0.2057	0.03	0.2415	0.02	0.2752	0.002	0.8893
SO_4^{2-}	0.02	0.6518	0.01	0.7	0.006	0.7933	0.00003	0.95	0.06	0.395	0.15	0.1588	0.24	0.06
Total porosity	0.42	0.0095	0.4	0.01	0.39	0.0129	0.37	0.02	0.29	0.0368	0.22	0.0761	0.08	0.3
K^+	0.19	0.1088	0.16	0.139	0.14	0.1647	0.14	0.1764	0.09	0.2664	0.1	0.245	0.27	0.045

Table S9. Fitting parameters for water uptake kinetics of BCPs by pseudo-first-order model at different relative humidity (RH) levels.

BCPs	33% RH				47% RH				94% RH			
	k_1[a] (10^{-5} s^{-1})	Q_e (cal)[b] (mg g^{-1})	Q_e (exp)[c] (mg g^{-1})	R^2	k_1[a] (10^{-5} s^{-1})	Q_e (cal)[b] (mg g^{-1})	Q_e (exp)[c] (mg g^{-1})	R^2	k_1[a] (10^{-5} s^{-1})	Q_e (cal)[b] (mg g^{-1})	Q_e (exp)[c] (mg g^{-1})	R^2
Amaranth	2±2	9±1	18±1	0.9879	2.01±0.03	22±2	30±1	0.9885	10±0	290±40	270±3	0.9993
Grass	3±2	10±2	16±3	0.9792	2±2	21±1	38±4	0.9359	0.9±0.1	120±10	180±6	0.9723
Peanuts	2±2	6±1	27±1	0.983	2±1	13±0	41±2	0.9154	10±0	100±10	140±4	0.9558
Pea	1±1	9±3	27±1	0.9979	2±3	15±2	45±6	0.9571	0.9±0.2	55±3	120±6	0.9258
Rice	0.4±0.1	5±2	21±4	0.9759	0.8±0.1	6±0	29±2	0.8805	1.4±0.1	25±0	55±3	0.8778
Wheat	1±1	9±2	21±5	0.948	3±1	15±4	40±4	0.9998	1.5±1.3	230±60	240±2	0.8017
Millet	2±1	13±0	38±5	0.9831	3±2	12±3	54±2	0.9804	1.3±0.6	96±7	190±7	0.8805
Corn	0.7±0.1	7±1	19±6	0.9042	3±1	15±2	28±0	0.9643	1.3±0.6	62±6	96±3	0.9663
Sorghum	1±1	12±1	30±13	0.9491	0.9±0.1	11±3	44±2	0.9709	1.3±0.6	130±12	190±10	0.9564
Bamboo	1±0	7±6	33±3	0.9159	0.6±0.4	10±2	50±8	0.9138	2±1	19±1	72±9	0.8948
Redpine	0.7±0.1	4.2±0.2	22±2	0.8172	5±3	20±6	39±1	0.8068	1±1	20±5	68±2	0.8252
Poplar	0.7±0.1	6.02±1.21	26±2	0.8745	2±1	8±2	33±2	0.8218	0.9±0.2	18±2	63±2	0.8771
Diesel engine soot	0.8±0.3	2.2±0.3	13±1	0.9932	0.8±0.4	8±3	30±7	0.9462	2±1	90±21	140±4	0.9686
Weifu diesel soot	0.4±0.1	14±5	21±14	0.8009	3±1	12±1	32±7	0.8926	6±1	31±7	69±6	0.9858
Household soot	1±0	2.12±0.01	9±1	0.8569	3±1	17±4	29±2	0.9524	1±1	410±40	420±20	0.9889

[a]Pseudo-first-order rate constant. [b]Model calculated maximum sorbed concentration at equilibrium. [c]Measured maximum sorbed concentration at equilibrium.

Table S10. Fitting parameters for water uptake kinetics of BCPs by pseudo-second-order model at different relative humidity (RH) levels.

BCPs	33% RH				47% RH				94% RH			
	k_2[a] (10^{-5} g mg^{-1}s^{-1})	Q_e (cal)[b] (mg g^{-1})	Q_e (exp)[c] (mg g^{-1})	R^2	k_2[a] (10^{-5} g mg^{-1}s^{-1})	Q_e (cal)[b] (mg g^{-1})	Q_e (exp)[c] (mg g^{-1})	R^2	k_2[a] (10^{-7} g mg^{-1}s^{-1})	Q_e (cal)[b] (mg g^{-1})	Q_e (exp)[c] (mg g^{-1})	R^2
Amaranth	0.5±0.1	18±1	18±1	0.9954	0.14±0.01	34±1	30±1	0.9963	0.31±0.02	330±11	260±4	0.9943
Grass	0.52±0.04	17±2	16±3	0.9963	0.20±0.03	40±3	38±4	0.9984	1.7±0.1	190±5	170±6	0.9975
Peanuts	2±1	28±0	27±1	0.995	0.6±0.2	41±2	41±2	0.9983	2.6±0.2	150±3	140±4	0.9974
Pea	0.8±0.2	28±1	27±1	0.9967	0.5±0.1	46±7	45±6	0.9987	5.3±0.4	120±5	120±6	0.9984
Rice	1.7±0.3	21±4	21±4	0.9955	5±2	28±2	29±2	0.9917	28±2	55±4	55±3	0.9985
Wheat	0.7±0.1	21±5	21±5	0.9945	1.2±0.1	37±9	40±4	0.9959	0.5±0.1	290±0	240±3	0.9889
Millet	0.6±0.2	39±5	38±5	0.9995	0.8±0.2	54±2	54±2	0.9997	3.1±0.2	190±7	180±7	0.9993
Corn	2±2	19±5	19±6	0.9986	0.36±0.01	29±1	28±0	0.9984	4.2±0.5	100±3	96±3	0.9959
Sorghum	0.34±0.03	29±6	30±13	0.9912	1.01±0.44	45±2	44±2	0.9986	1.7±0.1	210±11	190±10	0.9958
Bamboo	1.5±0.4	34±3	33±3	0.9978	4±2	50±8	50±8	0.9992	33±3	71±10	73±9	0.9961
Redpine	1.6±0.1	22±2	22±2	0.9938	0.43±0.01	40±1	39±1	0.9983	21±4	70±2	69±2	0.9991
Poplar	2±1	24±3	24±3	0.9996	0.55±0.04	33±2	32±2	0.9991	23±4	63±2	63±2	0.9985
Diesel engine soot	1.6±0.4	13±1	13±1	0.9931	0.6±0.1	30±4	30±4	0.9947	3.2±0.1	150±5	140±5	0.9987
Weifu soot	0.5±0.1	21±14	21±14	0.9706	0.9±0.3	31±7	32±7	0.9908	86±95	72±16	70±6	0.9954
Household soot	5±2	9±0	5±6	0.9948	0.20±0.03	32±2	28±2	0.9949	0.21±0.02	530±0	420±20	0.991

[a]Pseudo-second-order rate constant. [b]Model calculated maximum sorbed concentration at equilibrium. [c]Measured maximum sorbed concentration at equilibrium.

Table S11. Accuracy (R^2 and P) values for regression on pseudo-second-order rate constant against compositional and pore property parameters at different relative humidity (RH) levels.

Composition	33% RH		47% RH		94% RH	
	R^2	P	R^2	P	R^2	P
OC_{TGA}	0.47	0.0046	0.06	0.3845	0.28	0.0423
OC_{AE}	0.44	0.0070	0.10	0.2574	0.14	0.1672
EC	0.14	0.1700	0.05	0.4194	0.45	0.0061
Dissolved minerals	0.08	0.3100	0.19	0.1086	0.17	0.1302
NH_4^+	0.77	$<$0.0001	0.01	0.7118	0.06	0.3946
Cl^-	0.60	0.0007	0.08	0.3181	0.08	0.3118
$C_2O_4^{2-}$	0.05	0.4400	0.002	0.8848	0.004	0.5000
SO_4^{2-}	0.11	0.2286	0.10	0.2529	0.02	0.6618
Total porosity	0.03	0.5300	0.0001	0.9696	0.82	$<$0.0001
K^+	0.15	0.1509	0.13	0.1789	0.32	0.0266

II. Figures.

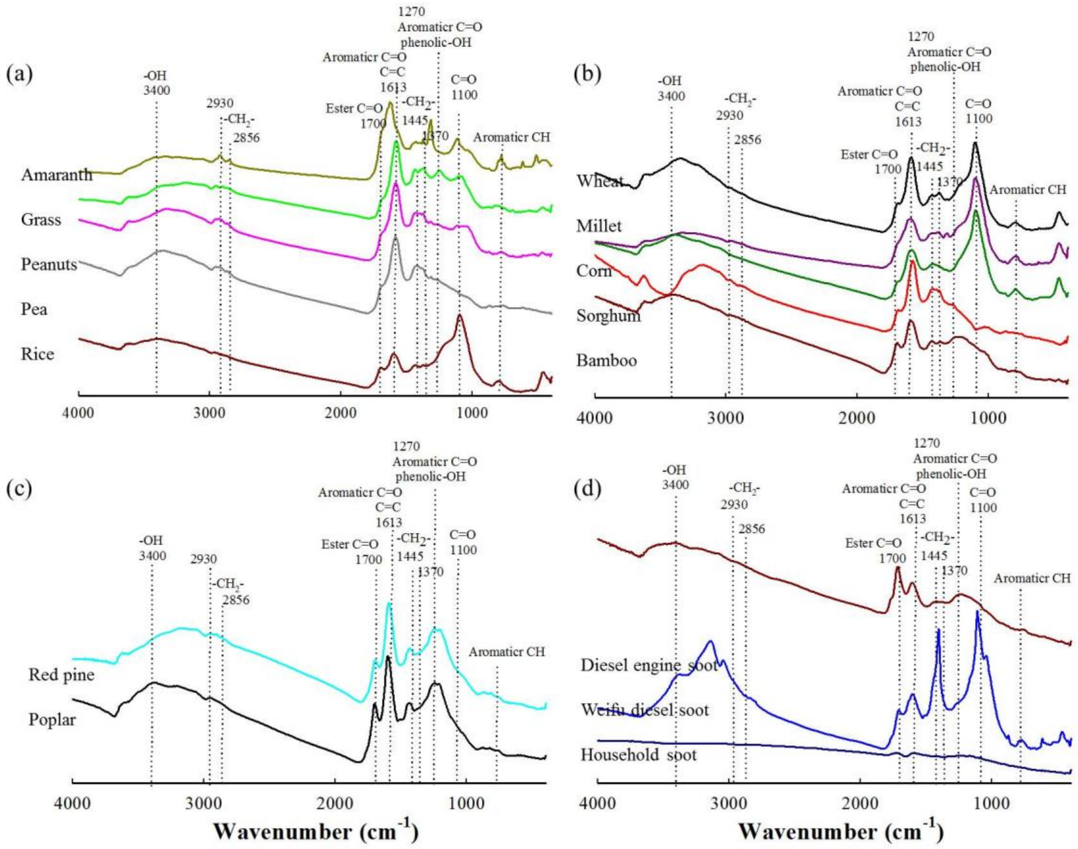

Figure S1. Fourier-transform infrared (FTIR) spectra of different BCPs. (a) Subgroup 1 of herbal BCPs. (b) Subgroup 2 of herbal BCPs. (c) Woody BCPs. (d) Soot BCPs.

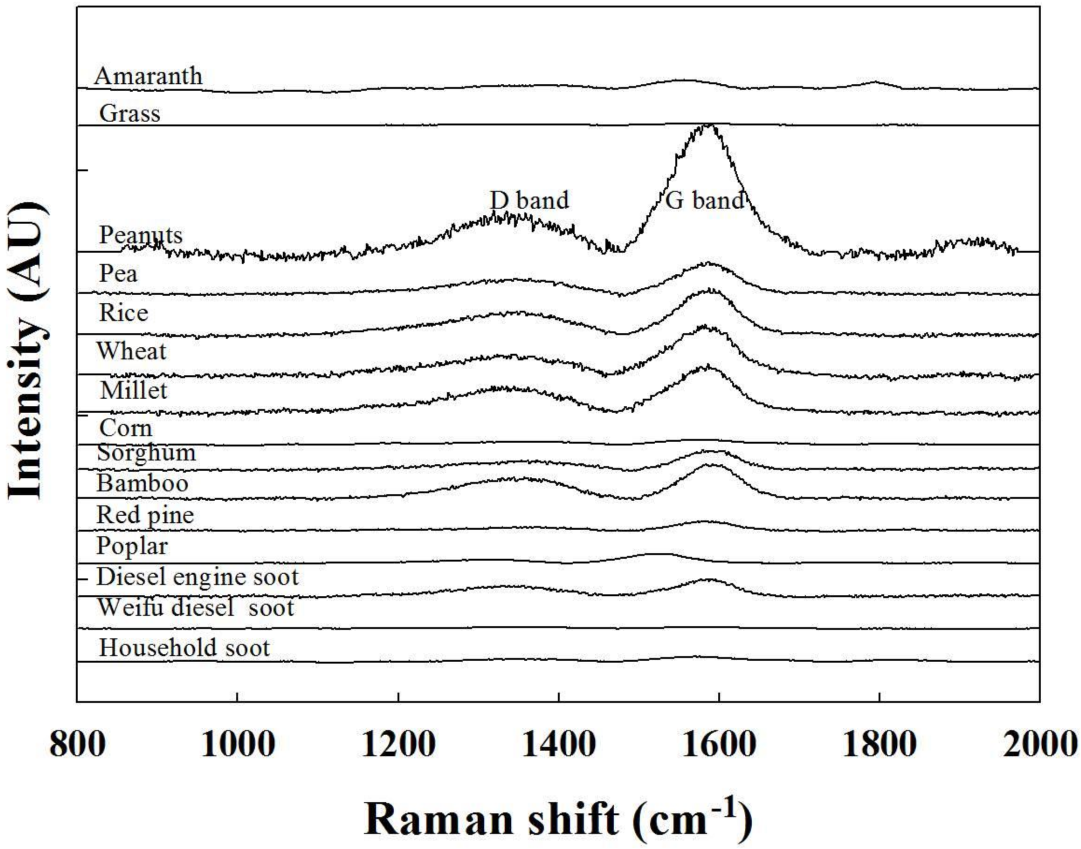

Figure S2. Raman spectra of different BCPs.

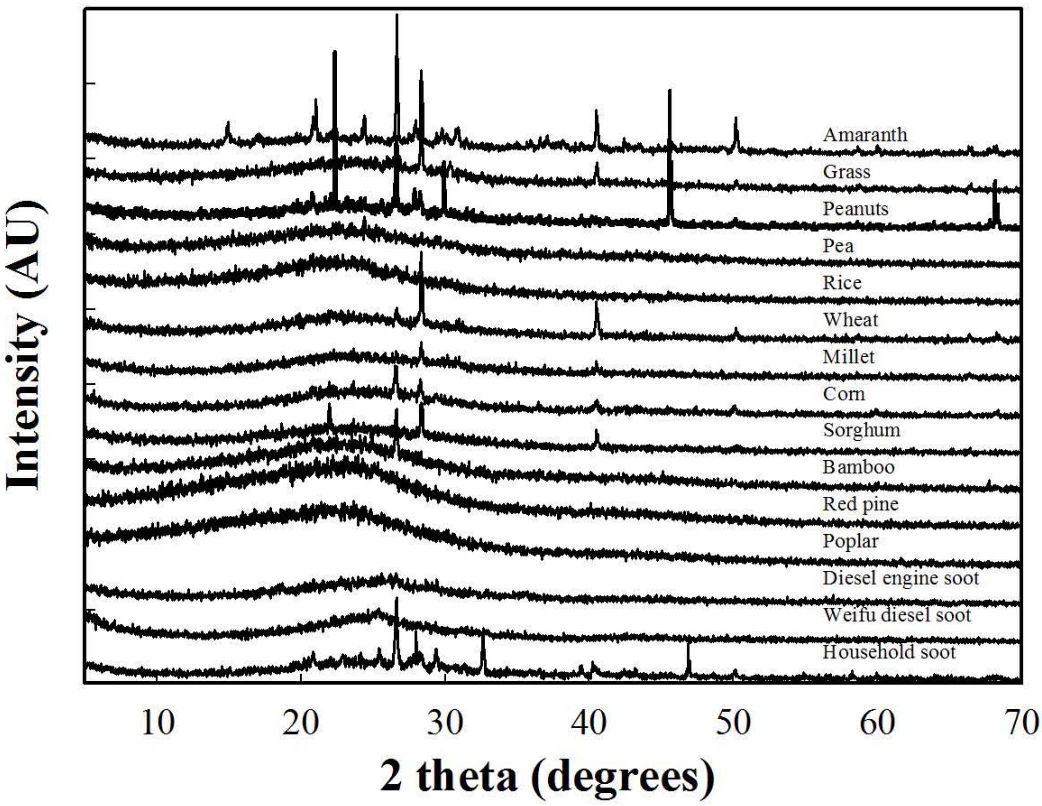

Figure S3. X-ray diffraction (XRD) profiles of different BCPs.

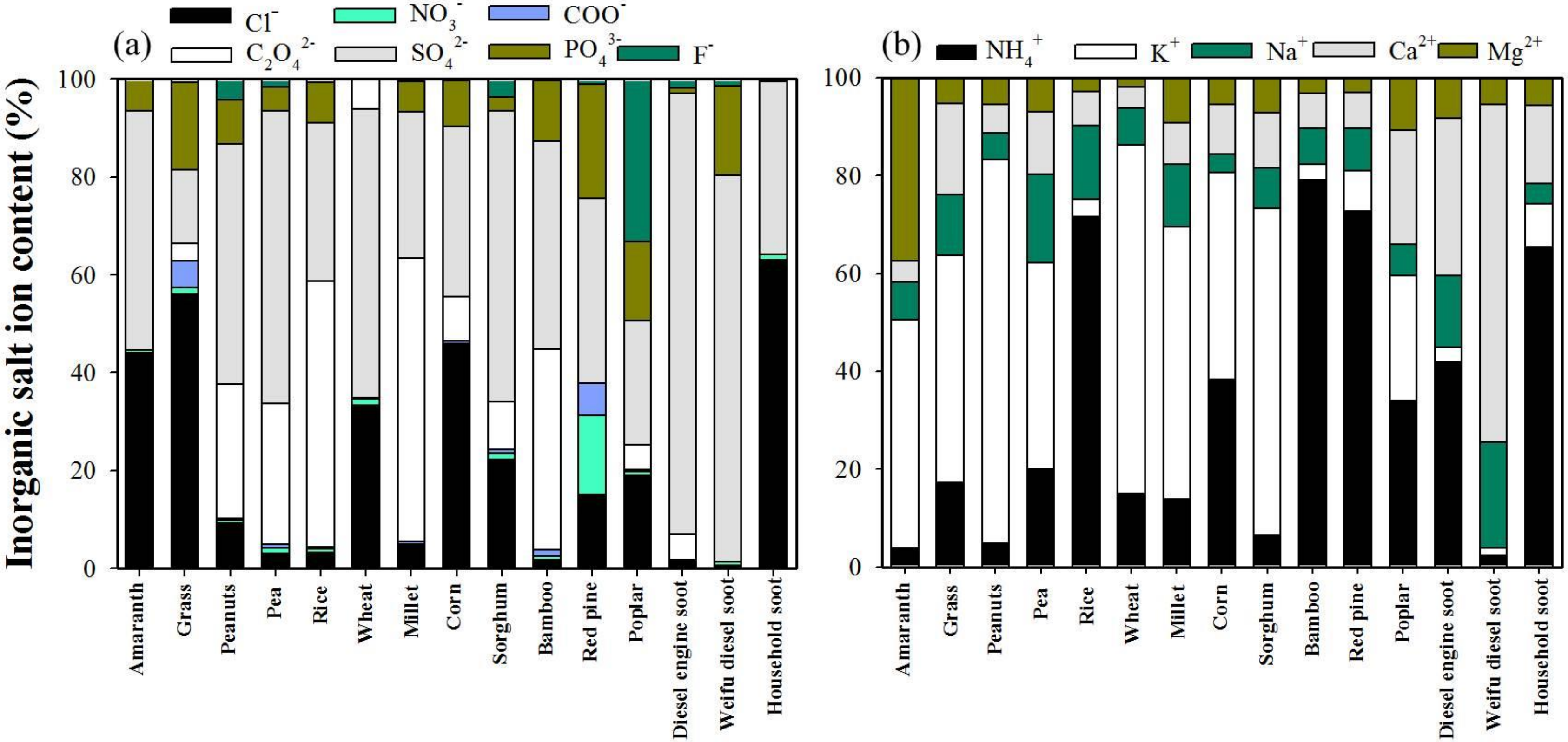

Figure S4. Compositional percentages of ionic constituents of different BCPs.

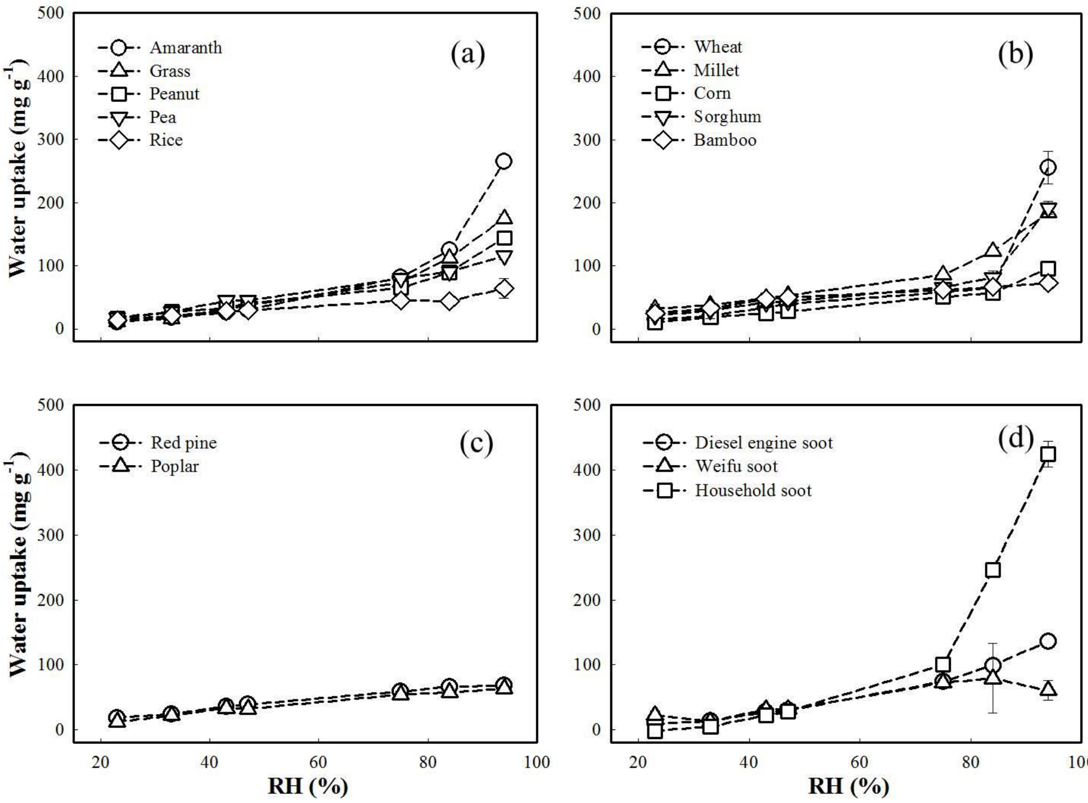

Figure S5. Sorption isotherms of water vapor plotted as equilibrium water uptake (mg g^{-1}) vs. relative humidity (RH, %) obtained by saturated aqueous salt solutions for different BCPs.

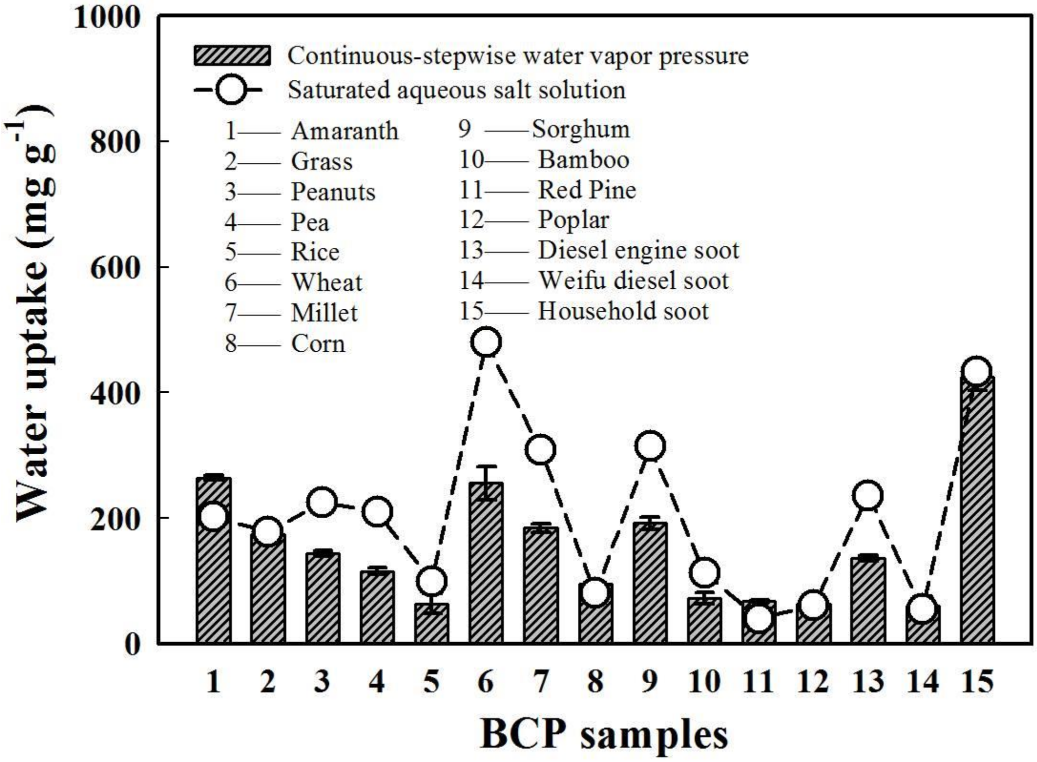

Figure S6. Comparison of equilibrium water uptake by BCPs at 94% relative humidity measured by two different gravimetric methods.

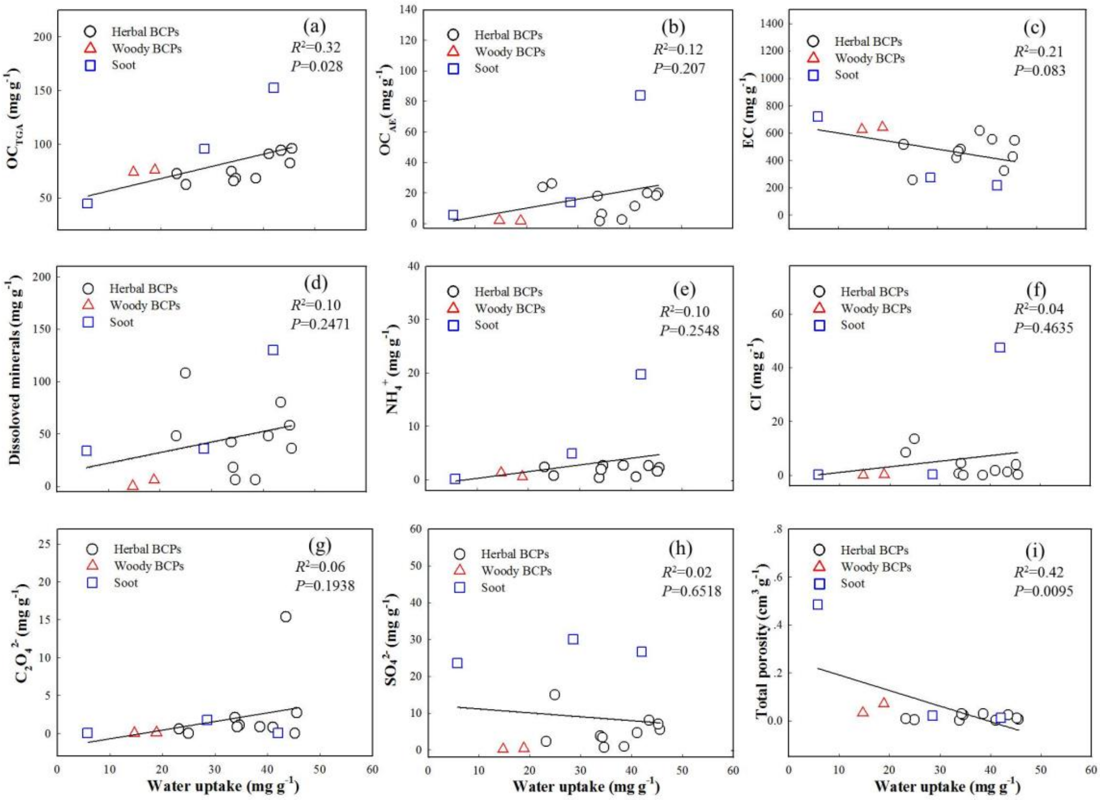

Figure S7. Relationships between equilibrium water uptake (mg g^{-1}) vs. compositional and pore property parameters for the group of BCPs at 23% relative humidity.

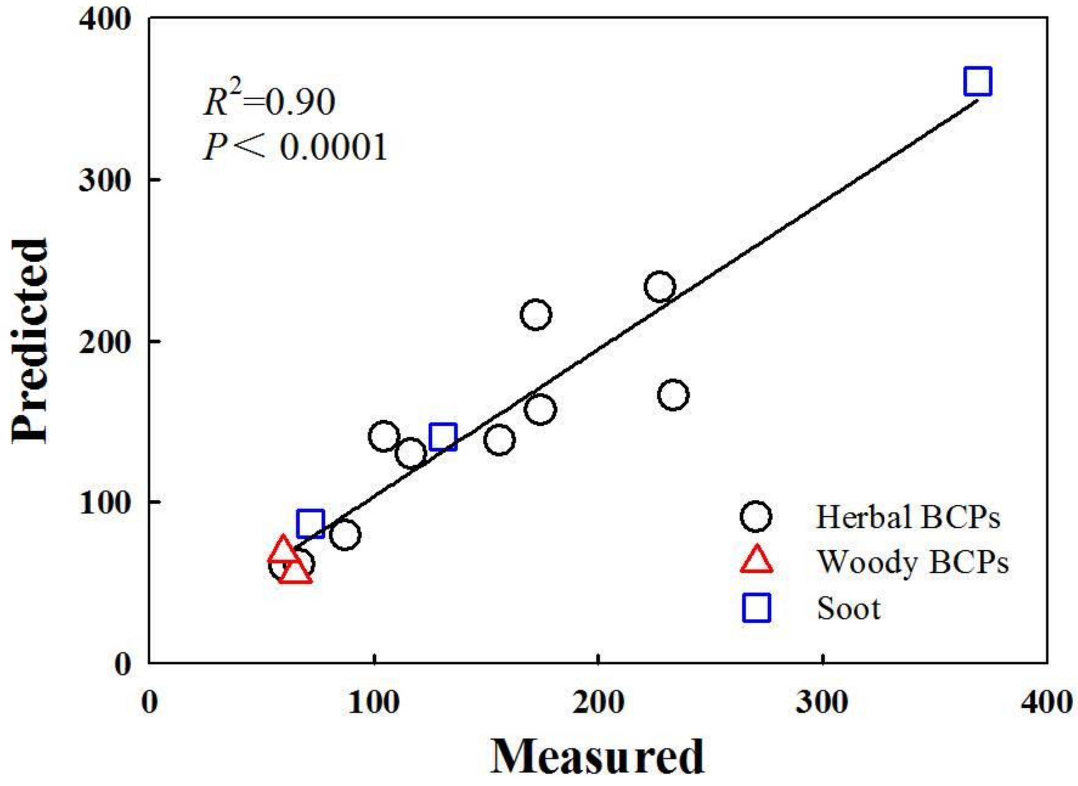

Figure S8. Relationship between measured values of equilibrium water uptake at 94% relative humidity vs. predicted values obtained by binary factor regression based on contents of OC_{TGA} and dissolved minerals for the group of BCPs. Regression equation: Uptake = 9.886OC_{TGA} + 17.459 DM − 16.839, where OC_{TGA} and DM are percentage contents of OC_{TGA} and dissolved minerals.

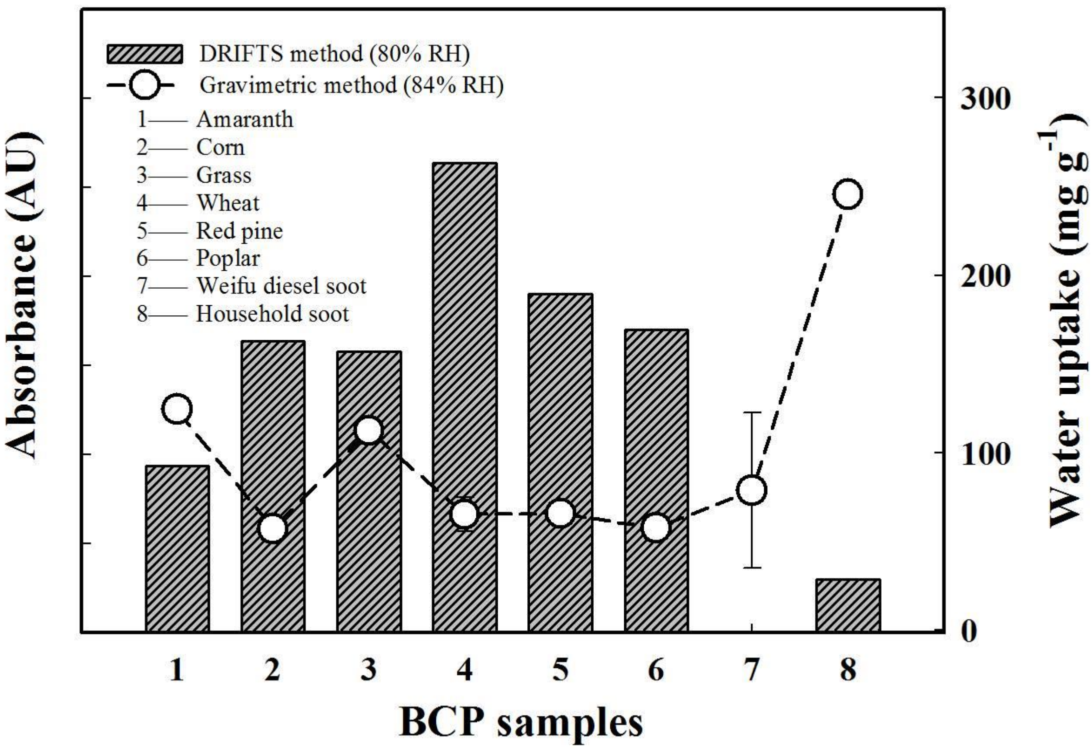

Figure S9. Comparison of equilibrium water uptake measured by gravimetric method and DRIFTS method for selected BCPs at high relative humidity.

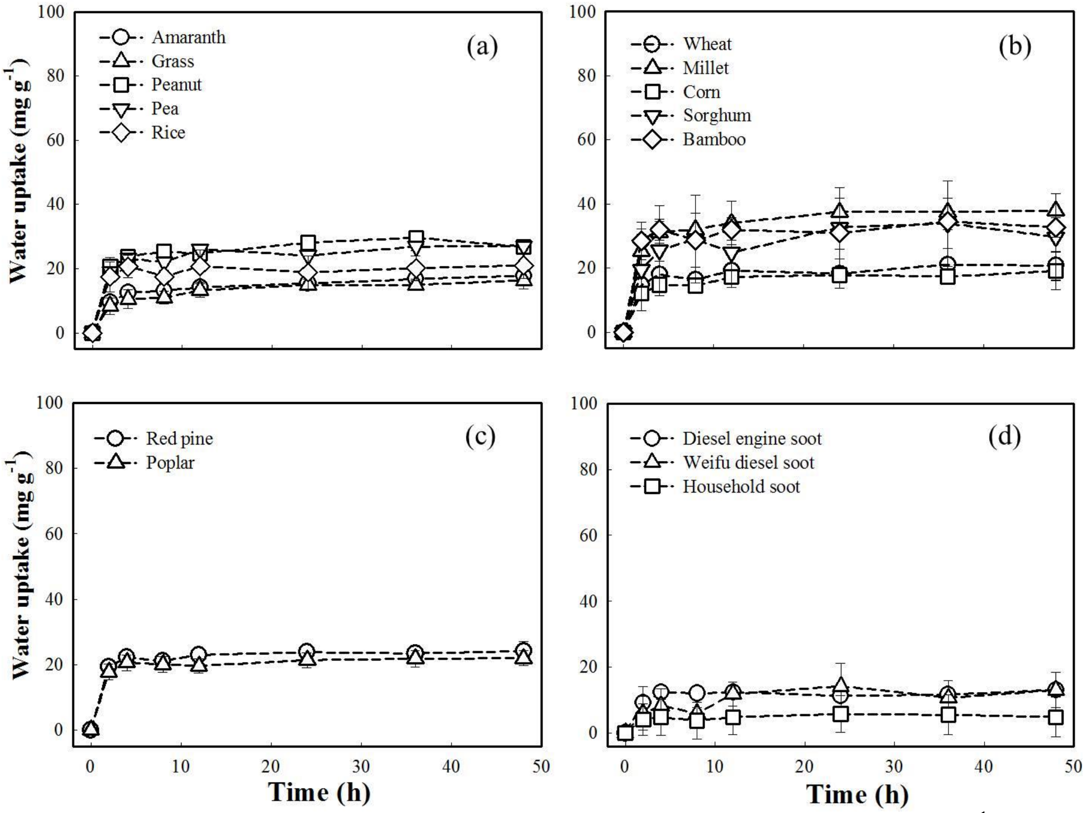

Figure S10. Sorption kinetics of water vapor plotted as water uptake (mg g^{-1}) vs. time (h) at 33% relative humidity.

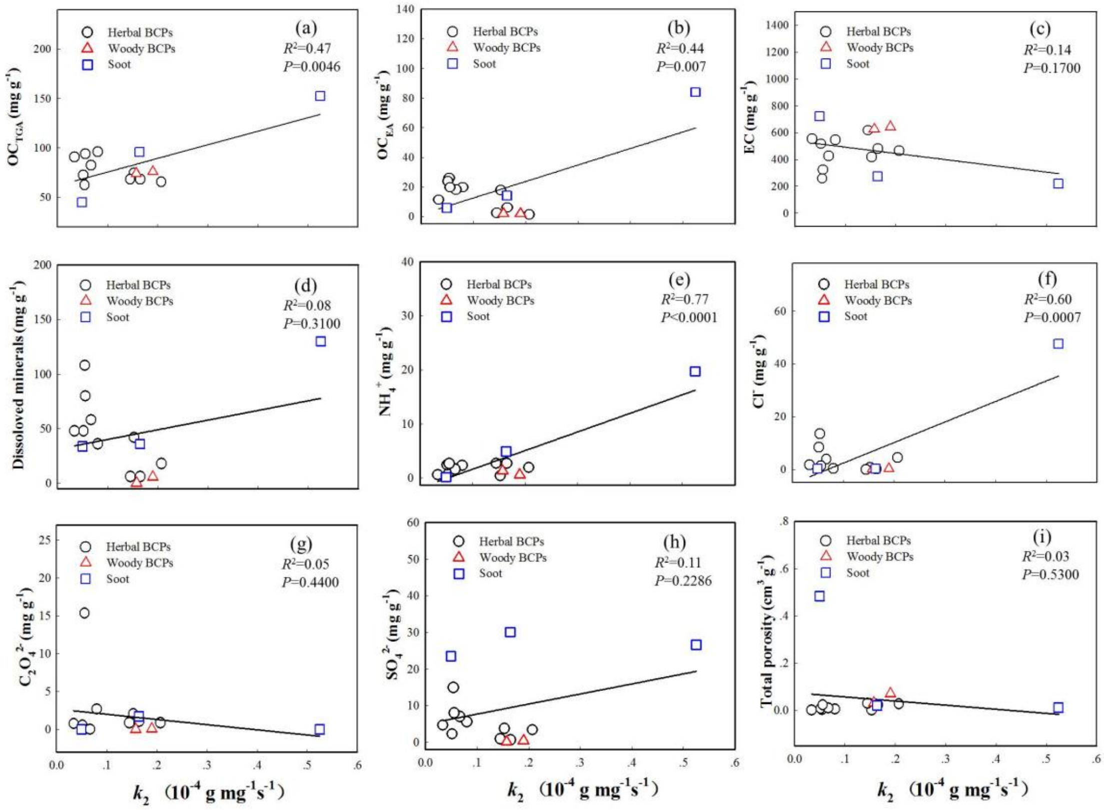

Figure S11. Relationships between pseudo-second water uptake rate constant (k_2) (g $mg^{-1}s^{-1}$) vs. compositional and pore property parameters for the group of BCPs at 33% relative humidity.