Supporting information

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Development of chemometrics method based on infrared spectroscopy for the determination of cement composition and process optimization[§]

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Table S2: Reference XRF results of major and minor oxides for calibration data and validation data

CALIBRATION DATA SET										
No	**Type**	**Name**	**CaO (w/w%)**	**SiO_2 (w/w%)**	**Al_2O_3 (w/w%)**	**Fe_2O_3 (w/w%)**	**MgO (w/w%)**	**SO_3 (w/w%)**	**Na_2O (w/w%)**	**K_2O (w/w%)**
1	IRON ORE	S42	0.61	50.53	1.15	42.42	0.05	0.72	0.02	0.09
2	IRON ORE	S4	1.41	29.86	1.85	59.38	0.12	1.28	0.35	0.13
3	IRON ORE	S33	4.36	32.82	2.51	48.77	0.21	0.93	0.41	0.21
4	IRON ORE	S43	4.58	31.84	1.43	56.4	0.11	1.07	0.15	0.12
5	CLAY	S9	5.33	54.22	15.64	5.88	2.09	0.14	2.41	2.52
6	TRASS	S28	9.42	51.21	14.02	5.24	2.11	1.48	2.26	2.6
7	CLAY	S70	5.6	52.05	16.2	6.13	2.31	0.16	1.11	3.2
8	CLAY	S75	7.39	55.42	12.73	4.93	2.31	0.14	0.9	2.56
9	CLAY	S73	9.22	49.11	14.46	5.83	2.53	0.35	1.11	2.71
10	CLAY	S74	9.96	50.51	14	5.48	2.05	0.23	0.87	2.75
11	ASH	S37	29.86	37.44	17.66	4.3	2.16	5.09	0.39	1.21
12	ASH	S6	37.33	32.25	14.51	3.9	1.85	6.53	0.37	1.04
13	GYPSUM	S19	33.22	1.21	0.29	0.1	2.93	37	0.12	0.06
14	GYPSUM	S45	33.4	0.28	0.02	0.02	0.88	43.48	0.03	0.01
15	GYPSUM	S76	34.02	0.82	0.13	0.11	0.27	42.45	0.05	0.02
16	GYPSUM	S44	34.35	0.61	0.06	0.05	4.38	33.19	0.02	0.02
17	GYPSUM	S49	34.97	0.76	0.1	0.12	0.06	41.99	0.05	0.02
18	GYPSUM	S46	36.4	1.03	0.27	0.12	9.13	16.51	0.03	0.07
19	GYPSUM	S14	36.5	0.74	0.13	0.12	3.54	33.56	0.04	0.03
20	RAW MEAL	S34	42.02	12.96	4.45	2.31	0.76	0.18	0.25	0.98
21	RAW MEAL	S36	42.05	12.98	4.42	2.28	0.75	0.18	0.6	0.98
22	RAW MEAL	S38	54.7	15.89	4.68	2.16	1	0.52	0.31	3.98
23	RAW MEAL	S39	55.27	16.28	4.74	2.39	0.99	0.5	0.28	3.38
24	RAW MEAL	S40	55.26	15.93	4.68	2.37	0.97	0.51	0.22	1.86
25	LIMESTONE	S10	54.09	1.47	0.75	0.2	0.64	0.17	0.06	0.07
26	LIMESTONE	S2	54.27	1.97	0.95	0.55	0.28	0.07	0.08	0.09
27	LIMESTONE	S32	54.29	1.57	0.88	0.23	0.28	0.1	0.07	0.08
28	LIMESTONE	S41	54.77	1.63	0.75	0.26	0.23	0.05	0.07	0.07
29	LIMESTONE	S21	55.05	1.43	0.57	0.29	0.33	0.49	0.09	0.07
30	LIMESTONE	S20	55.1	0.67	0.31	0.14	0.34	1.16	0.07	0.03
31	LIMESTONE	S1	55.48	1.03	0.52	0.18	0.19	0.05	0.07	0.05
32	LIMESTONE	S7	55.57	0.75	0.37	0.11	0.31	0.24	0.07	0.04
33	LIMESTONE	S15	55.69	0.5	0.28	0.14	0.4	0.15	0.07	0.03
34	CEM IV	S71	48.38	28.82	7.84	3.74	1.45	2.8	0.69	1.18

35	CEM IV	S79	49.76	28.36	7.98	2.87	1.46	3	0.75	1.17
36	CEM II	S22	56.01	22.31	6.28	3.05	1.41	3.66	0.56	1.05
37	CEM II	S29	56.39	22.32	6.31	3.02	1.39	3.36	0.57	1.03
38	CEM-I	S80	57.4	22.39	7.35	2.66	1.23	3.42	0.39	0.77
39	CEM-II	S25	58.56	21	7.08	2.82	1.35	2.98	0.38	0.86
40	CEM-II	S24	58.67	20.8	6.98	2.95	0.36	3.05	0.38	0.85
41	CEM-I	S77	60.38	19.75	6.99	2.43	1.34	2.84	0.47	0.85
42	CEM-I	S99	61.96	21.23	5.76	2.1	1.9	3.07	0.21	0.9
43	CEM-I	S103	62	20.48	5.65	2.22	1.45	4.21	0.21	0.85
44	CEM-I	S111	62.33	20.82	5.76	2.32	1.47	3.11	0.22	0.88
45	CEM-I	S92	62.46	20.24	5.62	2.26	1.52	3.32	0.21	0.86
46	CEM-II	S26	62.58	21.11	7.28	2.63	1.42	3.11	0.46	0.9
47	CEM-I	S109	62.76	20.21	5.53	2.1	2.02	3.45	0.16	0.85
48	CEM-I	S110	62.76	20.52	5.66	2.18	1.58	3.3	0.18	0.86
49	CEM-I	S18	62.99	18.87	5.45	2.94	1.35	3.33	0.38	0.84
50	CEM-I	S90	63.02	19.99	5.54	2.12	1.59	3.57	0.18	0.83
51	CEM-I	S105	63.06	20.32	5.37	2.12	1.44	3.55	0.17	0.83
52	CEM-I	S12	63.07	18.92	5.44	2.91	1.36	3.29	0.39	0.85
53	CEM-I	S13	63.1	18.98	5.34	2.84	1.36	3.47	0.37	0.85
54	CEM-I	S97	63.25	20.36	5.41	2.17	1.67	3.21	0.17	0.85
55	CEM-I	S106	63.31	20.29	5.45	2.38	1.46	3.28	0.17	0.81
56	CEM-I	S84	63.34	20.24	5.4	2.12	1.67	3.24	0.16	0.82
57	CEM-I	S89	63.42	19.83	5.23	2.35	1.54	3.62	0.17	0.83
58	CEM-I	S93	63.45	19.81	5.47	2.91	1.49	3.17	0.18	0.9
59	CEM-I	S88	63.48	20.21	5.58	2.08	1.34	3.22	0.19	0.78
60	CEM-I	S104	63.48	20.21	5.58	2.08	1.34	3.22	0.19	0.78
61	CEM-I	S30	63.49	19.07	5.48	2.8	1.38	3.25	0.4	0.88
62	CEM-I	S102	63.65	20.2	5.37	2.29	1.28	2.8	0.18	0.81
63	CEM-I	S95	63.7	20.01	5.33	2.12	1.41	3.37	0.19	0.8
64	CEM-I	S100	63.75	20.29	5.26	2.18	1.3	3.28	0.17	0.75
65	CEM-I	S81	64.59	20.87	5.14	2.93	2.01	3.42	0.25	0.78
66	CEM-I	S113	62.27	18.94	4.89	2.86	2.48	3.39	0.49	0.79
67	CEM-I	S91	64.89	19.16	5.26	2.85	1.3	2.82	0.2	0.87
68	CEM-I	S94	64.96	21.63	5.93	2.26	1.49	2.65	0.21	0.86
69	CEM-I	S83	65.05	20.76	5.23	2.83	1.85	3.29	0.24	0.76
70	CEM-I	S85	63.38	19.82	5.14	2.66	1.43	3.52	0.19	0.83
71	CEM-I	S112	63.13	18.78	5.16	2.88	1.98	3.25	0.38	0.84
72	CEM-I	S96	63.16	20.44	5.53	2.14	1.23	3.01	0.21	0.86
73	CEM-I	S114	62.17	19.13	4.72	3.13	1.73	2.82	0.38	0.81
74	CEM-I	S82	66.16	20.32	4.83	3.05	1.8	2.9	0.26	0.67
75	CLINKER	S60	65.75	21.49	5.81	3.8	1.04	0.35	0.34	0.92

76	CLINKER	S50	65.82	21.47	5.84	3.64	1.06	0.39	0.35	0.91
77	CLINKER	S56	65.89	21.43	5.76	3.65	1.01	0.46	0.34	0.94
78	CLINKER	S57	65.91	21.64	5.65	3.49	1.03	0.47	0.34	0.94
79	CLINKER	S16	65.92	21.21	5.74	3.62	1.05	0.41	0.34	1.01
80	CLINKER	S52	65.96	21.44	5.76	3.57	1.01	0.39	0.34	0.93
81	CLINKER	S54	66.03	21.43	5.75	3.59	1.04	0.4	0.33	0.92
82	CLINKER	S58	66.09	21.55	5.56	3.43	1.02	0.52	0.34	0.96
83	CLINKER	S67	66.16	21.49	5.64	3.46	1.01	0.44	0.34	0.95
84	CLINKER	S66	66.2	21.46	5.7	3.41	1.01	0.43	0.34	0.94
85	CLINKER	S53	66.22	21.32	5.71	3.49	1.09	0.4	0.33	0.92
86	CLINKER	S55	66.24	21.21	5.72	3.5	1.09	0.51	0.31	0.9
87	CLINKER	S68	66.24	21.56	5.61	3.37	1	0.44	0.34	0.93
88	CLINKER	S63	66.27	21.21	5.73	3.49	1.08	0.6	0.32	0.94
89	CLINKER	S59	66.38	21.15	5.72	3.52	1.04	0.4	0.33	0.96

VALIDATION DATA SET

No	Type	Name	CaO (w/w%)	SiO_2 (w/w%)	Al_2O_3 (w/w%)	Fe_2O_3 (w/w%)	MgO (w/w%)	SO_3 (w/w%)	Na_2O (w/w%)	K_2O (w/w%)
90	IRON ORE	S3	4.36	32.82	2.51	48.77	0.21	0.93	0.41	0.21
91	TRASS	S23	8.05	54.11	14.63	5.41	2.05	0.28	2.47	2.78
92	CLAY	S72	7.27	53.74	13.83	5.34	2.24	0.18	0.97	2.75
93	ASH	S5	30.38	37.9	16.85	4.24	2.02	5.14	0.42	1.24
94	GYPSUM	S48	34.21	0.3	0.03	0.02	3.53	34.92	0.02	0.02
95	GYPSUM	S47	35.98	0.56	0.08	0.06	5.09	27.28	0.04	0.03
96	RAW MEAL	S35	43	12.58	4.19	2.16	0.7	0.14	0.25	0.89
97	LIMESTONE	S8	54.87	1.34	0.5	0.97	0.2	0.06	0.07	0.06
98	LIMESTONE	S69	55.11	1.56	0.51	0.21	0.23	0.02	0.07	0.05
99	CEM-II	S31	54.76	23.74	7.37	3.16	1.39	3.56	0.56	1.06
100	CEM-I	S78	56.14	22.48	6.34	3.17	1.45	3.2	0.58	1.04
101	CEM-II	S27	58.48	20.82	6.89	3.03	1.35	3.08	0.38	0.88
102	CEM-II	S17	60.4	19.97	5.63	3.07	1.32	3.45	0.44	0.9
103	CEM-I	S87	62.28	21.07	5.66	2.18	1.47	3.42	0.2	0.87
104	CEM-I	S108	62.5	20.32	5.69	2.28	1.46	3.55	0.2	0.84
105	CEM-I	S11	63.03	18.78	5.31	2.86	1.4	3.42	0.36	0.84
106	CEM-I	S101	63.28	20.18	5.54	2.16	1.36	2.79	0.19	0.84
107	CEM-I	S86	63.46	20.12	5.52	2.05	1.25	3.06	0.2	0.78
108	CEM-I	S98	63.53	20.41	5.27	2.15	1.38	3.22	0.17	0.83
109	CLINKER	S61	65.87	21.41	5.76	3.79	1.05	0.34	0.36	0.9
110	CLINKER	S51	65.92	21.38	5.76	3.63	1.06	0.38	0.41	0.92
111	CLINKER	S65	66.18	21.33	5.68	3.65	1.02	0.39	0.33	0.92
112	CLINKER	S64	66.25	21.28	5.73	3.49	1.08	0.41	0.31	0.93
113	CLINKER	S62	66.29	21.3	5.7	3.49	1.04	0.37	0.33	0.97

Table S2: L.O.I results of samples for calibration data and validation data

Calibration Set				Validation Set	
No	**L.O.I (w/w%)**	**No**	**L.O.I (w/w%)**	**No**	**L.O.I (w/w%)**
1	1.03	35	3.88	68	1.03
2	1.52	36	4.13	69	2.86
3	2.60	37	4.40	70	3.00
4	2.63	38	4.45	71	3.03
5	2.83	39	4.45	72	3.11
6	2.84	40	4.45	73	3.17
7	2.86	41	4.53	74	3.42
8	2.90	42	4.56	75	3.86
9	2.90	43	5.08	76	4.57
10	2.95	44	5.10	77	6.44
11	3.00	45	5.16	78	6.77
12	3.00	46	5.48	79	15.10
13	3.01	47	6.66	80	21.93
14	3.03	48	6.69	81	25.33
15	3.07	49	8.17	82	34.57
16	3.07	50	8.99	83	42.15
17	3.11	51	14.75	84	42.72
18	3.11	52	17.36	85	42.86
19	3.12	53	21.88		
20	3.15	54	22.30		
21	3.15	55	25.07		
22	3.25	56	26.95		
23	3.32	57	27.32		
24	3.32	58	30.88		
25	3.41	59	34.29		
26	3.41	60	34.94		
27	3.48	61	36.44		
28	3.48	62	41.91		
29	3.55	63	42.50		
30	3.57	64	42.50		
31	3.64	65	42.58		
32	3.64	66	42.63		
33	42.81	67	43.48		
34	43.19				

Table S3: Comparison of the 95% reproducibility statics for the type of the materials used in this study with respect to SEP values obtained from PLS models based on FTIR-ATR spectra

Type of Materials	Parameters	CaO	SiO_2	Al_2O_3	Fe_2O_3	MgO	SO_3	Na_2O	K_2O	L.O.I
Limestone	Mean	42.72	6.52	1.58	8.55	10.68	0.60	0.09	0.45	39.98
	Min.	30.04	0.45	0.12	0.17	0.15	0.07	0.00	0.02	5.00
	Max.	55.40	12.58	3.03	17.05	20.51	1.18	0.17	0.88	46.90
	s_R	0.18	0.11	0.12	0.10	0.09	0.09	0.04	0.02	0.13
	R	0.50	0.31	0.34	0.28	0.25	0.25	0.11	0.06	0.36
	SEP	0.62	0.99	0.10	0.19	0.21	0.53	0.03	0.09	1.38
Clay-trass	Mean	28.79	61.08	18.83	2.33	1.50	1.69	5.30	5.60	5.88
	Min.	0.00	22.36	0.05	0.01	0.00	0.03	0.00	0.01	0.00
	Max.	57.58	99.79	37.60	4.64	2.98	3.36	10.59	11.20	13.90
	s_R	0.17	0.15	0.13	0.12	0.09	0.09	0.06	0.07	0.13
	R	0.48	0.42	0.36	0.34	0.25	0.25	0.17	0.20	0.36
	SEP	3.17	4.71	0.66	0.43	0.25	0.46	0.26	0.22	0.66
Gypsum	Mean	43.04	11.45	3.60	1.60	3.33	27.63	0.10	0.63	13.32
	Min.	28.50	0.63	0.14	0.11	1.74	3.36	0.01	0.03	1.59
	Max.	57.58	22.26	7.06	3.09	4.92	51.91	0.20	1.23	23.60
	s_R	0.18	0.14	0.11	0.09	0.09	0.18	0.04	0.05	0.12
	R	0.50	0.39	0.31	0.25	0.25	0.50	0.11	0.14	0.34
	SEP	3.85	2.32	0.33	0.15	0.55	1.94	0.02	0.10	1.98
Clinker	Mean	64.17	20.33	5.27	2.97	1.63	1.65	0.38	0.76	1.18
	Min.	62.17	18.80	4.71	2.33	1.23	0.48	0.29	0.56	0.18
	Max.	66.17	21.85	5.82	3.36	2.02	2.82	0.47	0.95	4.56
	s_R	0.22	0.15	0.16	0.10	0.10	0.15	0.03	0.04	0.13
	R	0.62	0.42	0.45	0.28	0.28	0.42	0.08	0.11	0.36
	SEP	1.29	0.61	0.36	0.25	0.26	0.58	0.13	0.10	None
Raw meal	Mean	45.97	9.56	3.81	1.47	1.15	0.15	0.15	0.53	0.00
	Min.	42.89	5.65	3.49	1.11	0.32	0.08	0.06	0.36	0.00
	Max.	49.05	13.47	4.12	1.82	1.98	0.22	0.24	0.70	0.00
	s_R	0.14	0.15	0.16	0.09	0.07	0.09	0.03	0.04	0.13
	R	0.39	0.42	0.45	0.25	0.20	0.25	0.08	0.11	0.36
	SEP	2.66	3.90	0.50	0.34	0.30	0.24	0.20	0.05	0.32
Fly ash	Mean	30.32	38.81	15.76	8.21	3.09	1.87	0.84	1.53	1.03
	Min.	3.05	22.26	7.06	3.09	1.01	0.38	0.19	0.41	0.23
	Max.	57.58	55.35	24.46	13.33	5.70	3.36	1.47	2.37	1.76
	s_R	0.12	0.12	0.14	0.08	0.06	0.08	0.04	0.04	0.13
	R	0.34	0.34	0.39	0.22	0.17	0.22	0.11	0.11	0.36
	SEP	1.85	2.01	1.08	0.03	0.49	0.20	0.14	0.03	2.12

s_R: Reproducibility standard deviation.

R: 95% reproducibility statics ($R = 2.8 \times s_R$)

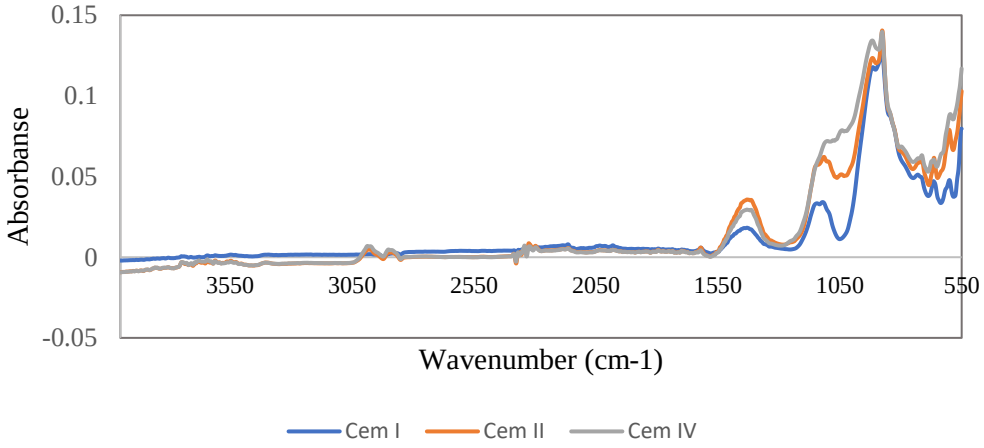

Figure S1: Mid-range spectra of Cem I, Cem II, Cem III types

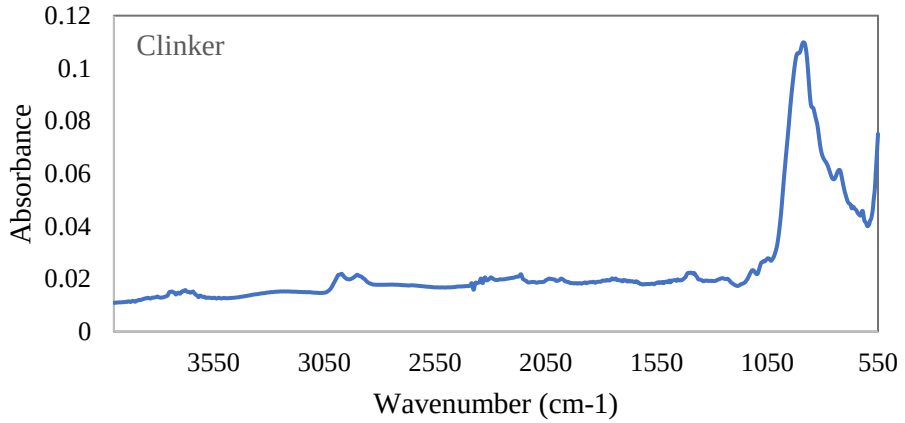

Figure S2: Mid-range spectrum of a clinker sample

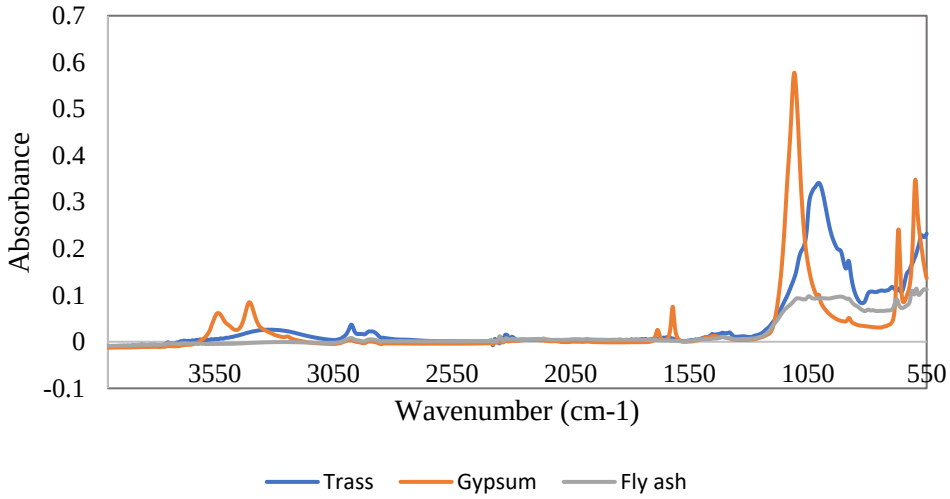

Figure S3: Mid-range spectra of additives with types

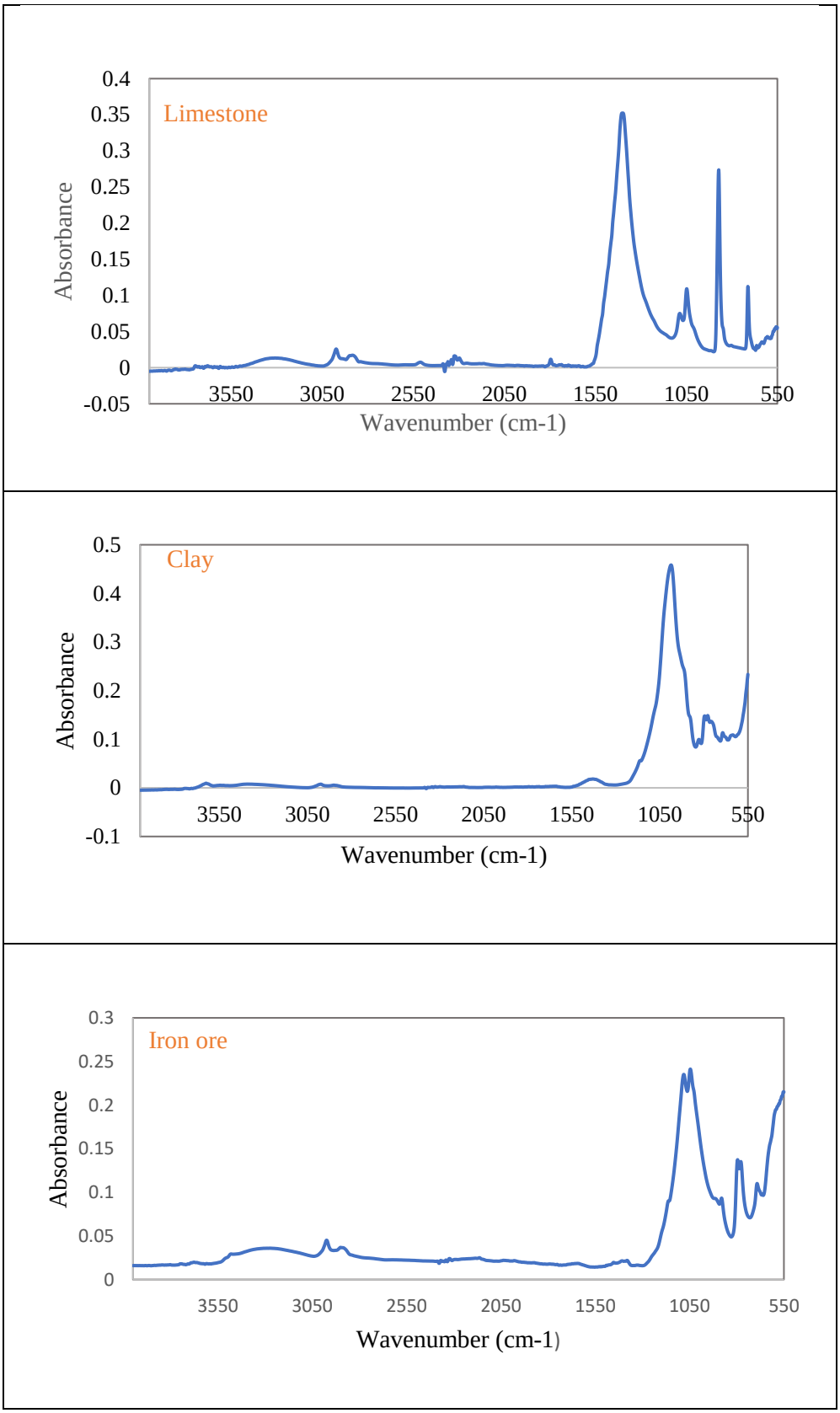

Figure S4: Mid-range spectrum of raw materials with type