

Characterisation of rare earth elements and toxic heavy metals in coal and coal fly ash

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Table S1: Absolute values (mean \pm standard deviation; in mg.kg⁻¹) of REEs in the various sequential extraction fractions for coal samples (OMC, OKC, ODC).

Sample/ Fractions	La	Ce	Pr	Nd	Sm	Y	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
OMC															
F1	0.01 \pm 0.00	0.01 \pm 0.00	0.00	0.01 \pm 0.00	0.00	0.01 \pm 0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
F2	0.82 \pm 0.02	2.37 \pm 0.06	0.33 \pm 0.01	1.61 \pm 0.04	0.33 \pm 0.01	2.54 \pm 0.07	0.08 \pm 0.00	0.43 \pm 0.01	0.06 \pm 0.00	0.33 \pm 0.01	0.06 \pm 0.00	0.16 \pm 0.01	0.02 \pm 0.00	0.10 \pm 0.00	0.01 \pm 0.00
F3	2.41 \pm 0.05	8.37 \pm 0.18	1.34 \pm 0.03	6.87 \pm 0.15	1.77 \pm 0.04	10.41 \pm 0.26	0.42 \pm 0.01	2.02 \pm 0.06	0.30 \pm 0.01	1.76 \pm 0.05	0.35 \pm 0.01	0.89 \pm 0.03	0.11 \pm 0.00	0.65 \pm 0.02	0.09 \pm 0.00
F4	3.42 \pm 0.07	8.00 \pm 0.20	0.89 \pm 0.02	3.30 \pm 0.07	0.61 \pm 0.01	1.40 \pm 0.03	0.11 \pm 0.00	0.49 \pm 0.01	0.06 \pm 0.00	0.33 \pm 0.01	0.06 \pm 0.00	0.14 \pm 0.00	0.02 \pm 0.00	0.09 \pm 0.04	0.01 \pm 0.00
Total	6.66	18.75	2.56	11.79	2.71	14.36	0.62	2.94	0.43	2.42	0.47	1.20	0.15	0.83	0.11
OKC															
F1	0.11 \pm 0.01	0.17 \pm 0.01	0.02 \pm 0.00	0.09 \pm 0.01	0.01 \pm 0.00	0.07 \pm 0.01	0.00	0.02 \pm 0.00	0.00	0.01 \pm 0.00	0.00	0.00	0.00	0.00	0.00
F2	0.71 \pm 0.04	1.35 \pm 0.10	0.14 \pm 0.01	0.56 \pm 0.05	0.10 \pm 0.01	0.58 \pm 0.05	0.03 \pm 0.00	0.12 \pm 0.01	0.02 \pm 0.00	0.01 \pm 0.01	0.02 \pm 0.00	0.05 \pm 0.00	0.01 \pm 0.00	0.03 \pm 0.00	0.00
F3	4.56 \pm 0.10	10.24 \pm 0.24	1.23 \pm 0.02	5.05 \pm 0.13	1.07 \pm 0.03	5.45 \pm 0.1	0.26 \pm 0.01	1.14 \pm 0.02	0.17 \pm 0.00	0.95 \pm 0.02	0.19 \pm 0.00	0.49 \pm 0.01	0.06 \pm 0.00	0.37 \pm 0.01	0.05 \pm 0.00
F4	2.32 \pm 0.08	4.79 \pm 0.16	0.52 \pm 0.02	1.94 \pm 0.08	0.35 \pm 0.02	0.94 \pm 0.03	0.07 \pm 0.00	0.31 \pm 0.01	0.04 \pm 0.00	0.20 \pm 0.00	0.04 \pm 0.00	0.09 \pm 0.00	0.01 \pm 0.00	0.06 \pm 0.00	0.01 \pm 0.00
Total	7.71	16.56	1.91	7.64	1.54	7.04	0.36	1.59	0.22	1.25	0.24	0.63	0.08	0.46	0.06
ODC															

F1	0.08 ± 0.01	0.13 ± 0.03	0.01 ± 0.00	0.06 ± 0.01	0.01 ± 0.00	0.09 ± 0.03	0.00	0.01 ± 0.00	0.00	0.01 ± 0.00	0.00	0.00	0.00	0.00	0.00
F2	1.52 ± 0.06	2.93 ± 0.11	0.32 ± 0.01	1.29 ± 0.04	0.23 ± 0.01	1.71 ± 0.05	0.06 ± 0.00	0.29 ± 0.01	0.04 ± 0.00	0.24 ± 0.01	0.05 ± 0.00	0.13 ± 0.00	0.02 ± 0.00	0.08 ± 0.00	0.01 ± 0.00
F3	4.45 ± 0.06	10.43 ± 0.14	1.24 ± 0.01	5.11 ± 0.04	1.07 ± 0.01	6.24 ± 0.10	0.27 ± 0.01	1.16 ± 0.02	0.17 ± 0.00	1.04 ± 0.02	0.21 ± 0.00	0.58 ± 0.01	0.08 ± 0.00	0.45 ± 0.01	0.07 ± 0.00
F4	6.02 ± 0.15	13.81 ± 0.36	1.47 ± 0.04	5.22 ± 0.14	0.91 ± 0.02	1.73 ± 0.04	0.18 ± 0.01	0.70 ± 0.01	0.09 ± 0.00	0.43 ± 0.01	0.07 ± 0.00	0.16 ± 0.01	0.02 ± 0.00	0.10 ± 0.00	0.01 ± 0.00
Total	12.08	27.29	3.04	11.68	2.22	9.77	0.51	2.16	0.30	1.71	0.33	0.88	0.11	0.64	0.09

F1: Acid Soluble Fraction; F2: Reducible Fraction; F3: Oxidisable Fraction; F4: Residual Fraction.

OMC: Omelewu Coal

OKC: Okaba Coal

ODC: Odagbo Coal

Table S2: Absolute values (mean \pm standard deviation; in mg.kg⁻¹) of toxic heavy metals in the various sequential extraction fractions for both coal and simulant fly ash samples (OMC, OMA, OKC, OKA, ODC and ODA).

Sample/Fractions	Cr	As	Pb	Cd	Th	U
OMC						
F1	0.15 \pm 0.05	0.12 \pm 0.04	0.36 \pm 0.00	0.01 \pm 0.00	0.001 \pm 0.00	0.002 \pm 0.00
F2	0.19 \pm 0.05	0.59 \pm 0.03	2.30 \pm 0.36	0.02 \pm 0.00	0.0003 \pm 0.00	0.004 \pm 0.00
F3	23.82 \pm 0.59	0.42 \pm 0.04	4.75 \pm 0.17	0.04 \pm 0.00	2.69 \pm 0.08	1.20 \pm 0.04
F4	0.76 \pm 0.09	0	1.62 \pm 0.09	0.001 \pm 0.00	1.85 \pm 0.02	0.18 \pm 0.00
Total	24.92	1.14	9.02	0.07	4.54	1.39
OMA						
F1	0.10 \pm 0.03	2.53 \pm 0.09	0.47 \pm 0.22	0.004 \pm 0.00	0.007 \pm 0.00	0.03 \pm 0.01
F2	0.15 \pm 0.02	1.03 \pm 0.14	0.68 \pm 0.15	0.001 \pm 0.00	0.001 \pm 0.00	0.001 \pm 0.00
F3	0.75 \pm 0.27	0.55 \pm 0.16	0.68 \pm 0.16	0.02.11 \pm 0.00	0.12 \pm 0.01	0.24 \pm 0.02
F4	5.00 \pm 0.57	0.27 \pm 0.08	0.48 \pm 0.13	0.004 \pm 0.00	3.09 \pm 0.29	0.32 \pm 0.03
Total	5.97	4.38	2.31	0.03	3.21	0.59
OKC						
F1	0.12 \pm 0.02	0.39 \pm 0.07	0.15 \pm 0.07	0.006 \pm 0.00	0.002 \pm 0.00	0.00
F2	0.15 \pm 0.05	0.55 \pm 0.02	0.86 \pm 0.13	0.007 \pm 0.00	0.00	0.00
F3	9.11 \pm 0.17	0.49 \pm 0.01	3.14 \pm 0.12	0.04 \pm 0.00	1.25 \pm 0.06	0.41 \pm 0.01
F4	0.70 \pm 0.38	0	0.50 \pm 0.03	0.001 \pm 0.00	0.70 \pm 0.05	0.07 \pm 0.00
Total	10.08	1.43	4.65	0.05	1.95	0.48
OKA						
F1	0.36 \pm 0.04	7.46 \pm 0.46	0.38 \pm 0.09	0.01 \pm 0.00	0.01 \pm 0.00	0.06 \pm 0.01
F2	0.15 \pm 0.01	4.79 \pm 0.05	0.18 \pm 0.07	0.002 \pm 0.00	0.0002 \pm 0.00	0.004 \pm 0.00

F3	0.67 ± 0.08	1.90 ± 0.14	0.60 ± 0.15	0.02 ± 0.00	0.80 ± 0.05	0.67 ± 0.04
F4	11.50 ± 0.90	2.03 ± 0.38	1.84 ± 0.01	0.01 ± 0.00	6.85 ± 0.24	1.23 ± 0.07
Total	12.68	16.18	2.99	0.04	7.66	1.97
ODC						
F1	0.09 ± 0.00	0.31 ± 0.06	0.33 ± 0.09	0.01 ± 0.7	0.004 ± 0.01	0.003 ± 0.00
F2	0.13 ± 0.02	0.51 ± 0.07	1.53 ± 0.08	0.005 ± 0.00	0.003 ± 0.00	0.003 ± 0.00
F3	12.06 ± 0.16	0.54 ± 0.02	4.76 ± 0.04	0.04 ± 0.00	1.43 ± 0.01	0.47 ± 0.01
F4	0.56 ± 0.01	0.00	1.24 ± 0.02	0.002 ± 0.00	1.61 ± 0.03	0.13 ± 0.004
Total	12.84	1.36	7.86	0.05	3.05	0.61
ODA						
F1	0.68 ± 0.02	13.21 ± 0.20	0.33 ± 0.15	0.01 ± 0.004	0.012 ± 0.00	0.29 ± 0.00
F2	0.24 ± 0.15	4.65 ± 0.30	0.27 ± 0.05	0.002 ± 0.000	0.004 ± 0.00	0.014 ± 0.00
F3	0.74 ± 0.07	2.27 ± 0.19	1.25 ± 0.04	0.02 ± 0.00	0.72 ± 0.03	0.78 ± 0.05
F4	14.90 ± 0.86	2.00 ± 0.10	6.79 ± 0.30	0.01 ± 0.00	6.43 ± 0.41	1.21 ± 0.08
Total	16.56	22.14	8.64	0.04	7.16	2.29

OMA: Omelewu simulant fly ash; OMC: Omelewu Coal

OKA: Okaba simulant fly ash; OKC: Okaba Coal

ODA: Odagbo simulant fly ash; ODC: Odagbo Coal