Monte Carlo comparison of conventional ternary diagrams with new log-ratio bivariate diagrams and an example of tectonic discrimination

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Supplementary equations

Equations for the alr transformation:

$$alr_1 = \ln\left(\frac{A_1}{A_3}\right), \tag{S1}$$

$$alr_2 = \ln\left(\frac{A_2}{A_3}\right). \tag{S2}$$

Equations for the clr transformation:

$$clr_1 = \ln\left(\frac{A_1}{(A_1 \times A_2 \times A_3)^{1/3}}\right), \tag{S3}$$

$$clr_2 = \ln\left(\frac{A_2}{(A_1 \times A_2 \times A_3)^{1/3}}\right), \tag{S4}$$

$$clr_3 = \ln\left(\frac{A_3}{(A_1 \times A_2 \times A_3)^{1/3}}\right). \tag{S5}$$

Equations for the ilr transformation:

$$ilr_1 = \sqrt{\frac{1}{2}} \ln\left(\frac{A_1}{A_2}\right), \tag{S6}$$

$$ilr_2 = \sqrt{\frac{2}{3}} \ln\left(\frac{\sqrt{A_1 \times A_2}}{A_3}\right). \tag{S7}$$

Equations for the variances $s^2_{A_{p2}}$ and $s^2_{A_{p3}}$:

$$s^2_{A_{p2}} \approx A^2_{p2}\left[\left(\frac{s_{A_2}}{A_2}\right)^2 + \left(\frac{(s_{A_1})^2 + (s_{A_2})^2 + (s_{A_3})^2 + 2(s_{(A_1)(A_2)(A_3)})^2}{(A_1 + A_2 + A_3)^2}\right) - \left(\frac{2(s_{(A_2)(A_1 A_2 A_3)})^2}{(A_2)^2 (A_1 + A_2 + A_3)^2}\right)\right], \tag{S8}$$

$$s^2_{A_{p3}} \approx A^2_{p3}\left[\left(\frac{s_{A_3}}{A_3}\right)^2 + \left(\frac{(s_{A_1})^2 + (s_{A_2})^2 + (s_{A_3})^2 + 2(s_{(A_1)(A_2)(A_3)})^2}{(A_1 + A_2 + A_3)^2}\right) - \left(\frac{2(s_{(A_3)(A_1 A_2 A_3)})^2}{(A_3)^2 (A_1 + A_2 + A_3)^2}\right)\right]. \tag{S9}$$

Equations for the DF1 and DF2 functions corresponding to the alr transformation from the complete dataset:

$$DF1_{alr} = (0.97253 \times alr_1) - (3.81560 \times alr_2) - 19.85906, \quad \text{(S10)}$$

$$DF2_{alr} = (-2.87457 \times alr_1) - (0.57851 \times alr_2) - 18.16119. \quad \text{(S11)}$$

Equations for the DF1 and DF2 functions corresponding to the clr_1–clr_2 transformation from the complete dataset:

$$DF1_{clr12} = (1.87054 \times clr_1) + (6.65866 \times clr_2) + 19.85906, \quad \text{(S12)}$$

$$DF2_{clr12} = (-6.32765 \times clr_1) - (4.03160 \times clr_2) - 18.16119. \quad \text{(S13)}$$

Equations for the DF1 and DF2 functions corresponding to the clr_2–clr_3 transformation from the complete dataset:

$$DF1_{clr23} = (-4.78812 \times clr_2) + (1.87054 \times clr_3) - 19.85906, \quad \text{(S14)}$$

$$DF2_{clr23} = (-2.29606 \times clr_2) - (6.32765 \times clr_3) + 18.16119. \quad \text{(S15)}$$

Equations for the DF1 and DF2 functions corresponding to the alr transformation from the complete dataset:

$$DF1_{ilr} = (3.38571 \times ilr_1) - (3.48203 \times ilr_2) - 19.85906, \quad \text{(S16)}$$

$$DF2_{ilr} = (-1.62356 \times ilr_1) - (4.22914 \times ilr_2) - 18.16119. \quad \text{(S17)}$$

Supplementary Table S1. Twenty-five data points involving three variables with errors equivalent to the relative standard deviation (RSD%) of 5% and the mean and standard deviation values simulated from the Monte Carlo procedure including 100,000 replications.

Id.	Assumed measured variables (A_i)			Assumed standard deviation (s_{A_i}) of the measured variables			Simulated mean $(\bar{x}_{A_i})_{\text{sim}}$ of the measured variables			Simulated standard deviation $(s_{A_i})_{\text{sim}}$ of the measured variables		
	A_1	A_2	A_3	s_{A_1}	s_{A_2}	s_{A_3}	$(\bar{x}_{A_1})_{\text{sim}}$	$(\bar{x}_{A_2})_{\text{sim}}$	$(\bar{x}_{A_3})_{\text{sim}}$	$(s_{A_1})_{\text{sim}}$	$(s_{A_2})_{\text{sim}}$	$(s_{A_3})_{\text{sim}}$
1	47.5	47.5	5	2.375	2.375	0.250	47.4958	47.5054	5.0000	2.3799	2.3801	0.2496
2	45	45	10	2.250	2.250	0.500	44.9960	45.0051	10.0000	2.2546	2.2548	0.4992
3	40	40	20	2.000	2.000	1.000	39.9965	40.0045	20.0000	2.0041	2.0043	0.9984
4	33.33	33.33	33.33	1.666	1.666	1.666	33.3271	33.3338	33.3298	1.6699	1.6701	1.6639
5	27.5	27.5	45	1.375	1.375	2.250	27.4976	27.5031	44.9998	1.3778	1.3780	2.2465
6	20	20	60	1.000	1.000	3.000	19.9982	20.0023	59.9997	1.0021	1.0022	2.9953
7	12.5	12.5	75	0.625	0.625	3.750	12.4989	12.5014	74.9996	0.6263	0.6263	3.7442
8	7.5	7.5	85	0.375	0.375	4.250	7.4993	7.5008	84.9996	0.3758	0.3758	4.2434
9	2.5	2.5	95	0.125	0.125	4.750	2.4998	2.5003	94.9996	0.1253	0.1253	4.7426
10	75	20	5	3.750	1.000	0.250	74.9934	20.0023	5.0000	3.7577	1.0022	0.2496
11	70	10	20 *	3.500	0.500	1.000	69.9938	10.0011	19.9999	3.5072	0.5011	0.9984
12	20	70	10 *	1.000	3.500	0.500	19.9982	70.0079	10.0000	1.0021	3.5075	0.4992
13	5	60	35 **	0.250	3.000	1.750	4.9996	60.0068	34.9998	0.2505	3.0065	1.7473
14	5	35	60 **	0.250	1.750	3.000	4.9996	35.0040	59.9997	0.2505	1.7538	2.9953
15	5	85	10	0.250	4.250	0.500	4.9996	85.0096	10.0000	0.2505	4.2592	0.4992
16	25	10	65	1.250	0.500	3.250	24.9978	10.0011	64.9997	1.2526	0.5011	3.2450
17	50	15	35	2.500	0.750	1.750	49.9956	15.0017	34.9998	2.5052	0.7516	1.7473
18	20	55	25	1.000	2.750	1.250	19.9982	55.0062	24.9999	1.0021	2.7559	1.2481
19	41	9	50	2.050	0.450	2.500	40.9964	9.0010	49.9998	2.0542	0.4510	2.4961
20	16	42	42	0.800	2.100	2.100	15.9986	42.0048	41.9998	0.8017	2.1045	2.0967
21	60	25	15	3.000	1.250	0.750	59.9947	25.0028	14.9999	3.0062	1.2527	0.7488
22	97	1	2	4.850	0.050	0.100	96.9914	1.0001	2.0000	4.8600	0.0501	0.0998
23	12.9	87	0.1	0.645	4.350	0.005	12.8989	87.0098	0.1000	0.6463	4.3594	0.0050
24	99.8	0.1	0.1	4.990	0.005	0.005	99.7912	0.1000	0.1000	5.0003	0.0050	0.0050
25	0.1	0.2	99.7	0.005	0.010	4.985	0.1000	0.2000	99.6995	0.0050	0.0100	4.9773

The data points identified by * and ** confirm the reproducibility of the simulation procedure as demonstrated by the very similar mean and standard deviation values for these pairs of simulations. The symbols are explained in the text.

Supplementary Table S2. Twenty-five data points involving three variables with errors equivalent to the relative standard deviation (RSD) of 5%,in addition to the final propagated standard deviation and %RSD values for the ternary variable simulated from the Monte Carlo procedure including 100,000 replications.

Id.	Measured (A_i) or plotted (A_{pi}) variables			Standard deviation (s_{A_i}) of the measured variables			Final propagated standard deviation in ternary plot			Final relative standard deviation (%RSD) in ternary plot		
	A_1 or A_{p1}	A_2 or A_{p2}	A_3 or A_{p3}	s_{A_1}	s_{A_2}	s_{A_3}	$s_{A_{p1}}$	$s_{A_{p2}}$	$s_{A_{p3}}$	$RSD_{A_{p1}}$	RSD_{Ap_2}	$RSD_{A_{p3}}$
1	47.5	47.5	5	2.375	2.375	0.250	1.691	1.691	0.292	3.56	3.56	5.84
2	45	45	10	2.250	2.250	0.500	1.620	1.620	0.553	3.60	3.60	5.53
3	40	40	20	2.000	2.000	1.000	1.504	1.504	0.982	3.76	3.76	4.91
4	33.33	33.33	33.33	1.666	1.666	1.666	1.366	1.366	1.366	4.10	4.10	4.10
5	27.5	27.5	45	1.375	1.375	2.250	1.238	1.238	1.521	4.50	4.50	3.38
6	20	20	60	1.000	1.000	3.000	1.024	1.024	1.476	5.12	5.12	2.46
7	12.5	12.5	75	0.625	0.625	3.750	0.728	0.728	1.155	5.82	5.82	1.54
8	7.5	7.5	85	0.375	0.375	4.250	0.474	0.474	0.790	6.32	6.32	0.93
9	2.5	2.5	95	0.125	0.125	4.750	0.171	0.171	0.294	6.85	6.85	0.31
10	75	20	5	3.750	1.000	0.250	1.222	1.102	0.308	1.63	5.51	6.16
11	70	10	20 *	3.500	0.500	1.000	1.316	0.581	1.072	1.88	5.81	5.36
12	20	70	10 *	1.000	3.500	0.500	1.072	1.316	0.581	5.36	1.88	5.81
13	5	60	35 **	0.250	3.000	1.750	0.295	1.608	1.558	5.90	2.68	4.45
14	5	35	60 **	0.250	1.750	3.000	0.295	1.558	1.608	5.90	4.45	2.68
15	5	85	10	0.250	4.250	0.500	0.321	0.799	0.623	6.42	0.94	6.23
16	25	10	65	1.250	0.500	3.250	1.250	0.571	1.443	5.00	5.71	2.22
17	50	15	35	2.500	0.750	1.750	1.575	0.788	1.463	3.15	5.25	4.18
18	20	55	25	1.000	2.750	1.250	1.006	1.529	1.192	5.03	2.78	4.77
19	41	9	50	2.050	0.450	2.500	1.603	0.504	1.640	3.91	5.60	3.28
20	16	42	42	0.800	2.100	2.100	0.826	1.546	1.546	5.16	3.68	3.68
21	60	25	15	3.000	1.250	0.750	1.494	1.220	0.806	2.49	4.88	5.37
22	97	1	2	4.850	0.050	0.100	0.184	0.070	0.139	0.19	6.98	6.93
23	12.9	87	0.1	0.645	4.350	0.005	0.798	0.800	0.007	6.19	0.92	6.69
24	99.8	0.1	0.1	4.990	0.005	0.005	0.010	0.007	0.007	0.01	7.11	7.10
25	0.1	0.2	99.7	0.005	0.010	4.985	0.007	0.014	0.020	7.10	7.10	0.02

The data points identified by * and ** confirm the reproducibility of the simulation procedure. For these pairs, the exact same final standard deviation and RSD% results were determined for equal values of the measured or plotted ternary variables independent of the location of the ternary component, whether A_1, A_2, or A_3. The symbols are explained in the text.

Supplementary Table S3. Twenty-five data points involving three variables and the synthesis of statistical information for bivariate additive log-ratio (alr) and isometric log-ratio (ilr) transformed plots from Monte Carlo simulations.

Id.	Assumed measured variable (A_i)			Additive $\log_e$-ratio transformation (alr) mean		Final standard deviation in additive-type (alr) bivariate plot		Centered $\log_e$-ratio transformation (clr) mean			Final standard deviation in centered-type (clr) bivariate plot			Isometric $\log_e$-ratio transformation (ilr) mean		Final standard deviation in isometric-type (ilr) bivariate plot	
	A_1	A_2	A_3	alr_1	alr_2	s_{alr_1}	s_{alr_2}	clr_1	clr_2	clr_3	s_{clr_1}	s_{clr_2}	s_{clr_3}	ilr_1	ilr_2	s_{ilr_1}	s_{ilr_2}
1	47.5	47.5	5	+2.25120	+2.25140	0.07106	0.07112	+0.75033	+0.75053	-1.50087	0.04103	0.04107	0.04104	-0.00014	+1.83818	0.05028	0.05027
2	45	45	10	+1.50398	+1.50419	0.07106	0.07112	+0.50126	+0.50146	-1.00272	0.04103	0.04107	0.04104	-0.00014	+1.22808	0.05028	0.05027
3	40	40	20	+0.69305	+0.69326	0.07106	0.07112	+0.23095	+0.23115	-0.46210	0.04103	0.04107	0.04104	-0.00014	+0.56596	0.05028	0.05027
4	33.33	33.33	33.33	-0.00009	+0.00011	0.07106	0.07112	-0.00010	+0.00010	-0.00001	0.04103	0.04107	0.04104	-0.00014	+0.00001	0.05028	0.05027
5	27.5	27.5	45	-0.49257	-0.49237	0.07106	0.07112	-0.16426	-0.16406	+0.32831	0.04103	0.04107	0.04104	-0.00014	-0.40210	0.05028	0.05027
6	20	20	60	-1.09871	-1.09850	0.07106	0.07112	-0.36630	-0.36610	+0.73240	0.04103	0.04107	0.04104	-0.00014	-0.89701	0.05028	0.05027
7	12.5	12.5	75	-1.79185	-1.79165	0.07106	0.07112	-0.59735	-0.59715	+1.19450	0.04103	0.04107	0.04104	-0.00014	-1.46296	0.05028	0.05027
8	7.5	7.5	85	-2.42784	-2.42764	0.07106	0.07112	-0.80935	-0.80915	+1.61849	0.04103	0.04107	0.04104	-0.00014	-1.98224	0.05028	0.05027
9	2.5	2.5	95	-3.63768	-3.63748	0.07106	0.07112	-1.21263	-1.21242	+2.42505	0.04103	0.04107	0.04104	-0.00014	-2.97007	0.05028	0.05027
10	75	20	5	+2.70796	+1.38640	0.07106	0.07112	+1.34317	+0.02162	-1.36479	0.04103	0.04107	0.04104	+0.93448	+1.67152	0.05028	0.05027
11	70	10	20	+1.25267	-0.69304	0.07106	0.07112	+1.06613	-0.87958	-0.18654	0.04103	0.04107	0.04104	+1.37582	+0.22847	0.05028	0.05027
12	20	70	10	+0.69305	+1.94602	0.07106	0.07112	-0.18664	+1.06633	-0.87969	0.04103	0.04107	0.04104	-0.88598	+1.07740	0.05028	0.05027
13	5	60	35	-1.94600	+0.53911	0.07106	0.07112	-1.47704	+1.00807	+0.46897	0.04103	0.04107	0.04104	-1.75724	-0.57436	0.05028	0.05027
14	5	35	60	-2.48500	-0.53889	0.07106	0.07112	-1.47704	+0.46907	+1.00796	0.04103	0.04107	0.04104	-1.37611	-1.23450	0.05028	0.05027
15	5	85	10	-0.69324	+2.14018	0.07106	0.07112	-1.17555	+1.65786	-0.48231	0.04103	0.04107	0.04104	-2.00353	+0.59071	0.05028	0.05027
16	25	10	65	-0.95561	-1.87169	0.07106	0.07112	-0.01317	-0.92926	+0.94243	0.04103	0.04107	0.04104	+0.64777	-1.15424	0.05028	0.05027
17	50	15	35	+0.35658	-0.84719	0.07106	0.07112	+0.52012	-0.68365	+0.16354	0.04103	0.04107	0.04104	+0.85119	-0.20029	0.05028	0.05027
18	20	55	25	-0.22324	+0.78857	0.07106	0.07112	-0.41168	+0.60012	-0.18844	0.04103	0.04107	0.04104	-0.71545	+0.23079	0.05028	0.05027
19	41	9	50	-0.19854	-1.71469	0.07106	0.07112	+0.43920	-1.07694	+0.63774	0.04103	0.04107	0.04104	+1.07208	-0.78107	0.05028	0.05027
20	16	42	42	-0.96517	+0.00011	0.07106	0.07112	-0.64349	+0.32180	+0.32169	0.04103	0.04107	0.04104	-0.68256	-0.39399	0.05028	0.05027
21	60	25	15	+1.38620	+0.51093	0.07106	0.07112	+0.75382	-0.12144	-0.63238	0.04103	0.04107	0.04104	+ 0.61891	+0.77450	0.05028	0.05027
22	97	1	2	+3.88147	-0.69304	0.07106	0.07112	+2.81866	-1.75585	-1.06281	0.04103	0.04107	0.04104	+3.23467	+1.30167	0.05028	0.05027
23	12.9	87	0.1	+4.85972	+6.76860	0.07106	0.07112	+0.98361	+2.89250	-3.87611	0.04103	0.04107	0.04104	-1.34978	+4.74724	0.05028	0.05027
24	99.8	0.1	0.1	+6.90566	+0.00011	0.07106	0.07112	+4.60374	-2.30181	-2.30192	0.04103	0.04107	0.04104	+4.88296	+2.81927	0.05028	0.05027
25	0.1	0.2	99.7	-6.90484	-6.21149	0.07106	0.07112	-2.53273	-1.83938	+4.37211	0.04103	0.04107	0.04104	-0.49027	-5.35472	0.05028	0.05027

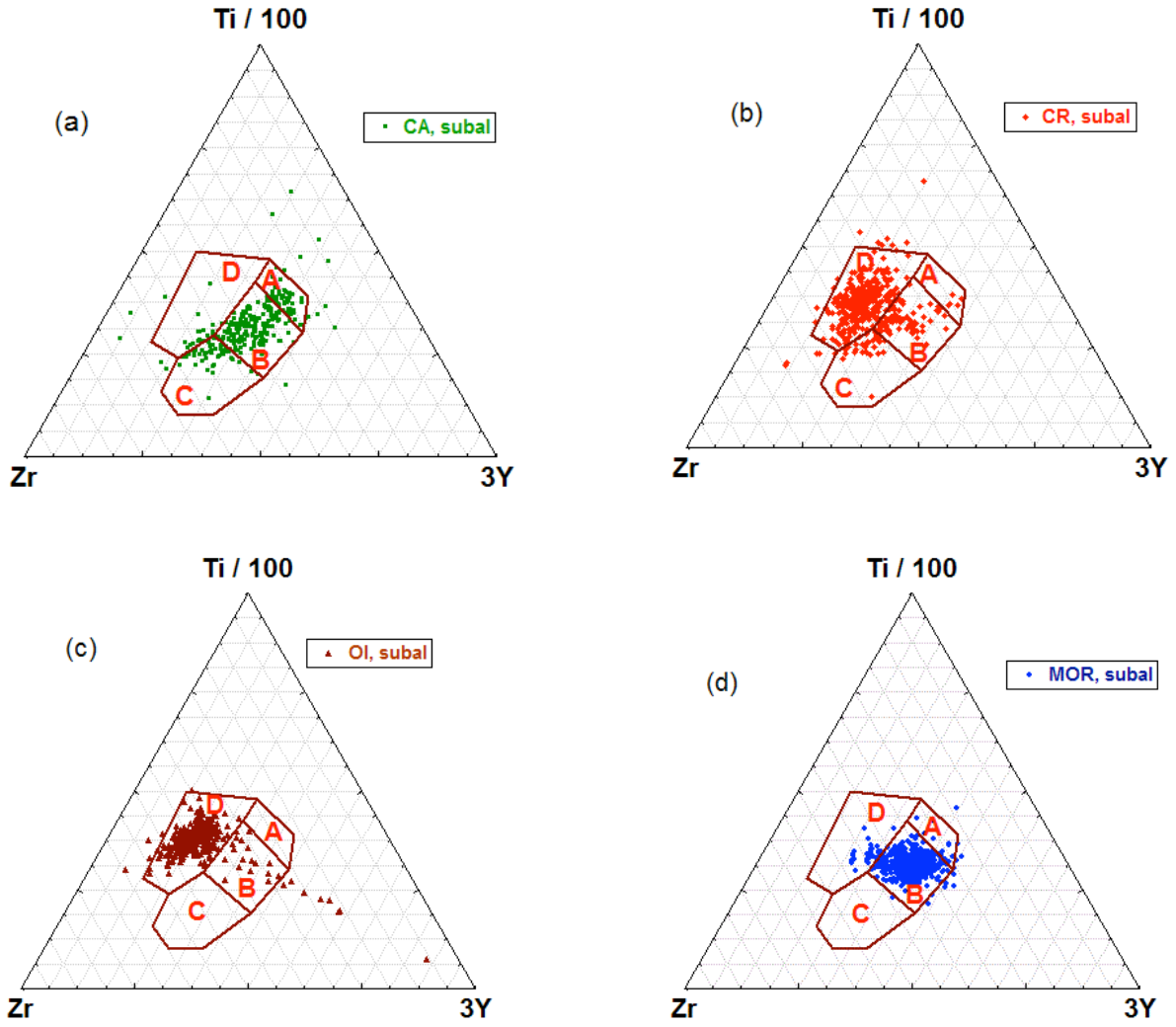

Fig. S1. Evaluation of the Zr–3Y–Ti/100 ternary diagram of Pearce and Cann (1973) from an extensive database of 3743 basalt samples from different tectonic settings. The original fields A–D are as follows: A: island arc tholeiites; B: overlap region of island arc tholeiite, calc–alkali basalt, and mid-ocean ridge basalt; C: calc–alkaline basalt; and D: within-plate basalt. The centroids for each of the three tectonic settings computed from the Monte Carlo procedure including 100,000 replications for the data of Table 2 are shown in Fig. 2a only; they were the same in all diagrams. (a) continental arc (CA) subalkaline (subal) rocks; (b) continental rift (CR) subal rocks; (c) ocean island (OI) subal rocks; and (c) mid-ocean ridge (MOR) subal rocks.

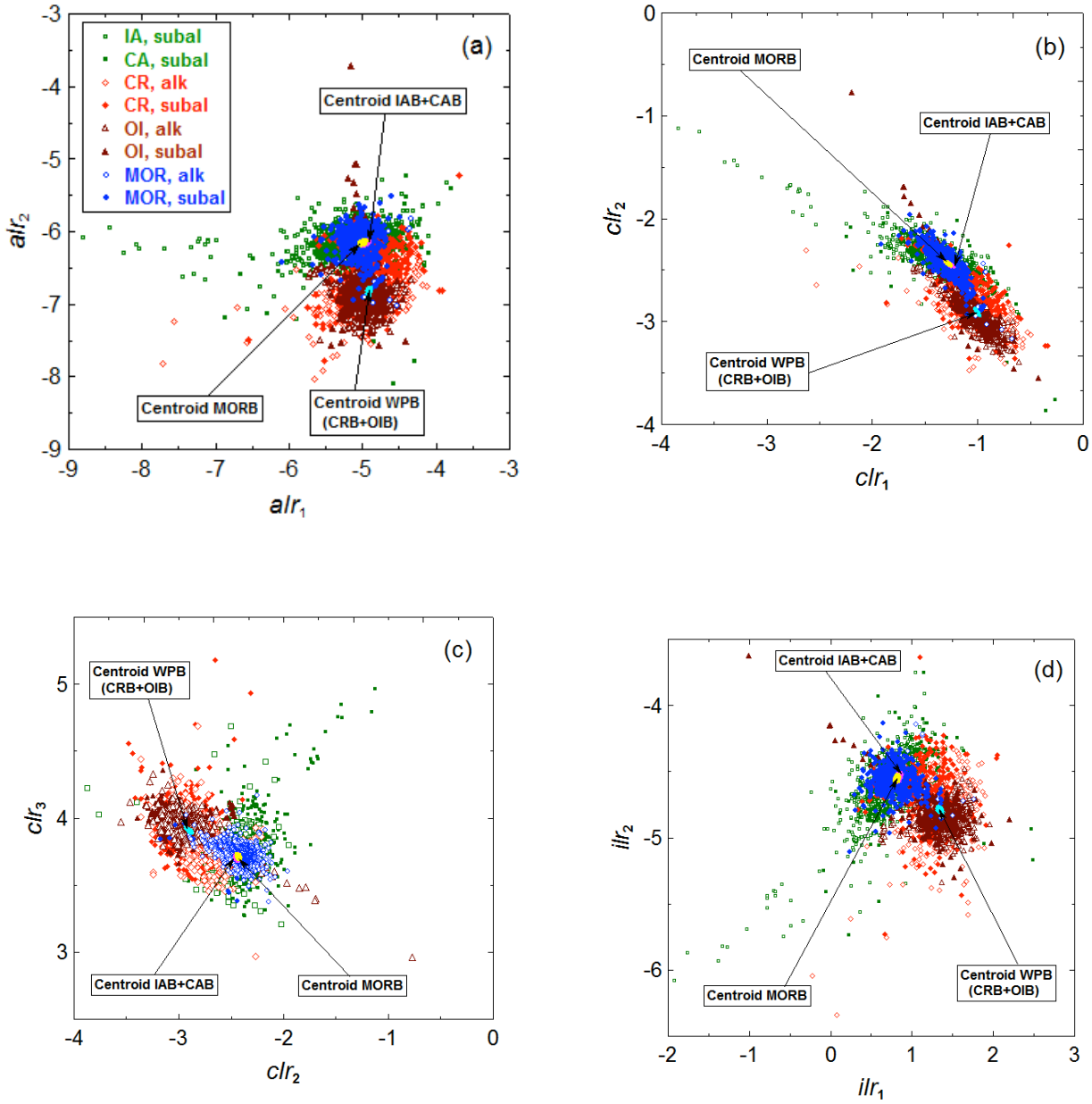

Fig. S2. Bivariate (x–y-type) plot of transformed data for Zr, Y, and $(TiO_2)_{adj}$ from the compiled dataset. Island arc (IA), continental arc (CA), continental rift (CR), ocean island (OI), and mid-ocean ridge (MOR) are identified in addition to basalt (B), subalkaline (subal), and alkaline (alk). The subscript $_{adj}$ refers to the adjusted data from SINCLAS (Verma et al., 2002) or IgRoCS (Verma and Rivera-Gómez, 2013). The centroids for each of the three tectonic settings estimated from the Monte Carlo procedure including 100,000 replications for the data of Table 3 are also shown. The complete datasets were used for each tectonic setting. (a) Additive log-ratio (alr) transformation of Aitchison (1986); equations (5) and (6) give the alr1–alr2 computations. (b) First and second variables of centered log-ratio (clr) transformation of Aitchison (1986); equations (7) and (8) give the clr1–clr2 computations. (c) Second and third variables of centered log-ratio (clr) transformation of Aitchison (1986); equations (8) and (9) give the clr2–clr3 computations. (d) Isometric log-ratio (ilr) transformation of Egozcue et al. (2003); equations (10) and (11) give the ilr1–ilr2 computations.

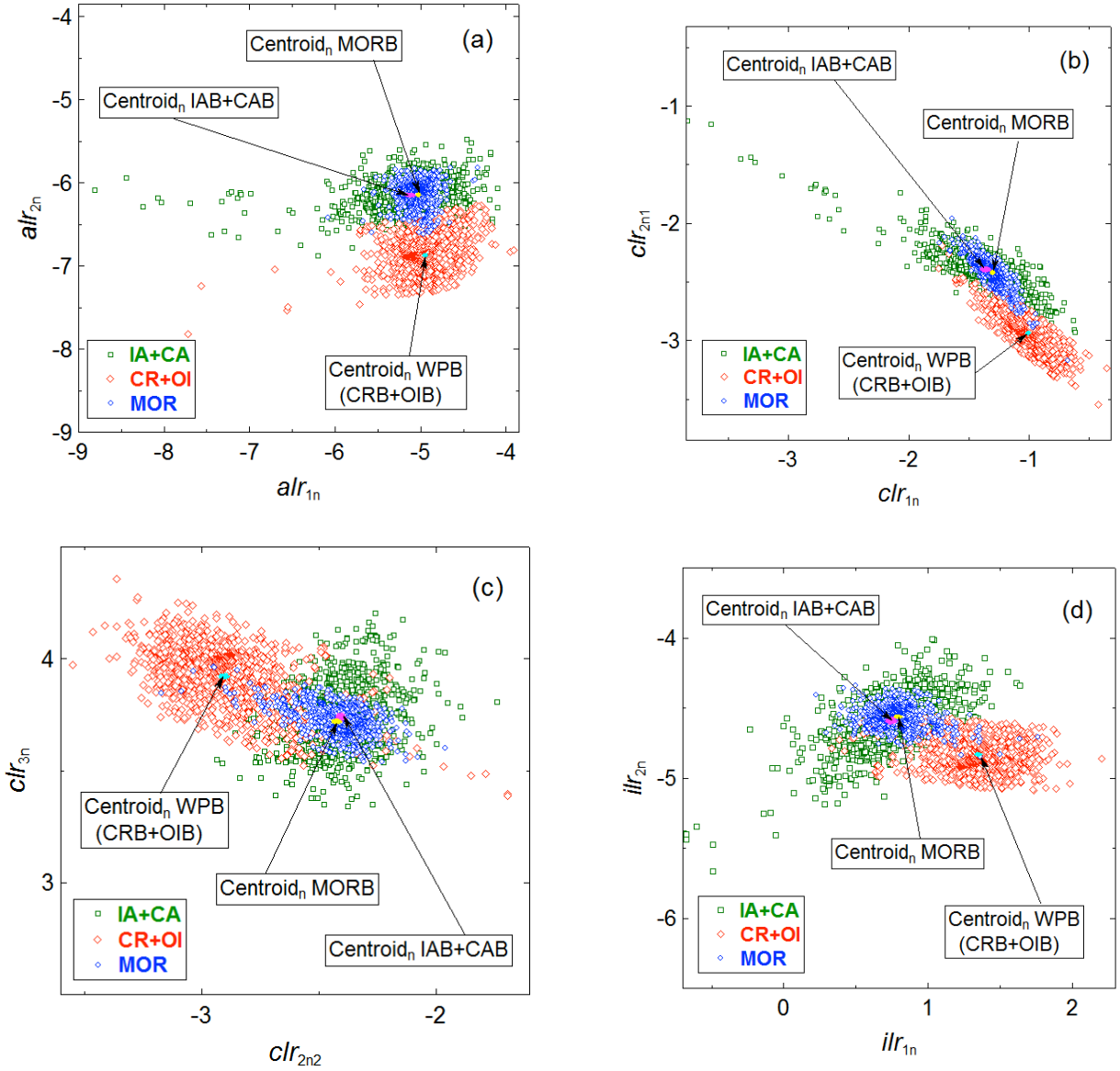

Fig. S3. Bivariate plot of transformed data for Zr, Y, and $(TiO_2)_{adj}$ from the compiled database after the separation of bivariate discordant outliers for each pair of transformed variables (normally distributed dataset); island arc (IA), continental arc (CA), continental rift (CR), ocean island (OI), and mid-ocean ridge (MOR) are indicated in addition to basalt (B), subalkaline (subal), and alkaline, alk. The subscript $_{adj}$ refers to the adjusted data from SINCLAS (Verma et al., 2002) or IgRoCS (Verma and Rivera-Gómez, 2013). The centroids for each of the three tectonic settings estimated from the Monte Carlo procedure including 100,000 replications for the data of Table 3 are also shown, where subscript $_n$ refers to normally distributed variables. The differences between Figs. S2a–d and S3a–d are such that the latter figures are based on the normally distributed log-transformed data. (a) Additive log-ratio (alr) transformation of Aitchison (1986); equations (5) and (6) give the alr1–alr2 computations. (b) First and second variables of centered log-ratio (clr) transformation of Aitchison (1986); equations (7) and (8) give the clr1–clr2 computations. (c) Second and third variables of centered log-ratio (clr) transformation of Aitchison (1986); equations (8) and (9) give the clr2–clr3 computations. (d) Isometric log-ratio (ilr) transformation of Egozcue et al. (2003); equations (10) and (11) give the ilr1–ilr2 computations.