

Supporting Information

Table S1. Numerical data for Figure 3.

Z	Element	% L.C.	% H.C.	Data set
55	Cs	66.9	33.19	1,057
56	Ba	85.1	14.9	2,231
57	La	90.7	9.3	3,612
58	Ce	84.7	15.3	2,905
59	Pr	96.0	4.0	2,271
60	Nd	88.6	11.4	3,880
62	Sm	81.9	18.1	3,485
63	Eu	93.8	6.2	5,515
64	Gd	96.2	3.8	4,895
65	Tb	96.9	3.1	4,440
66	Dy	95.7	4.3	5,755
67	Ho	95.1	4.9	1,688
68	Er	88.4	11.5	2,884
69	Tm	87.3	12.7	599
70	Yb	66.4	33.6	3,252
71	Lu	60.9	39.1	1,185
72	Hf	32.5	67.5	1,024
73	Ta	17.4	82.7	1,704
74	W	3.2	96.8	42,180
75	Re	2.2	97.8	10,727
76	Os	9.8	90.2	2,678
77	Ir	1.6	98.4	6,764
78	Pt	0.4	99.6	20,775
79	Au	0.0	100.0	13,813
80	Hg	2.1	97.9	7,917

L.C. is the percentage of atomic centers with coordination numbers equal or lower than 6; H.C. is the percentage of atomic centers with coordination numbers higher than 6.

Table S2. Numerical data for Figure 4.

Z	Element	% L.C.	% H.C.	Data set
19	K	10.6	89.4	8,998
20	Ca	6.8	93.2	3,651
21	Sc	13.6	86.4	1,146
22	Ti	7.0	93.0	9,649
23	V	13.8	86.2	16,510
24	Cr	11.1	88.9	9,874
25	Mn	4.3	95.7	31,558
26	Fe	16.4	83.6	38,359
27	Co	15.2	84.8	44,108
28	Ni	40.1	59.9	46,840
29	Cu	46.9	54.0	96,984
30	Zn	47.9	52.1	50,899
31	Ga	74.6	25.4	8,826
32	Ge	79.0	21.0	11,946
33	As	90.2	9.8	12,258
34	Se	98.0	2.0	29,443
35	Br	99.3	0.7	9,900

L.C. is the percentage of atomic centers with coordination numbers equal or less than 4; H.C. is the percentage of atomic centers with coordination numbers higher than 4.

Table S3. Numerical data for Figure 5.

Z	Element	% M-O	Data set
55	Cs	82.1	1,057
56	Ba	92.1	2,231
57	La	84.1	3,612
58	Ce	81.1	2,905
59	Pr	90.7	2,271
60	Nd	87.1	3,880
62	Sm	78.0	3,485
63	Eu	92.0	5,515
64	Gd	94.0	4,895
65	Tb	93.7	4,440
66	Dy	92.2	5,755
67	Ho	90.4	1,688
68	Er	87.4	2,884
69	Tm	80.2	599
70	Yb	76.7	3,252
71	Lu	64.9	1,185
72	Hf	41.6	1,024
73	Ta	36.2	1,704
74	W	42.9	42,180
75	Re	35.7	10,727
76	Os	18.5	2,678
77	Ir	18.6	6,764
78	Pt	13.5	20,775
79	Au	3.4	13,813
80	Hg	18.4	7,917

% M-O is the percentage of crystal structures of a given element that presents at least one M-O bond.