



STRUCTURAL SCIENCE  
CRYSTAL ENGINEERING  
MATERIALS

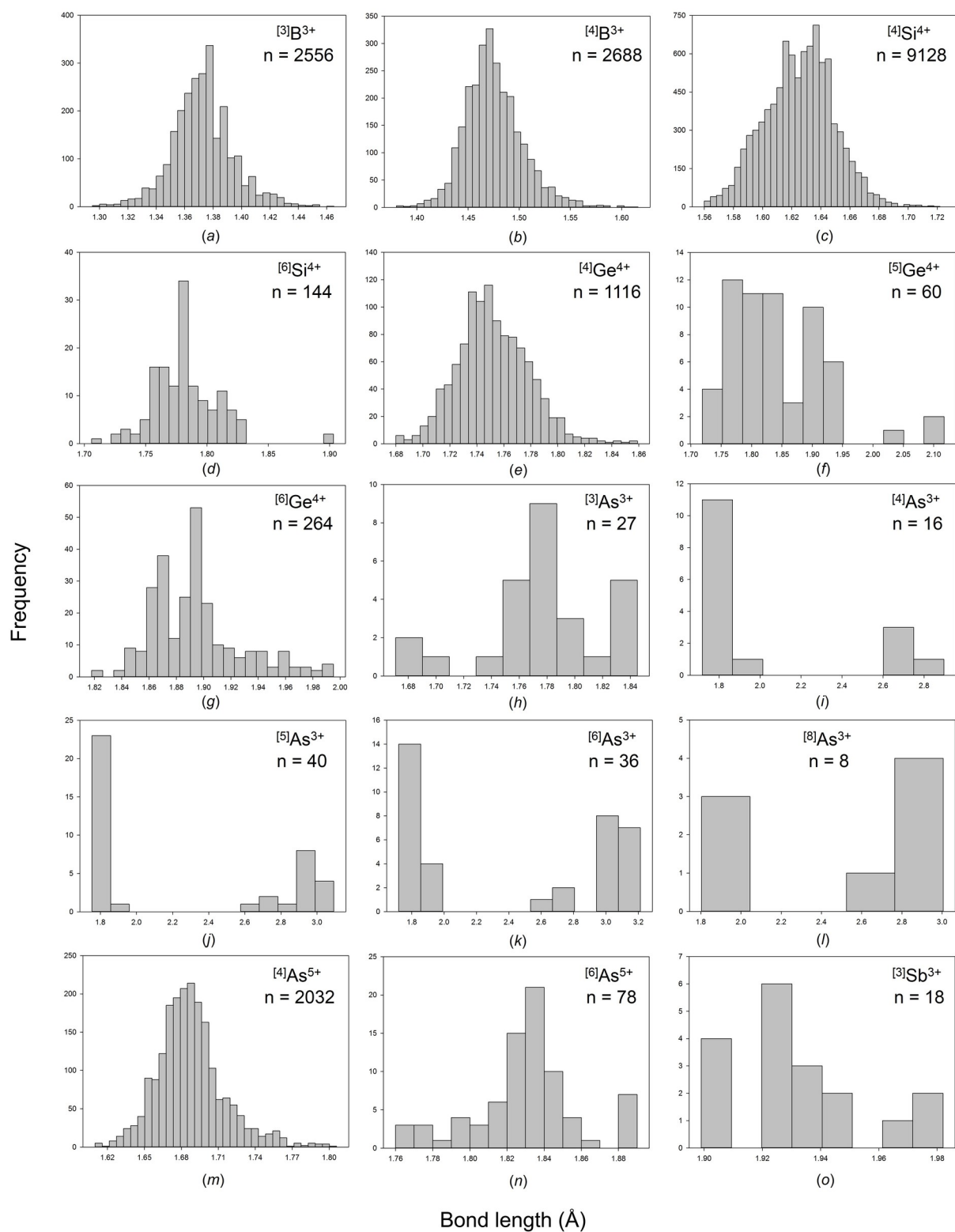
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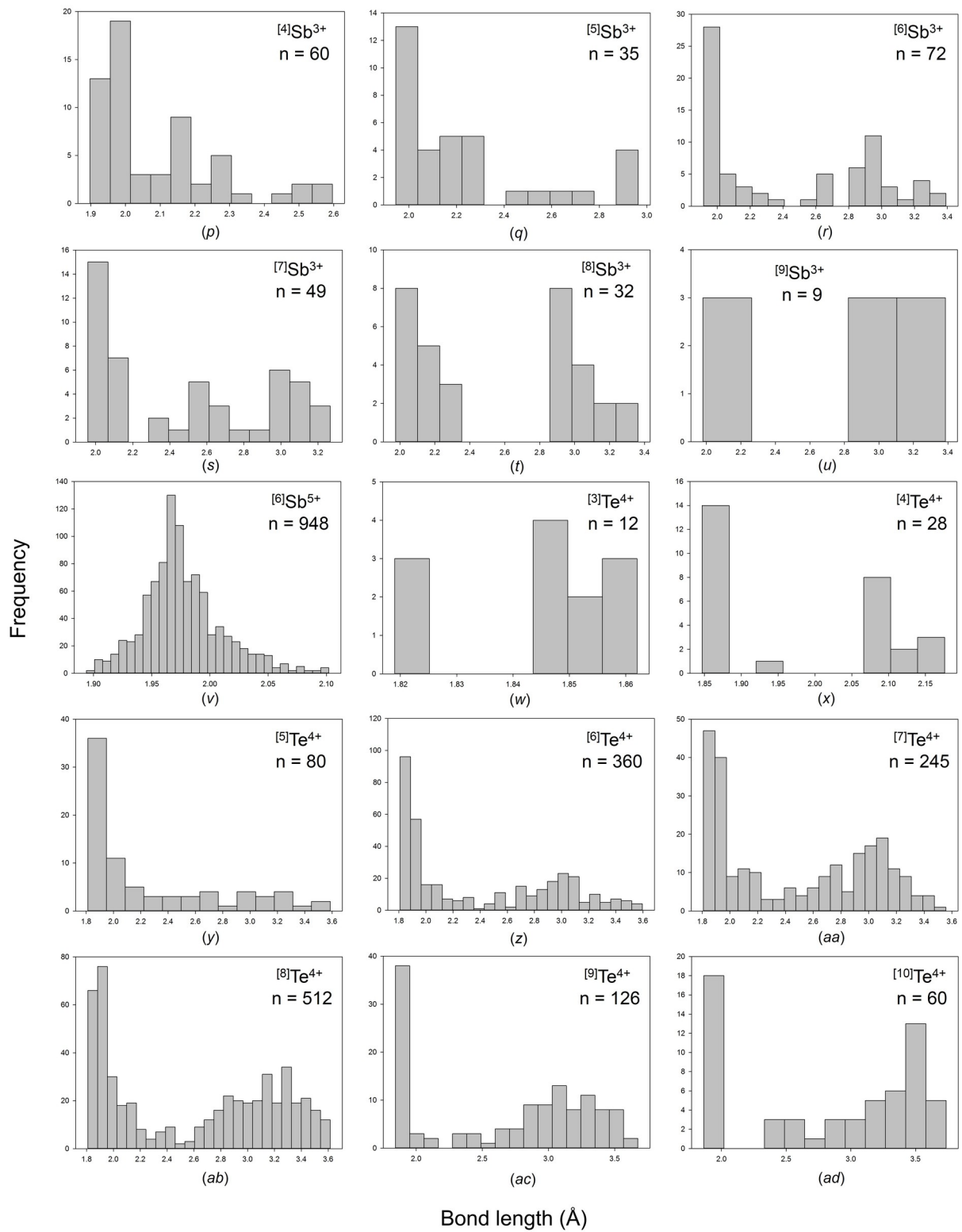
**Supporting information for article:**

**Bond-length distributions for ions bonded to oxygen: metalloids  
and post-transition metals**

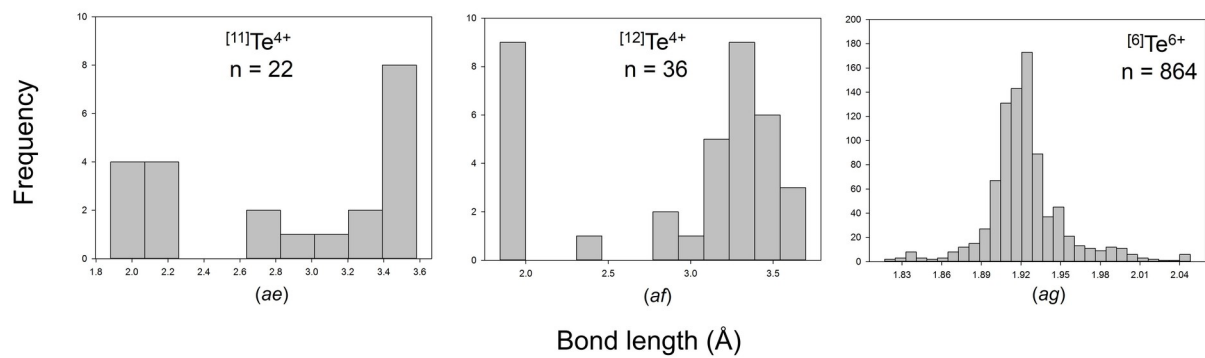
**Olivier Charles Gagné and Frank Christopher Hawthorne**

**Figure S1** Bond-length distributions for all configurations of the metalloid ions bonded to  $O^{2-}$ : (a)  $^{[3]}B^{3+}$ , (b)  $^{[4]}B^{3+}$ , (c)  $^{[4]}Si^{4+}$ , (d)  $^{[6]}Si^{4+}$ , (e)  $^{[4]}Ge^{4+}$ , (f)  $^{[5]}Ge^{4+}$ , (g)  $^{[6]}Ge^{4+}$ , (h)  $^{[3]}As^{3+}$ , (i)  $^{[4]}As^{3+}$ , (j)  $^{[5]}As^{3+}$ , (k)  $^{[6]}As^{3+}$ , (l)  $^{[8]}As^{3+}$ , (m)  $^{[4]}As^{5+}$ , (n)  $^{[6]}As^{5+}$ , (o)  $^{[3]}Sb^{3+}$ , (p)  $^{[4]}Sb^{3+}$ , (q)  $^{[5]}Sb^{3+}$ , (r)  $^{[6]}Sb^{3+}$ , (s)  $^{[7]}Sb^{3+}$ , (t)  $^{[8]}Sb^{3+}$ , (u)  $^{[9]}Sb^{3+}$ , (v)  $^{[6]}Sb^{5+}$ , (w)  $^{[3]}Te^{4+}$ , (x)  $^{[4]}Te^{4+}$ , (y)  $^{[5]}Te^{4+}$ , (z)  $^{[6]}Te^{4+}$ , (aa)  $^{[7]}Te^{4+}$ , (ab)  $^{[8]}Te^{4+}$ , (ac)  $^{[9]}Te^{4+}$ , (ad)  $^{[10]}Te^{4+}$ , (ae)  $^{[11]}Te^{4+}$ , (af)  $^{[12]}Te^{4+}$ , (ag)  $^{[6]}Te^{6+}$ .

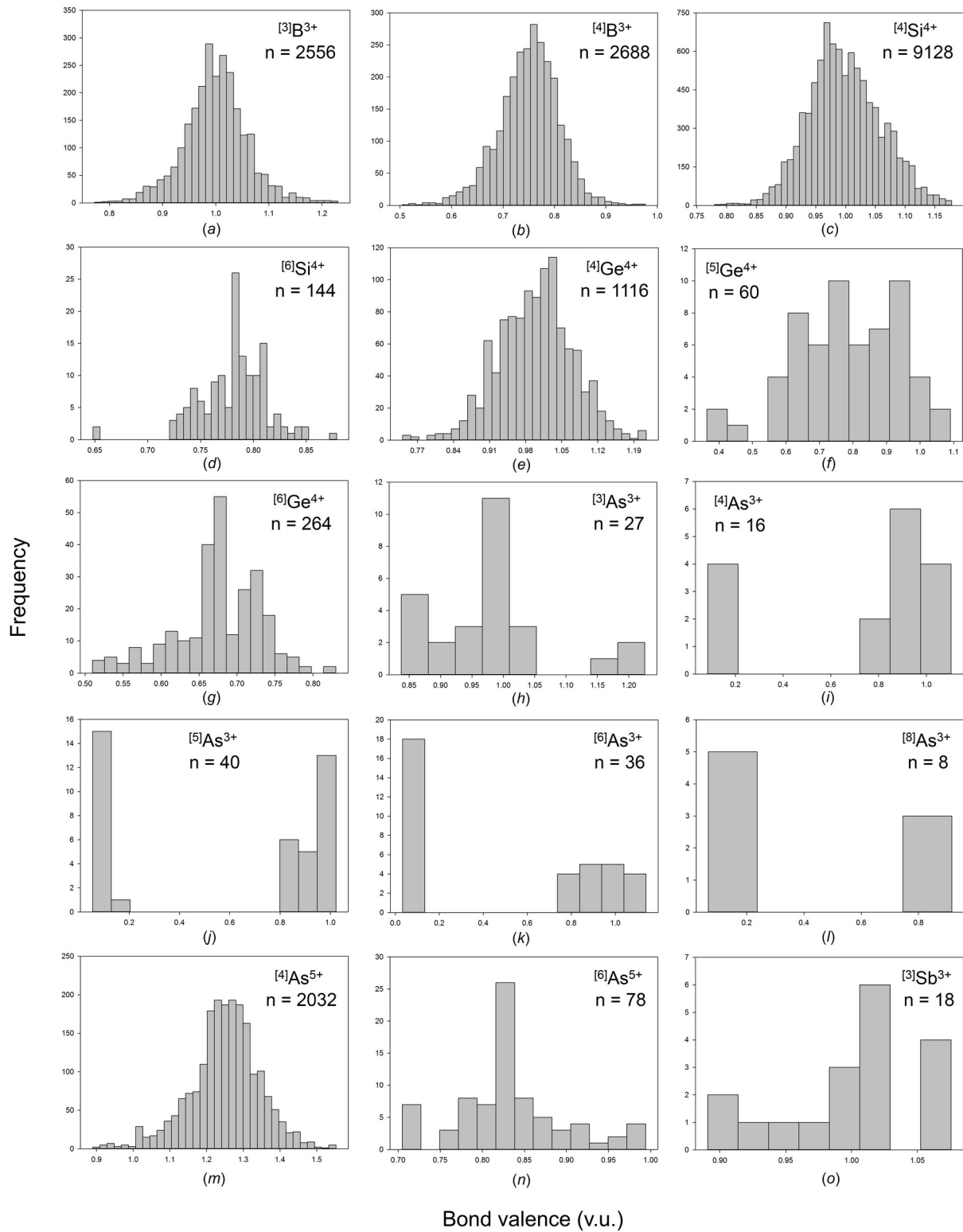


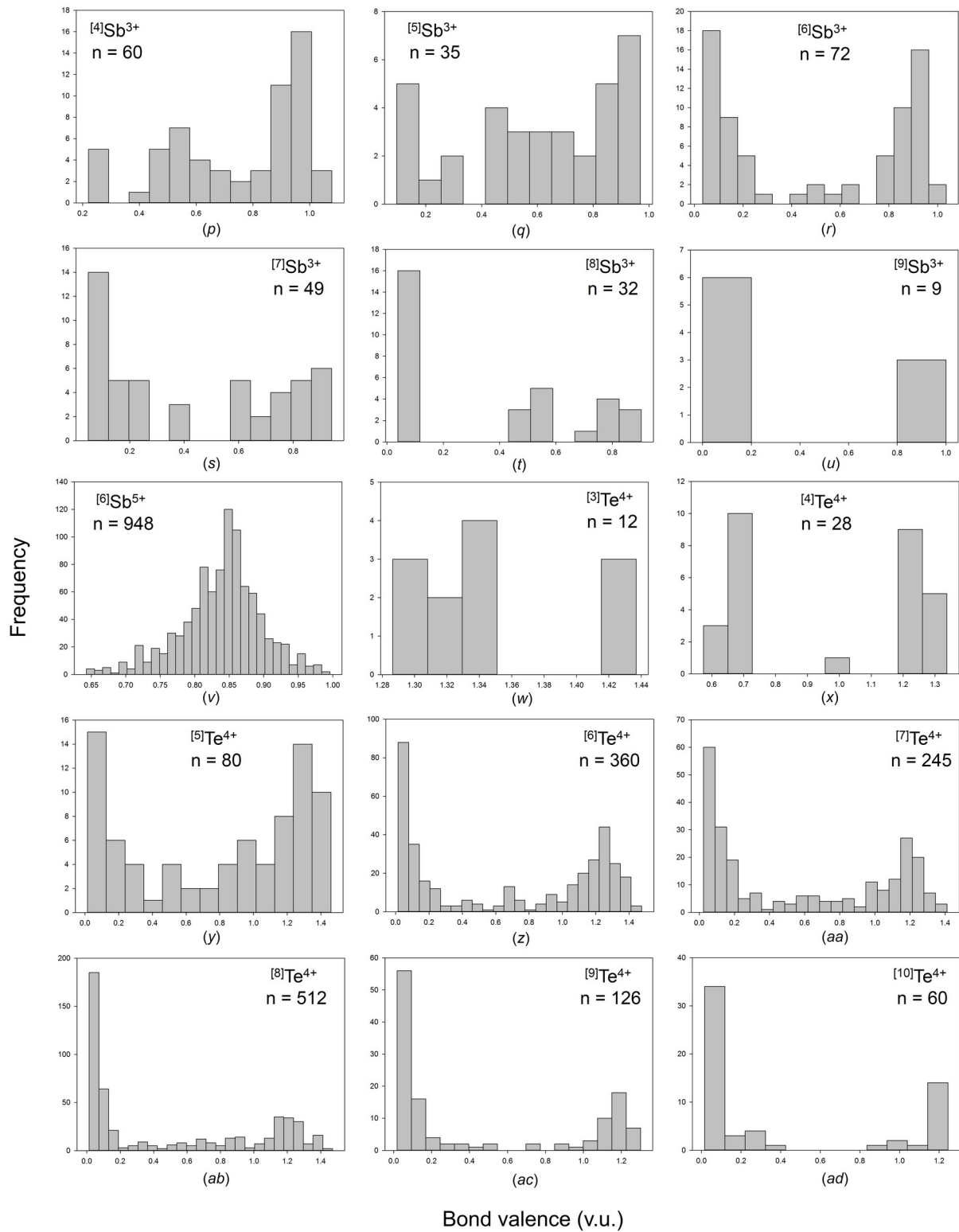


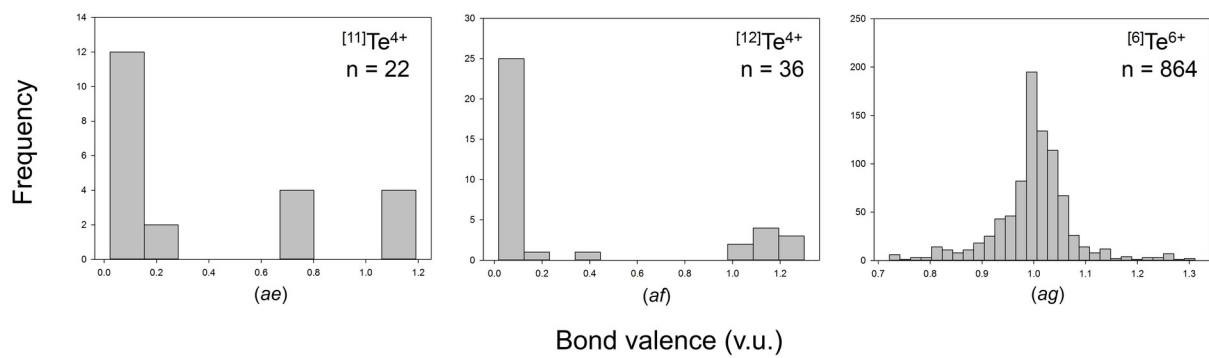




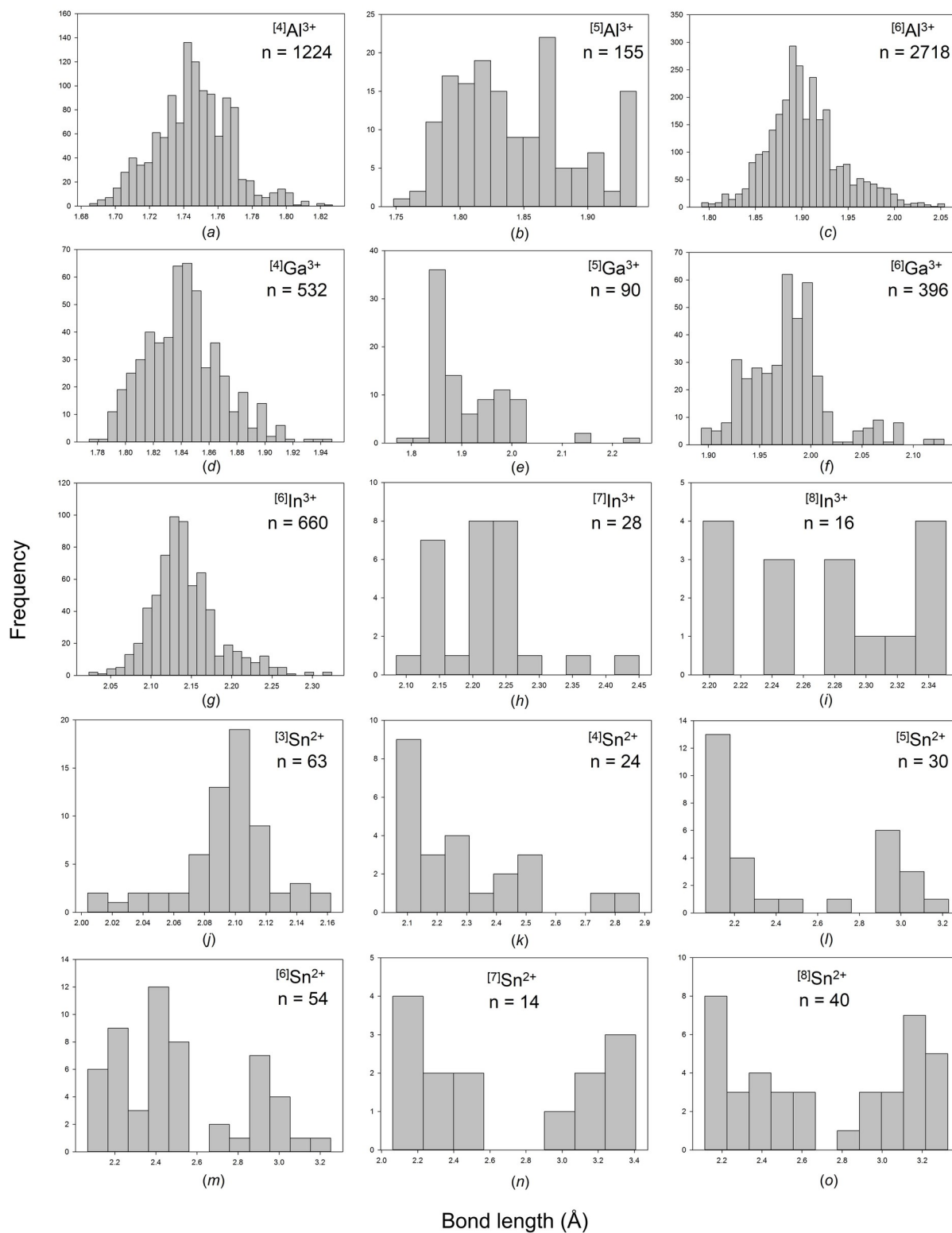
**Figure S2** Bond-valence distributions for all configurations of the metalloid ions bonded to O<sup>2-</sup>: (a) <sup>[3]</sup>B<sup>3+</sup>, (b) <sup>[4]</sup>B<sup>3+</sup>, (c) <sup>[4]</sup>Si<sup>4+</sup>, (d) <sup>[6]</sup>Si<sup>4+</sup>, (e) <sup>[4]</sup>Ge<sup>4+</sup>, (f) <sup>[5]</sup>Ge<sup>4+</sup>, (g) <sup>[6]</sup>Ge<sup>4+</sup>, (h) <sup>[3]</sup>As<sup>3+</sup>, (i) <sup>[4]</sup>As<sup>3+</sup>, (j) <sup>[5]</sup>As<sup>3+</sup>, (k) <sup>[6]</sup>As<sup>3+</sup>, (l) <sup>[8]</sup>As<sup>3+</sup>, (m) <sup>[4]</sup>As<sup>5+</sup>, (n) <sup>[6]</sup>As<sup>5+</sup>, (o) <sup>[3]</sup>Sb<sup>3+</sup>, (p) <sup>[4]</sup>Sb<sup>3+</sup>, (q) <sup>[5]</sup>Sb<sup>3+</sup>, (r) <sup>[6]</sup>Sb<sup>3+</sup>, (s) <sup>[7]</sup>Sb<sup>3+</sup>, (t) <sup>[8]</sup>Sb<sup>3+</sup>, (u) <sup>[9]</sup>Sb<sup>3+</sup>, (v) <sup>[6]</sup>Sb<sup>5+</sup>, (w) <sup>[3]</sup>Te<sup>4+</sup>, (x) <sup>[4]</sup>Te<sup>4+</sup>, (y) <sup>[5]</sup>Te<sup>4+</sup>, (z) <sup>[6]</sup>Te<sup>4+</sup>, (aa) <sup>[7]</sup>Te<sup>4+</sup>, (ab) <sup>[8]</sup>Te<sup>4+</sup>, (ac) <sup>[9]</sup>Te<sup>4+</sup>, (ad) <sup>[10]</sup>Te<sup>4+</sup>, (ae) <sup>[11]</sup>Te<sup>4+</sup>, (af) <sup>[12]</sup>Te<sup>4+</sup>, (ag) <sup>[6]</sup>Te<sup>6+</sup>.

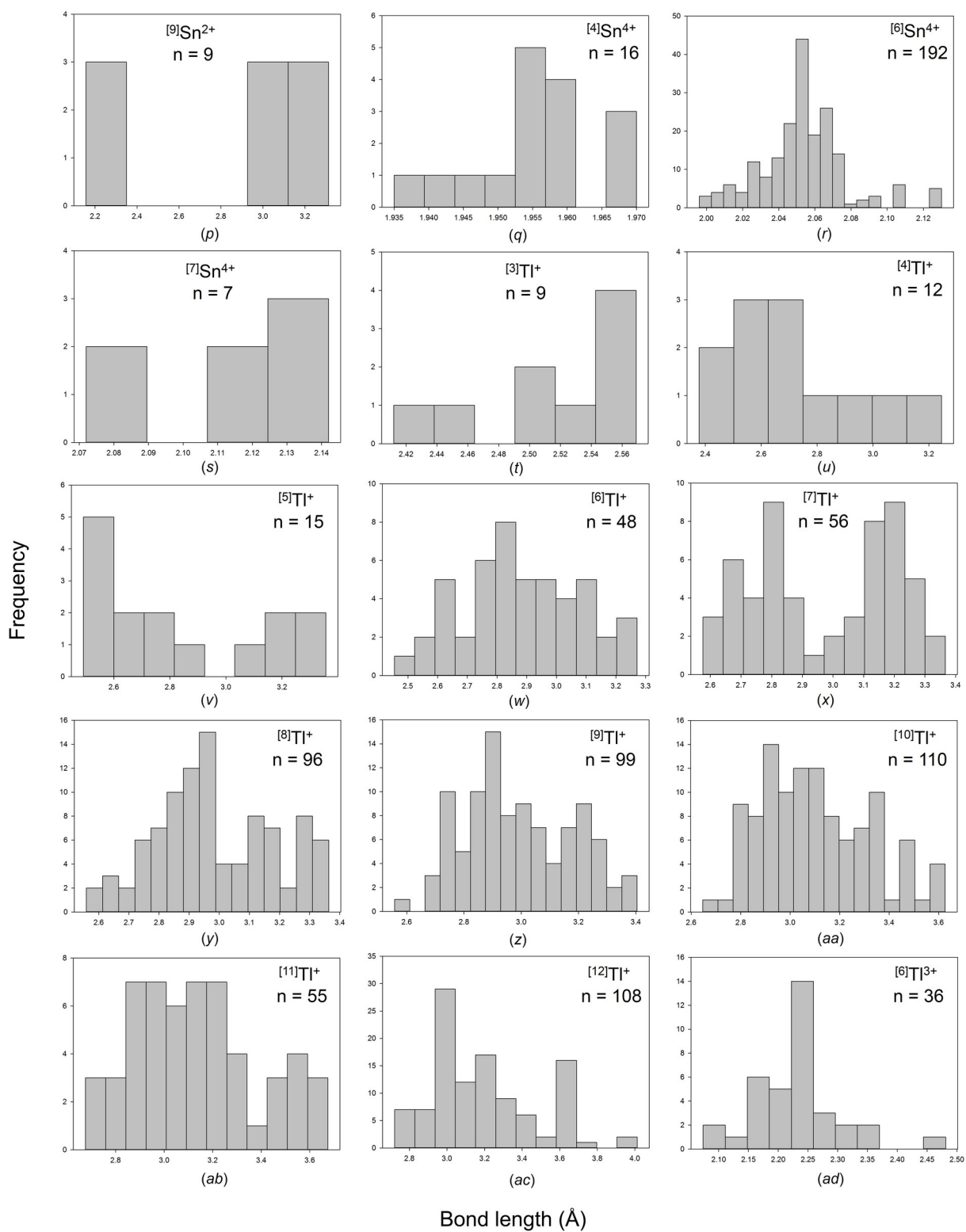




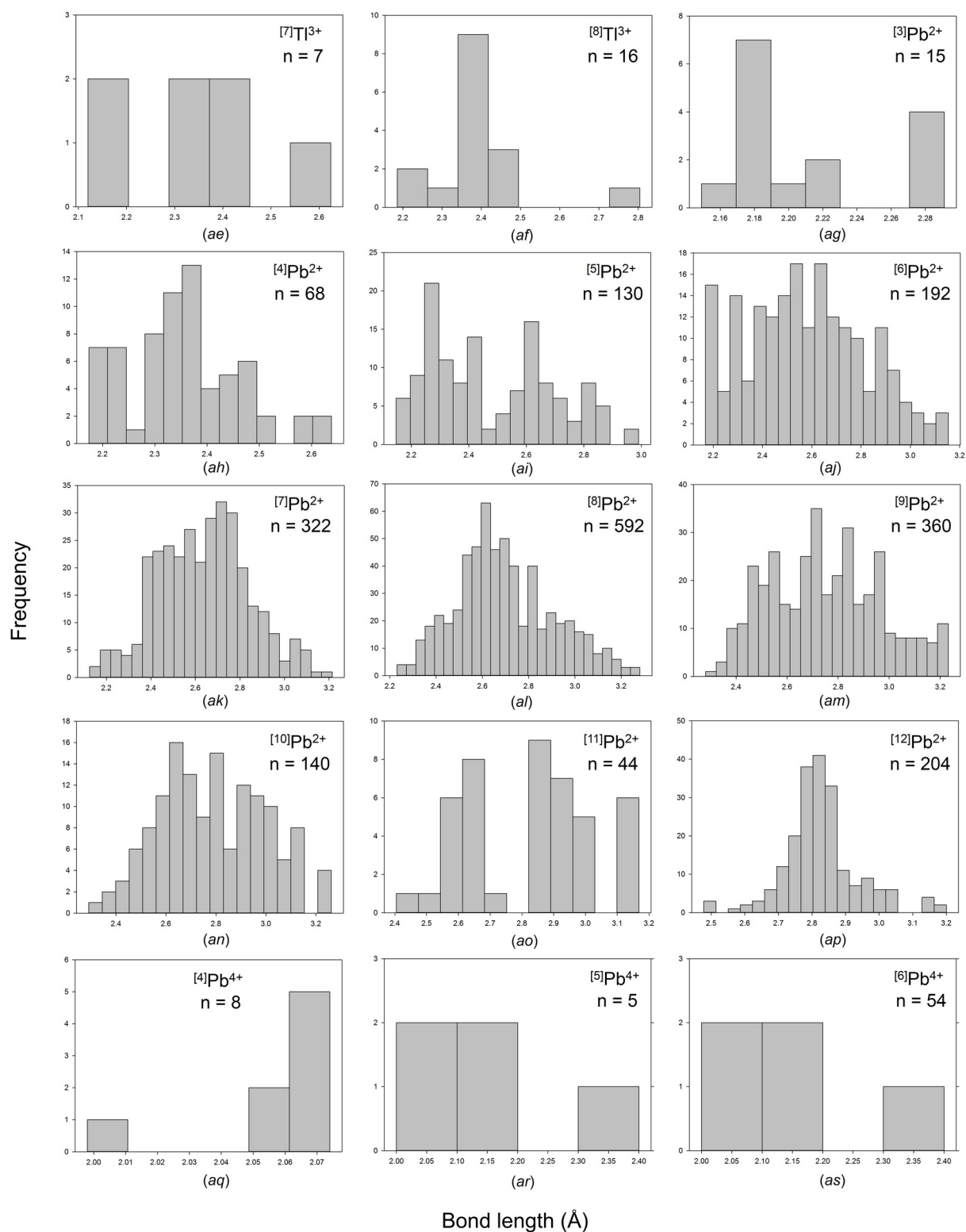


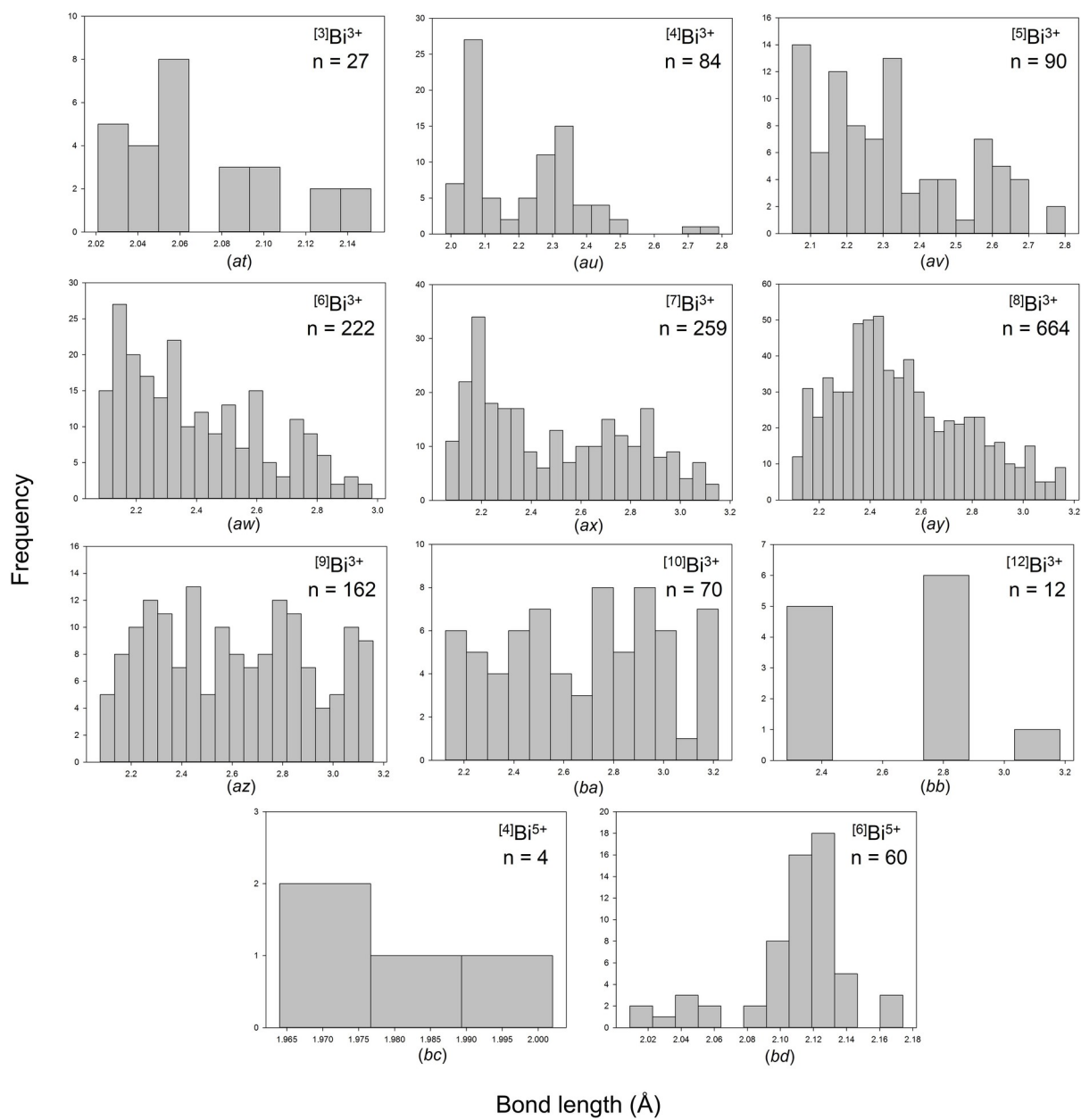
**Figure S3** Bond-length distributions for all configurations of the post-transition-metal ions bonded to O<sup>2-</sup>: (a) <sup>[4]</sup>Al<sup>3+</sup>, (b) <sup>[5]</sup>Al<sup>3+</sup>, (c) <sup>[6]</sup>Al<sup>3+</sup>, (d) <sup>[4]</sup>Ga<sup>3+</sup>, (e) <sup>[5]</sup>Ga<sup>3+</sup>, (f) <sup>[6]</sup>Ga<sup>3+</sup>, (g) <sup>[6]</sup>In<sup>3+</sup>, (h) <sup>[7]</sup>In<sup>3+</sup>, (i) <sup>[8]</sup>In<sup>3+</sup>, (j) <sup>[3]</sup>Sn<sup>2+</sup>, (k) <sup>[4]</sup>Sn<sup>2+</sup>, (l) <sup>[5]</sup>Sn<sup>2+</sup>, (m) <sup>[6]</sup>Sn<sup>2+</sup>, (n) <sup>[7]</sup>Sn<sup>2+</sup>, (o) <sup>[8]</sup>Sn<sup>2+</sup>, (p) <sup>[9]</sup>Sn<sup>2+</sup>, (q) <sup>[4]</sup>Sn<sup>4+</sup>, (r) <sup>[6]</sup>Sn<sup>4+</sup>, (s) <sup>[7]</sup>Sn<sup>4+</sup>, (t) <sup>[3]</sup>Tl<sup>+</sup>, (u) <sup>[4]</sup>Tl<sup>+</sup>, (v) <sup>[5]</sup>Tl<sup>+</sup>, (w) <sup>[6]</sup>Tl<sup>+</sup>, (x) <sup>[7]</sup>Tl<sup>+</sup>, (y) <sup>[8]</sup>Tl<sup>+</sup>, (z) <sup>[9]</sup>Tl<sup>+</sup>, (aa) <sup>[10]</sup>Tl<sup>+</sup>, (ab) <sup>[11]</sup>Tl<sup>+</sup>, (ac) <sup>[12]</sup>Tl<sup>+</sup>, (ad) <sup>[6]</sup>Tl<sup>3+</sup>, (ae) <sup>[7]</sup>Tl<sup>3+</sup>, (af) <sup>[8]</sup>Tl<sup>3+</sup>, (ag) <sup>[3]</sup>Pb<sup>2+</sup>, (ah) <sup>[4]</sup>Pb<sup>2+</sup>, (ai) <sup>[5]</sup>Pb<sup>2+</sup>, (aj) <sup>[6]</sup>Pb<sup>2+</sup>, (ak) <sup>[7]</sup>Pb<sup>2+</sup>, (al) <sup>[8]</sup>Pb<sup>2+</sup>, (am) <sup>[9]</sup>Pb<sup>2+</sup>, (an) <sup>[10]</sup>Pb<sup>2+</sup>, (ao) <sup>[11]</sup>Pb<sup>2+</sup>, (ap) <sup>[12]</sup>Pb<sup>2+</sup>, (aq) <sup>[4]</sup>Pb<sup>4+</sup>, (ar) <sup>[5]</sup>Pb<sup>4+</sup>, (as) <sup>[6]</sup>Pb<sup>4+</sup>, (at) <sup>[3]</sup>Bi<sup>3+</sup>, (au) <sup>[4]</sup>Bi<sup>3+</sup>, (av) <sup>[5]</sup>Bi<sup>3+</sup>, (aw) <sup>[6]</sup>Bi<sup>3+</sup>, (ax) <sup>[7]</sup>Bi<sup>3+</sup>, (ay) <sup>[8]</sup>Bi<sup>3+</sup>, (az) <sup>[9]</sup>Bi<sup>3+</sup>, (ba) <sup>[10]</sup>Bi<sup>3+</sup>, (bb) <sup>[12]</sup>Bi<sup>3+</sup>, (bc) <sup>[4]</sup>Bi<sup>5+</sup>, (bd) <sup>[6]</sup>Bi<sup>5+</sup>.



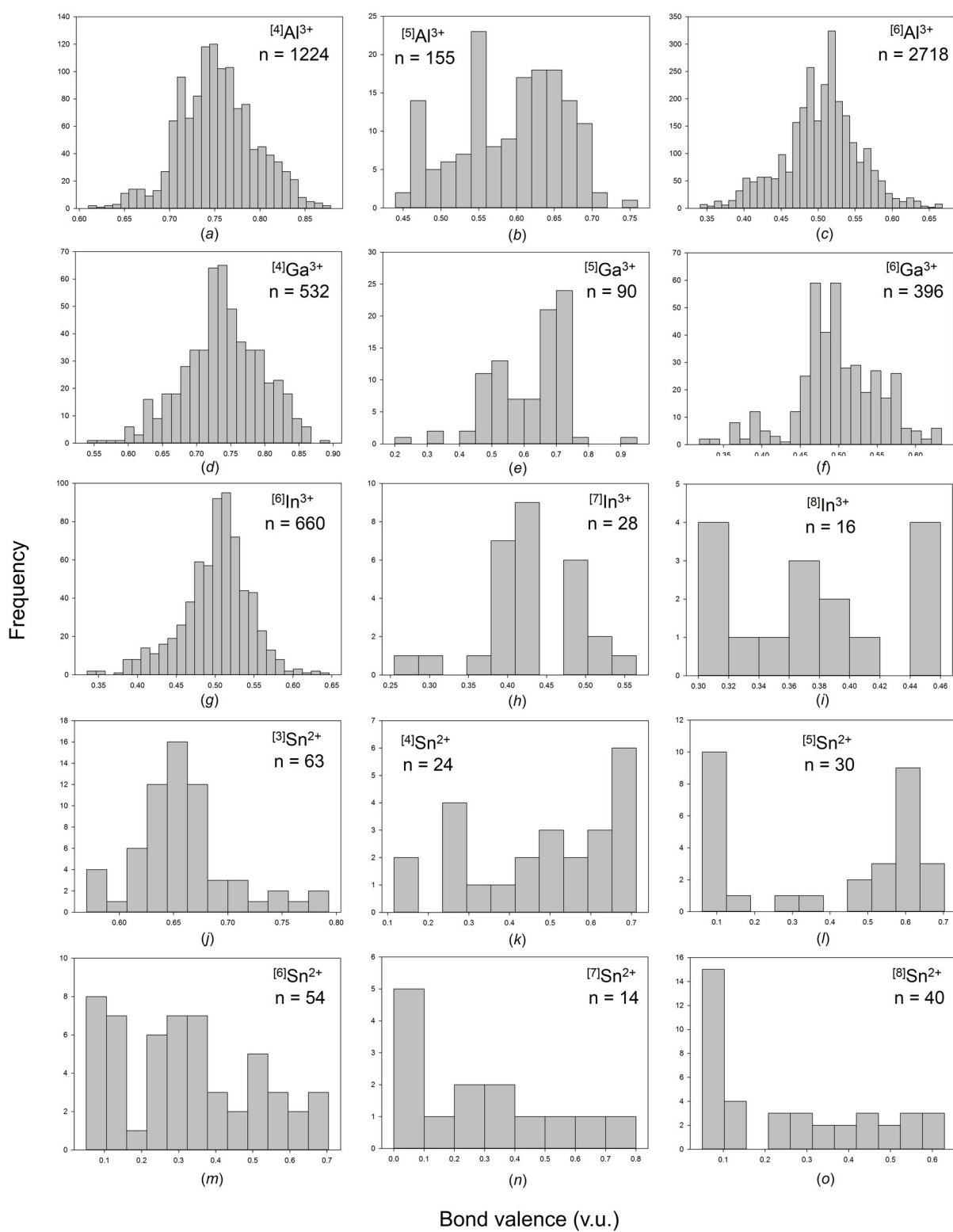


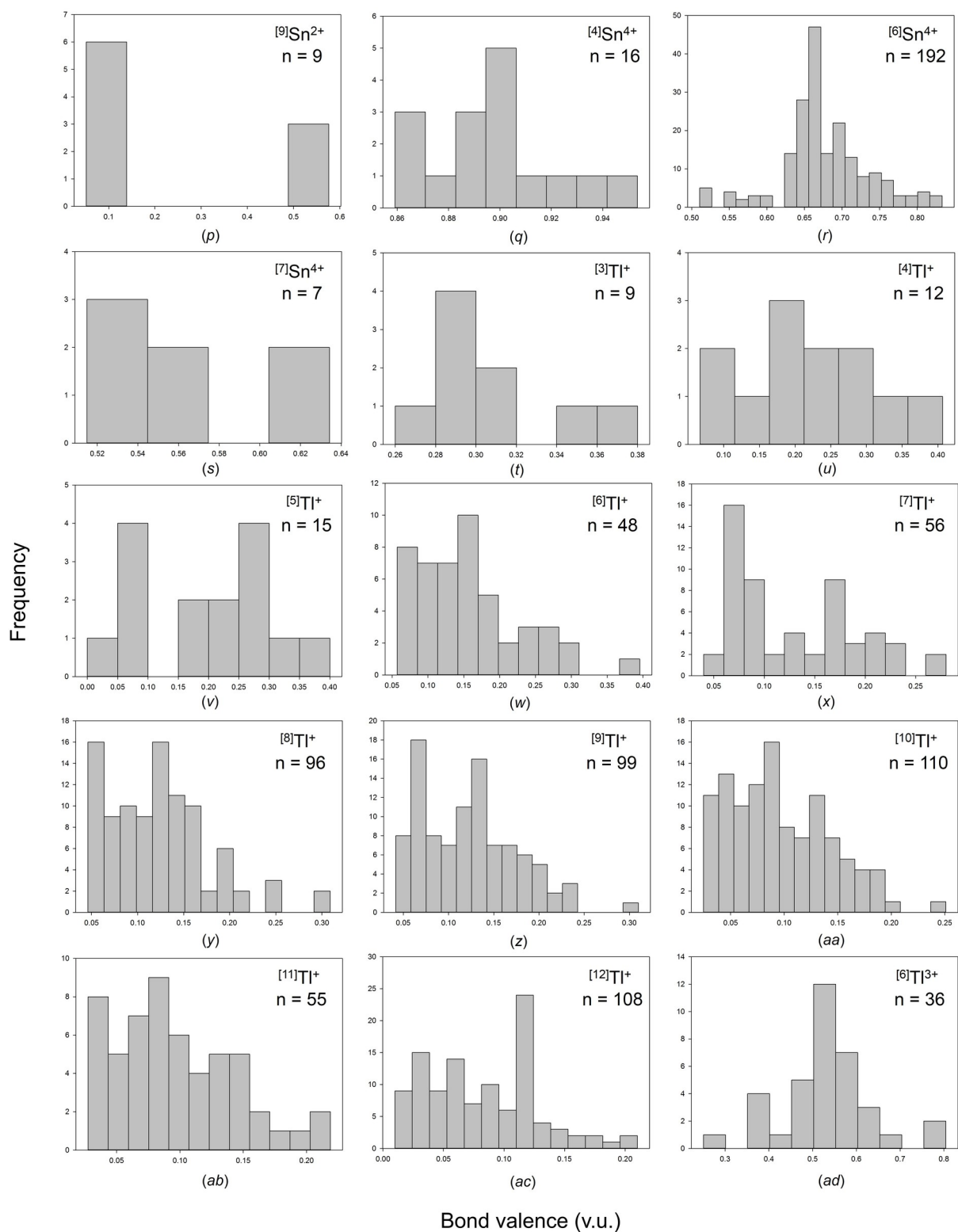


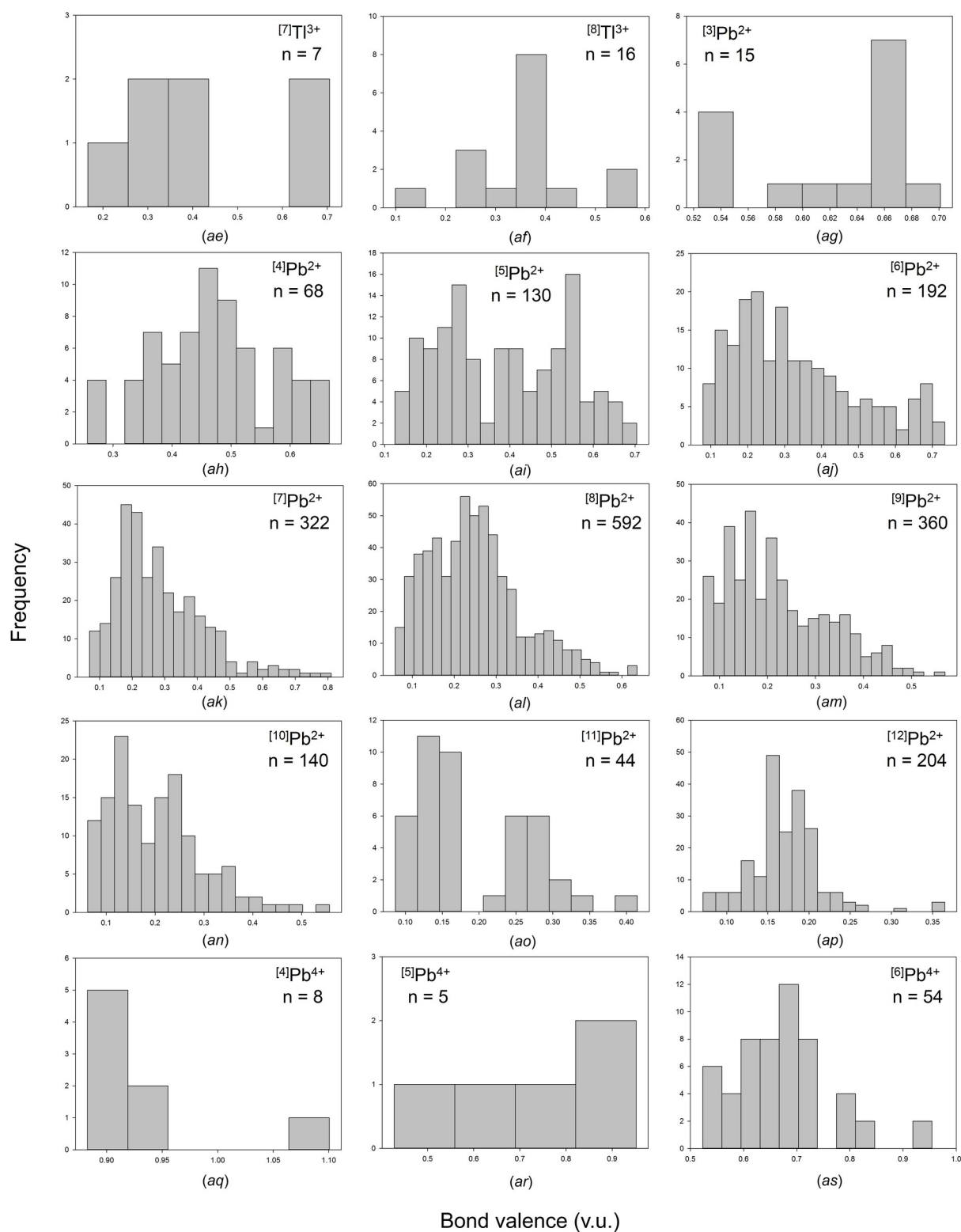


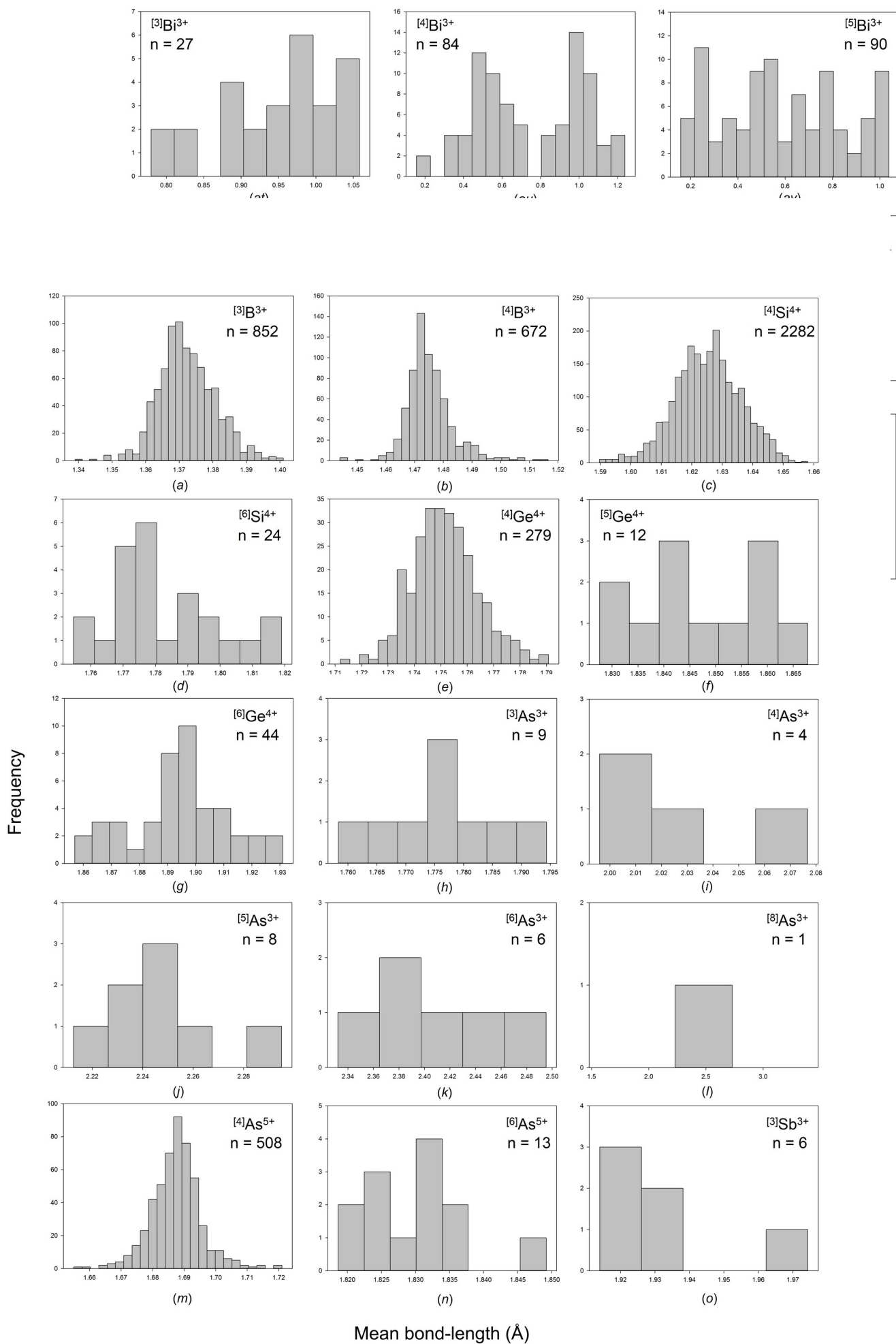


**Figure S4** Bond-valence distributions for all configurations of the post-transition-metal ions bonded to  $O^{2-}$ : (a)  $^{[4]}Al^{3+}$ , (b)  $^{[5]}Al^{3+}$ , (c)  $^{[6]}Al^{3+}$ , (d)  $^{[4]}Ga^{3+}$ , (e)  $^{[5]}Ga^{3+}$ , (f)  $^{[6]}Ga^{3+}$ , (g)  $^{[6]}In^{3+}$ , (h)  $^{[7]}In^{3+}$ , (i)  $^{[8]}In^{3+}$ , (j)  $^{[3]}Sn^{2+}$ , (k)  $^{[4]}Sn^{2+}$ , (l)  $^{[5]}Sn^{2+}$ , (m)  $^{[6]}Sn^{2+}$ , (n)  $^{[7]}Sn^{2+}$ , (o)  $^{[8]}Sn^{2+}$ , (p)  $^{[9]}Sn^{2+}$ , (q)  $^{[4]}Sn^{4+}$ , (r)  $^{[6]}Sn^{4+}$ , (s)  $^{[7]}Sn^{4+}$ , (t)  $^{[3]}Tl^{+}$ , (u)  $^{[4]}Tl^{+}$ , (v)  $^{[5]}Tl^{+}$ , (w)  $^{[6]}Tl^{+}$ , (x)  $^{[7]}Tl^{+}$ , (y)  $^{[8]}Tl^{+}$ , (z)  $^{[9]}Tl^{+}$ , (aa)  $^{[10]}Tl^{+}$ , (ab)  $^{[11]}Tl^{+}$ , (ac)  $^{[12]}Tl^{+}$ , (ad)  $^{[6]}Tl^{3+}$ , (ae)  $^{[7]}Tl^{3+}$ , (af)  $^{[8]}Tl^{3+}$ , (ag)  $^{[3]}Pb^{2+}$ , (ah)  $^{[4]}Pb^{2+}$ , (ai)  $^{[5]}Pb^{2+}$ , (aj)  $^{[6]}Pb^{2+}$ , (ak)  $^{[7]}Pb^{2+}$ , (al)  $^{[8]}Pb^{2+}$ , (am)  $^{[9]}Pb^{2+}$ , (an)  $^{[10]}Pb^{2+}$ , (ao)  $^{[11]}Pb^{2+}$ , (ap)  $^{[12]}Pb^{2+}$ , (aq)  $^{[4]}Pb^{4+}$ , (ar)  $^{[5]}Pb^{4+}$ , (as)  $^{[6]}Pb^{4+}$ , (at)  $^{[3]}Bi^{3+}$ , (au)  $^{[4]}Bi^{3+}$ , (av)  $^{[5]}Bi^{3+}$ , (aw)  $^{[6]}Bi^{3+}$ , (ax)  $^{[7]}Bi^{3+}$ , (ay)  $^{[8]}Bi^{3+}$ , (az)  $^{[9]}Bi^{3+}$ , (ba)  $^{[10]}Bi^{3+}$ , (bb)  $^{[12]}Bi^{3+}$ , (bc)  $^{[4]}Bi^{5+}$ , (bd)  $^{[6]}Bi^{5+}$ .



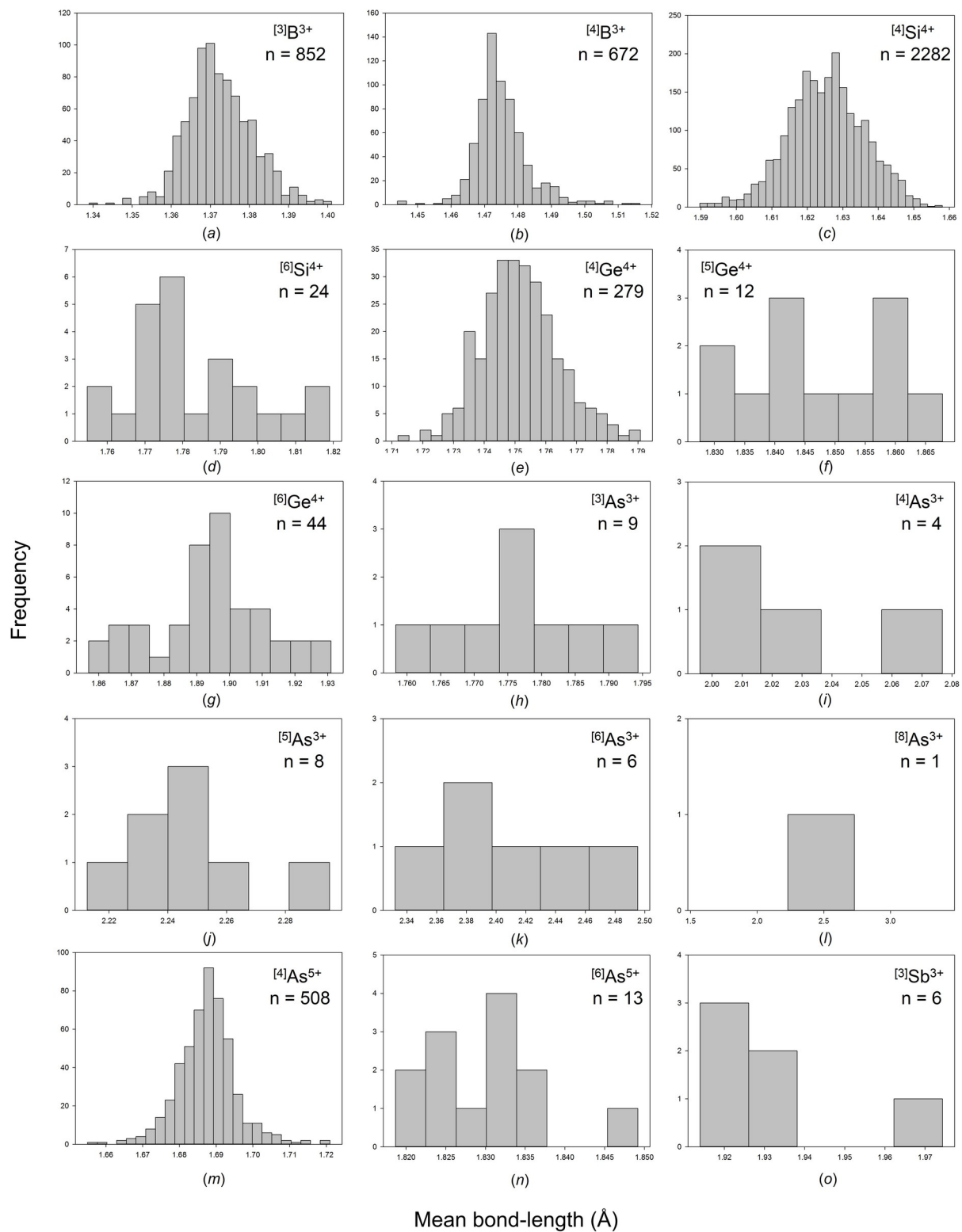


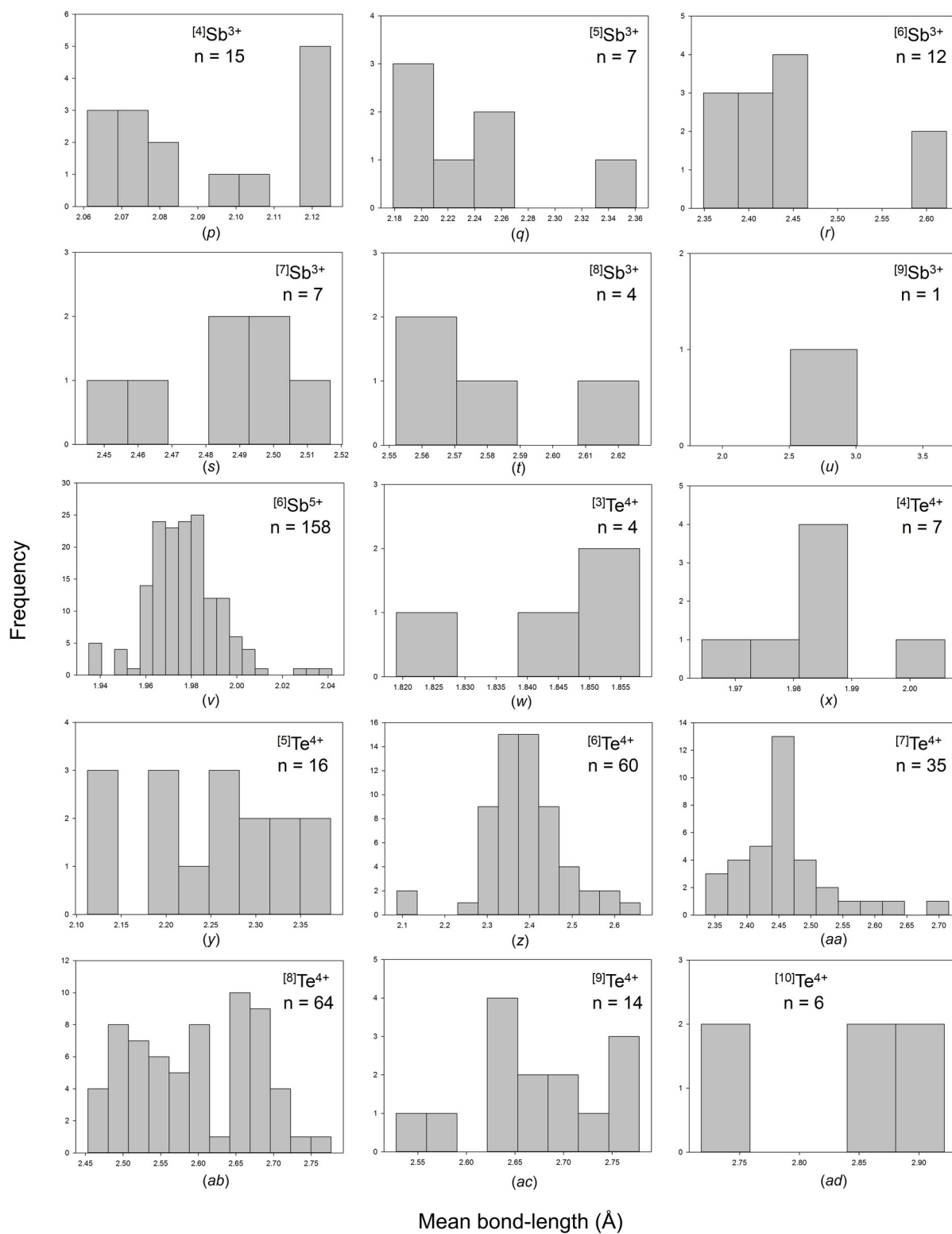


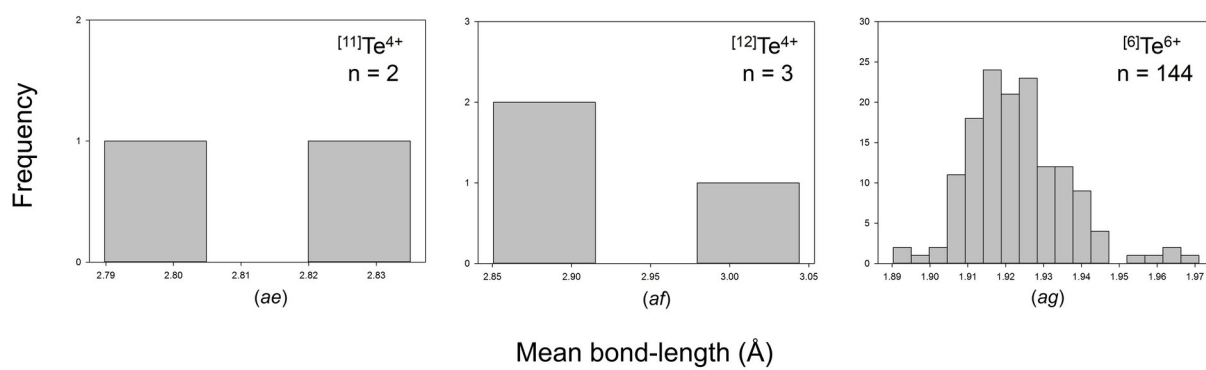


**Figure S5** Mean-bond-length distributions for all configurations of the metalloid ions bonded to  $O^{2-}$ : (a)  $^{[3]}B^{3+}$ , (b)  $^{[4]}B^{3+}$ , (c)  $^{[4]}Si^{4+}$ , (d)  $^{[6]}Si^{4+}$ , (e)  $^{[4]}Ge^{4+}$ , (f)  $^{[5]}Ge^{4+}$ , (g)  $^{[6]}Ge^{4+}$ , (h)  $^{[3]}As^{3+}$ , (i)  $^{[4]}As^{3+}$ , (j)  $^{[5]}As^{3+}$ , (k)  $^{[6]}As^{3+}$ , (l)  $^{[8]}As^{3+}$ , (m)  $^{[4]}As^{5+}$ , (n)  $^{[6]}As^{5+}$ , (o)  $^{[3]}Sb^{3+}$ , (p)  $^{[4]}Sb^{3+}$ , (q)  $^{[5]}Sb^{3+}$ , (r)  $^{[6]}Sb^{3+}$ , (s)  $^{[7]}Sb^{3+}$ , (t)  $^{[8]}Sb^{3+}$ , (u)  $^{[9]}Sb^{3+}$ , (v)  $^{[6]}Sb^{5+}$ , (w)  $^{[3]}Te^{4+}$ , (x)  $^{[4]}Te^{4+}$ , (y)  $^{[5]}Te^{4+}$ , (z)  $^{[6]}Te^{4+}$ , (aa)  $^{[7]}Te^{4+}$ , (ab)  $^{[8]}Te^{4+}$ , (ac)  $^{[9]}Te^{4+}$ , (ad)  $^{[10]}Te^{4+}$ , (ae)  $^{[11]}Te^{4+}$ , (af)  $^{[12]}Te^{4+}$ , (ag)  $^{[6]}Te^{6+}$ .

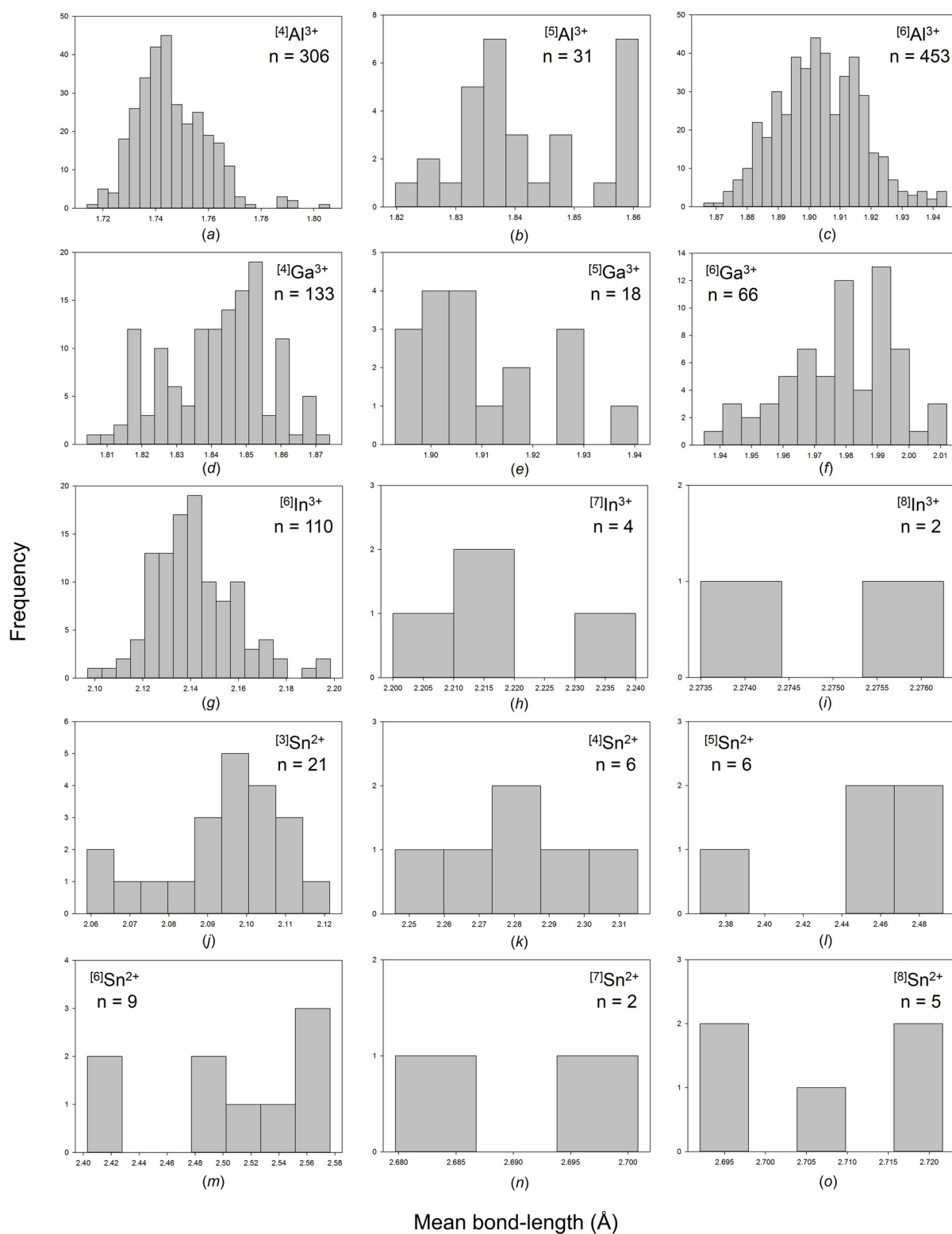


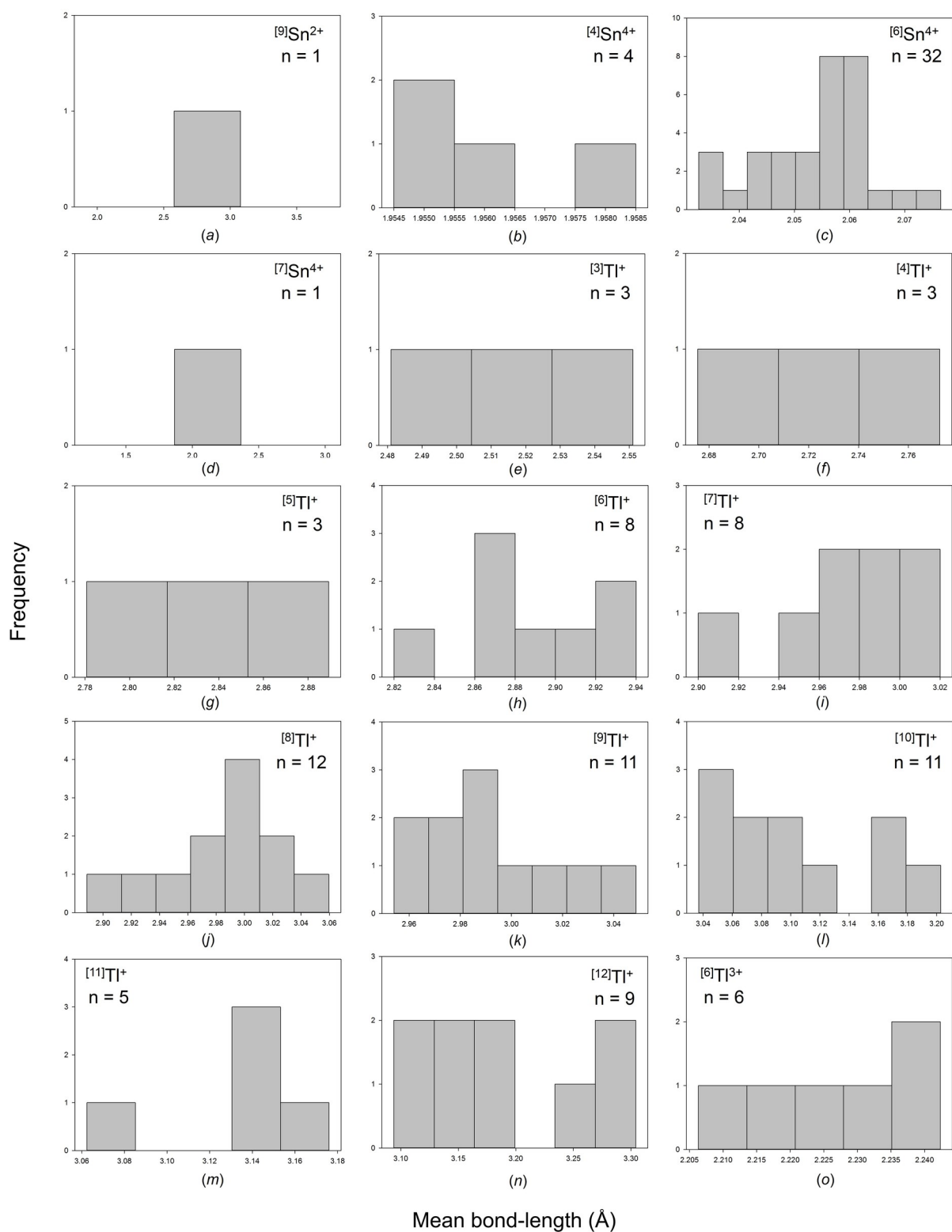


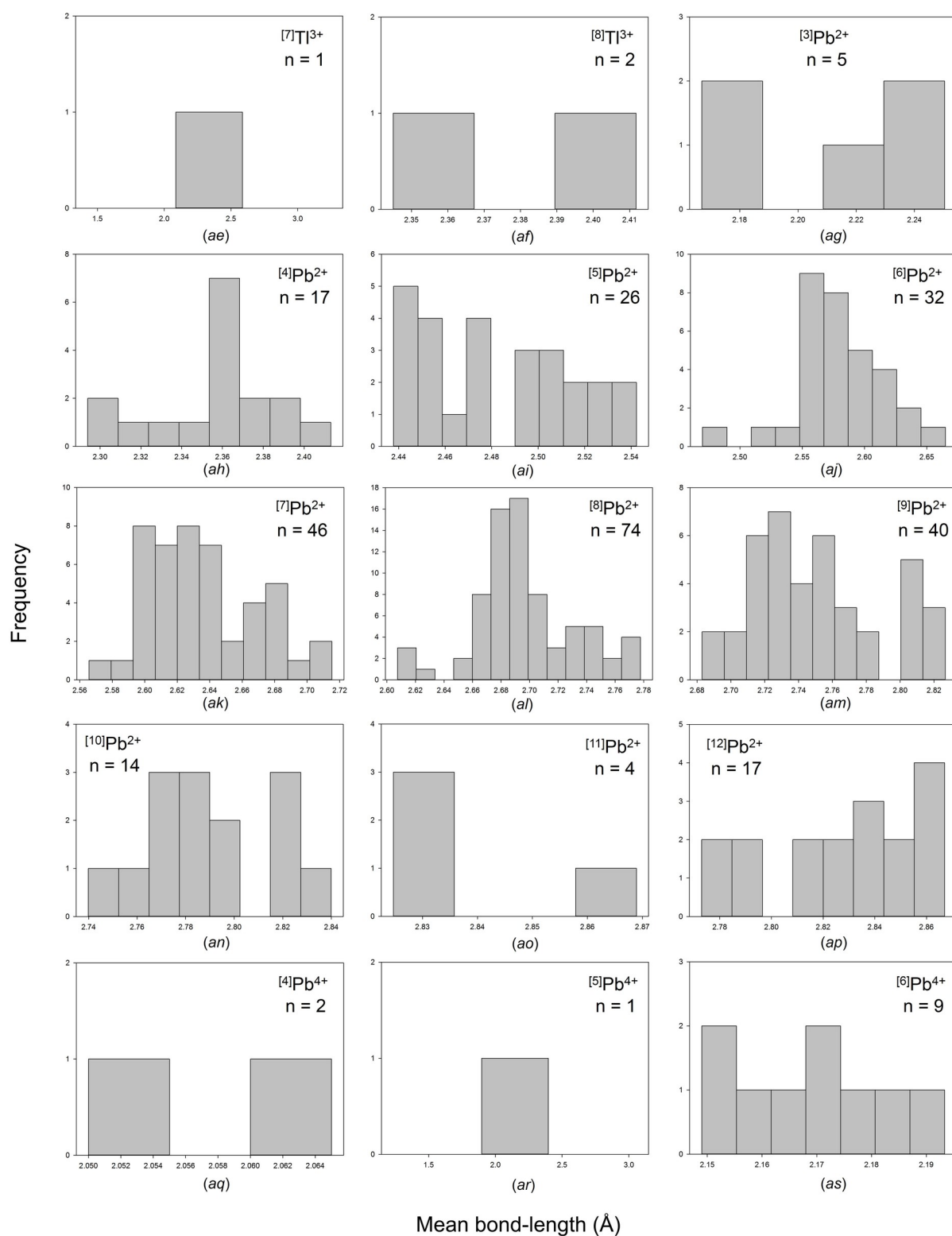


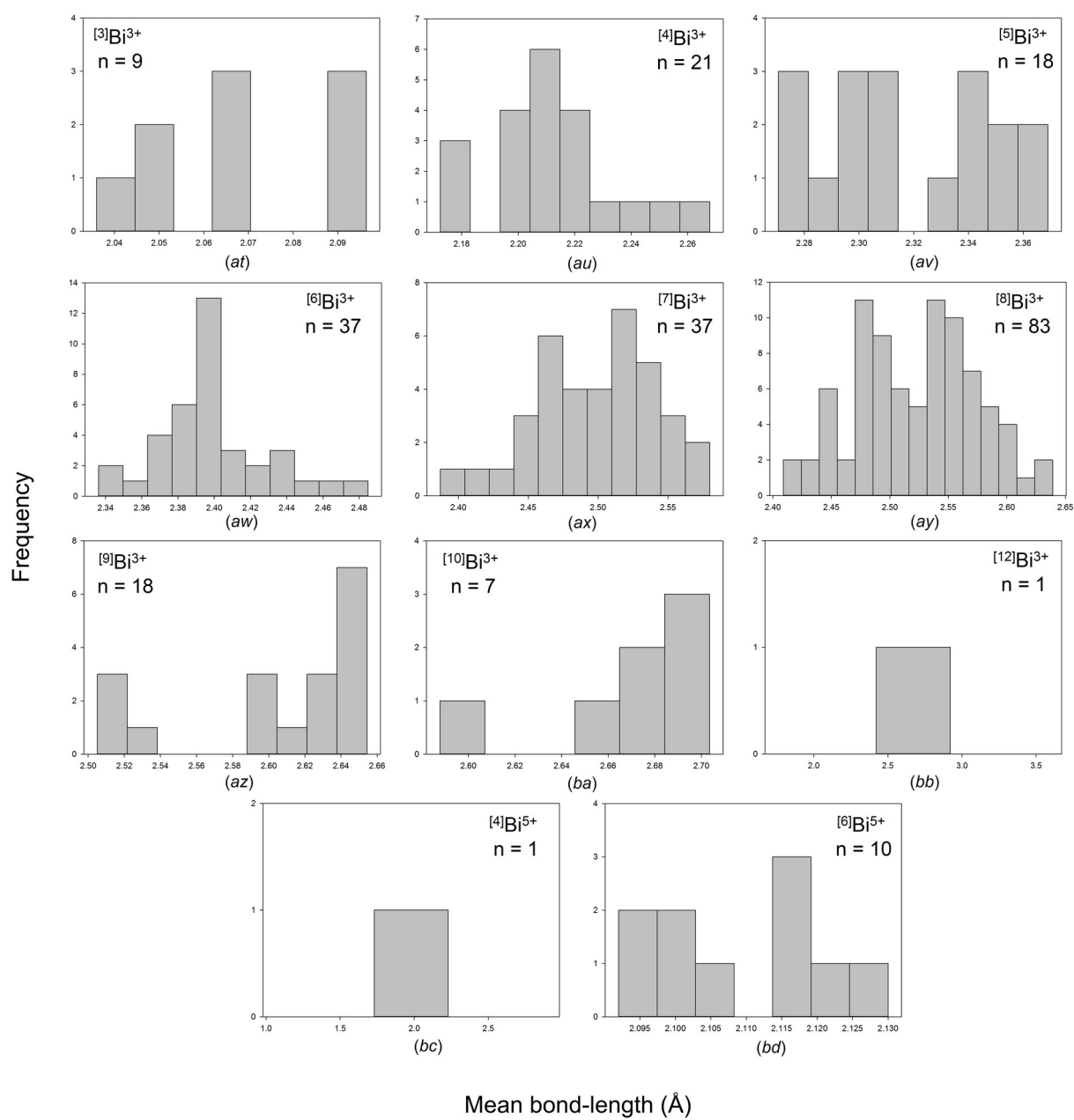


**Figure S6** Mean-bond-length distributions for all configurations of the post-transition-metal ions bonded to O<sup>2-</sup>: (a) <sup>[4]</sup>Al<sup>3+</sup>, (b) <sup>[5]</sup>Al<sup>3+</sup>, (c) <sup>[6]</sup>Al<sup>3+</sup>, (d) <sup>[4]</sup>Ga<sup>3+</sup>, (e) <sup>[5]</sup>Ga<sup>3+</sup>, (f) <sup>[6]</sup>Ga<sup>3+</sup>, (g) <sup>[6]</sup>In<sup>3+</sup>, (h) <sup>[7]</sup>In<sup>3+</sup>, (i) <sup>[8]</sup>In<sup>3+</sup>, (j) <sup>[3]</sup>Sn<sup>2+</sup>, (k) <sup>[4]</sup>Sn<sup>2+</sup>, (l) <sup>[5]</sup>Sn<sup>2+</sup>, (m) <sup>[6]</sup>Sn<sup>2+</sup>, (n) <sup>[7]</sup>Sn<sup>2+</sup>, (o) <sup>[8]</sup>Sn<sup>2+</sup>, (p) <sup>[9]</sup>Sn<sup>2+</sup>, (q) <sup>[4]</sup>Sn<sup>4+</sup>, (r) <sup>[6]</sup>Sn<sup>4+</sup>, (s) <sup>[7]</sup>Sn<sup>4+</sup>, (t) <sup>[3]</sup>Tl<sup>+</sup>, (u) <sup>[4]</sup>Tl<sup>+</sup>, (v) <sup>[5]</sup>Tl<sup>+</sup>, (w) <sup>[6]</sup>Tl<sup>+</sup>, (x) <sup>[7]</sup>Tl<sup>+</sup>, (y) <sup>[8]</sup>Tl<sup>+</sup>, (z) <sup>[9]</sup>Tl<sup>+</sup>, (aa) <sup>[10]</sup>Tl<sup>+</sup>, (ab) <sup>[11]</sup>Tl<sup>+</sup>, (ac) <sup>[12]</sup>Tl<sup>+</sup>, (ad) <sup>[6]</sup>Tl<sup>3+</sup>, (ae) <sup>[7]</sup>Tl<sup>3+</sup>, (af) <sup>[8]</sup>Tl<sup>3+</sup>, (ag) <sup>[3]</sup>Pb<sup>2+</sup>, (ah) <sup>[4]</sup>Pb<sup>2+</sup>, (ai) <sup>[5]</sup>Pb<sup>2+</sup>, (aj) <sup>[6]</sup>Pb<sup>2+</sup>, (ak) <sup>[7]</sup>Pb<sup>2+</sup>, (al) <sup>[8]</sup>Pb<sup>2+</sup>, (am) <sup>[9]</sup>Pb<sup>2+</sup>, (an) <sup>[10]</sup>Pb<sup>2+</sup>, (ao) <sup>[11]</sup>Pb<sup>2+</sup>, (ap) <sup>[12]</sup>Pb<sup>2+</sup>, (aq) <sup>[4]</sup>Pb<sup>4+</sup>, (ar) <sup>[5]</sup>Pb<sup>4+</sup>, (as) <sup>[6]</sup>Pb<sup>4+</sup>, (at) <sup>[3]</sup>Bi<sup>3+</sup>, (au) <sup>[4]</sup>Bi<sup>3+</sup>, (av) <sup>[5]</sup>Bi<sup>3+</sup>, (aw) <sup>[6]</sup>Bi<sup>3+</sup>, (ax) <sup>[7]</sup>Bi<sup>3+</sup>, (ay) <sup>[8]</sup>Bi<sup>3+</sup>, (az) <sup>[9]</sup>Bi<sup>3+</sup>, (ba) <sup>[10]</sup>Bi<sup>3+</sup>, (bb) <sup>[12]</sup>Bi<sup>3+</sup>, (bc) <sup>[4]</sup>Bi<sup>5+</sup>, (bd) <sup>[6]</sup>Bi<sup>5+</sup>.



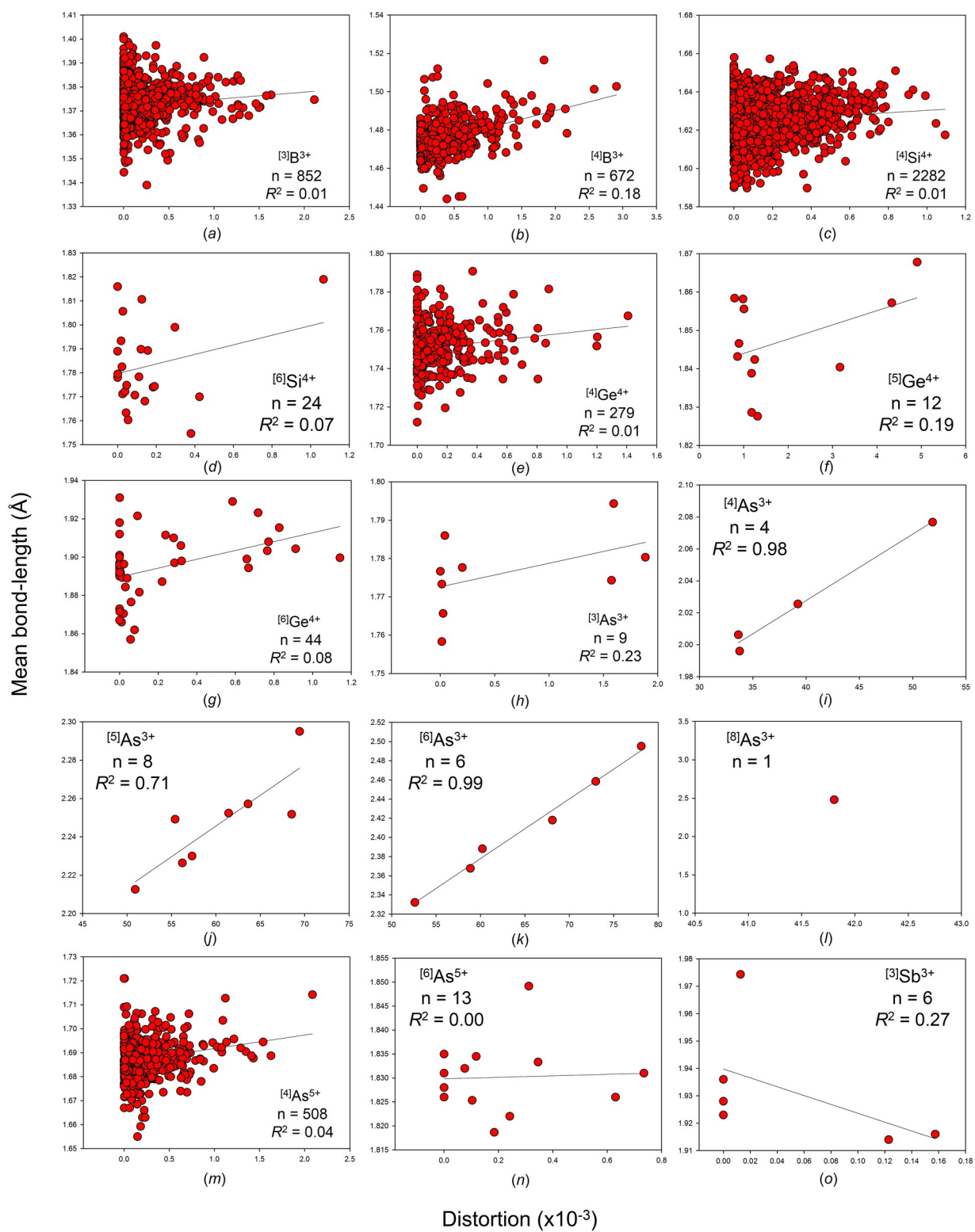


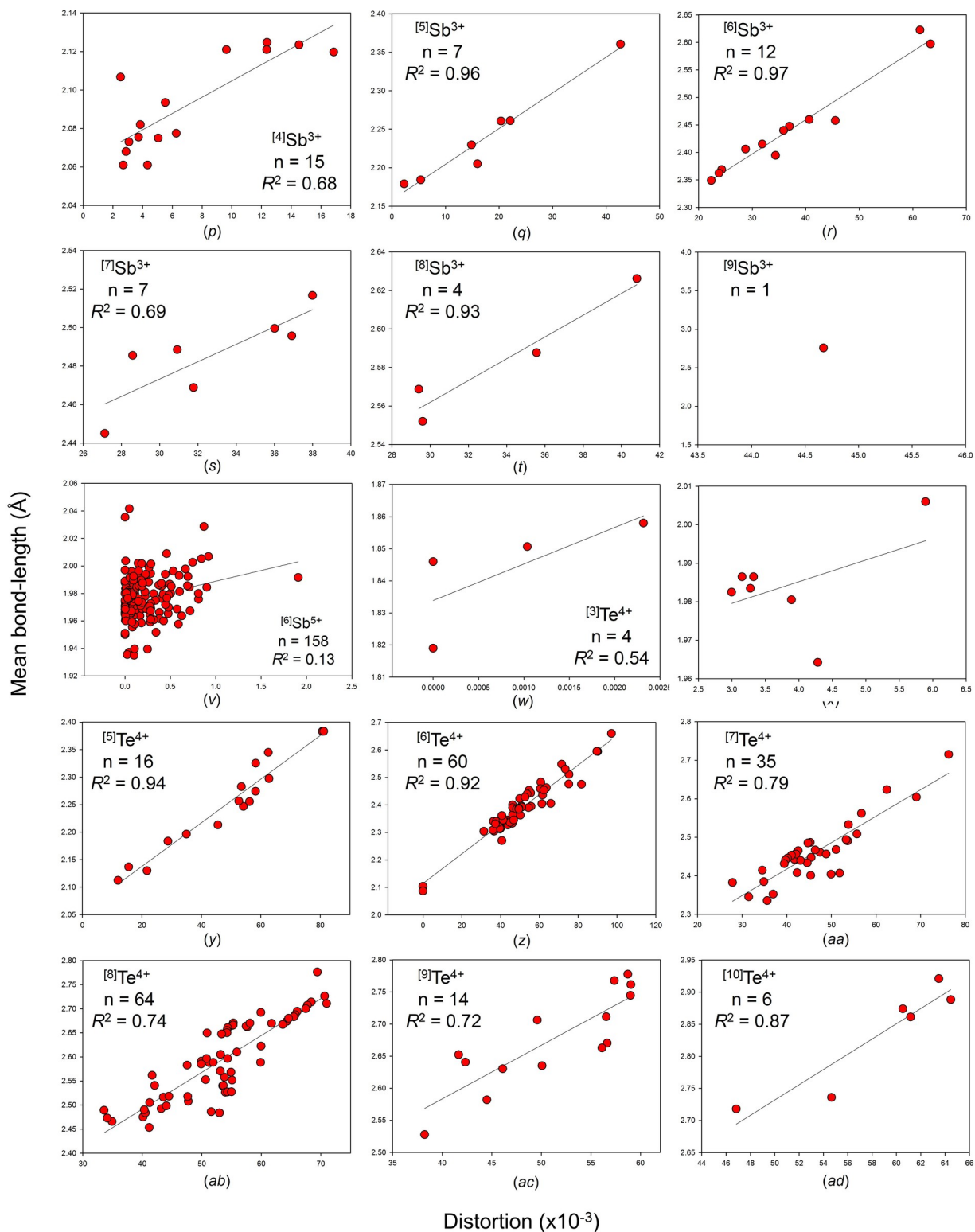


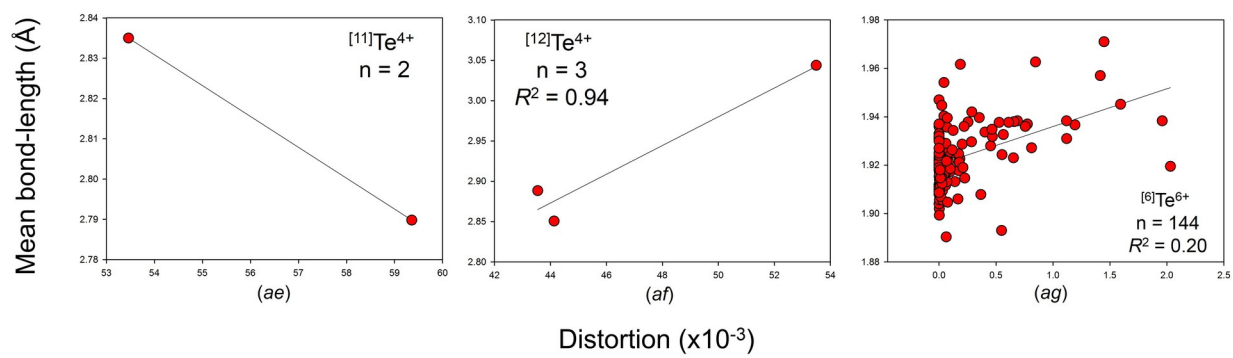




**Figure S7** The effect of bond-length distortion on mean bond-length for all configurations of the metalloid ions bonded to  $O^{2-}$ : (a)  $^{[3]}B^{3+}$ , (b)  $^{[4]}B^{3+}$ , (c)  $^{[4]}Si^{4+}$ , (d)  $^{[6]}Si^{4+}$ , (e)  $^{[4]}Ge^{4+}$ , (f)  $^{[5]}Ge^{4+}$ , (g)  $^{[6]}Ge^{4+}$ , (h)  $^{[3]}As^{3+}$ , (i)  $^{[4]}As^{3+}$ , (j)  $^{[5]}As^{3+}$ , (k)  $^{[6]}As^{3+}$ , (l)  $^{[8]}As^{3+}$ , (m)  $^{[4]}As^{5+}$ , (n)  $^{[6]}As^{5+}$ , (o)  $^{[3]}Sb^{3+}$ , (p)  $^{[4]}Sb^{3+}$ , (q)  $^{[5]}Sb^{3+}$ , (r)  $^{[6]}Sb^{3+}$ , (s)  $^{[7]}Sb^{3+}$ , (t)  $^{[8]}Sb^{3+}$ , (u)  $^{[9]}Sb^{3+}$ , (v)  $^{[6]}Sb^{5+}$ , (w)  $^{[3]}Te^{4+}$ , (x)  $^{[4]}Te^{4+}$ , (y)  $^{[5]}Te^{4+}$ , (z)  $^{[6]}Te^{4+}$ , (aa)  $^{[7]}Te^{4+}$ , (ab)  $^{[8]}Te^{4+}$ , (ac)  $^{[9]}Te^{4+}$ , (ad)  $^{[10]}Te^{4+}$ , (ae)  $^{[11]}Te^{4+}$ , (af)  $^{[12]}Te^{4+}$ , (ag)  $^{[6]}Te^{6+}$ .







**Figure S8** The effect of bond-length distortion on mean bond-length for all configurations of the post-transition-metal ions bonded to  $O^{2-}$ : (a)  $^{[4]}Al^{3+}$ , (b)  $^{[5]}Al^{3+}$ , (c)  $^{[6]}Al^{3+}$ , (d)  $^{[4]}Ga^{3+}$ , (e)  $^{[5]}Ga^{3+}$ , (f)  $^{[6]}Ga^{3+}$ , (g)  $^{[6]}In^{3+}$ , (h)  $^{[7]}In^{3+}$ , (i)  $^{[8]}In^{3+}$ , (j)  $^{[3]}Sn^{2+}$ , (k)  $^{[4]}Sn^{2+}$ , (l)  $^{[5]}Sn^{2+}$ , (m)  $^{[6]}Sn^{2+}$ , (n)  $^{[7]}Sn^{2+}$ , (o)  $^{[8]}Sn^{2+}$ , (p)  $^{[9]}Sn^{2+}$ , (q)  $^{[4]}Sn^{4+}$ , (r)  $^{[6]}Sn^{4+}$ , (s)  $^{[7]}Sn^{4+}$ , (t)  $^{[3]}Tl^{+}$ , (u)  $^{[4]}Tl^{+}$ , (v)  $^{[5]}Tl^{+}$ , (w)  $^{[6]}Tl^{+}$ , (x)  $^{[7]}Tl^{+}$ , (y)  $^{[8]}Tl^{+}$ , (z)  $^{[9]}Tl^{+}$ , (aa)  $^{[10]}Tl^{+}$ , (ab)  $^{[11]}Tl^{+}$ , (ac)  $^{[12]}Tl^{+}$ , (ad)  $^{[6]}Tl^{3+}$ , (ae)  $^{[7]}Tl^{3+}$ , (af)  $^{[8]}Tl^{3+}$ , (ag)  $^{[3]}Pb^{2+}$ , (ah)  $^{[4]}Pb^{2+}$ , (ai)  $^{[5]}Pb^{2+}$ , (aj)  $^{[6]}Pb^{2+}$ , (ak)  $^{[7]}Pb^{2+}$ , (al)  $^{[8]}Pb^{2+}$ , (am)  $^{[9]}Pb^{2+}$ , (an)  $^{[10]}Pb^{2+}$ , (ao)  $^{[11]}Pb^{2+}$ , (ap)  $^{[12]}Pb^{2+}$ , (aq)  $^{[4]}Pb^{4+}$ , (ar)  $^{[5]}Pb^{4+}$ , (as)  $^{[6]}Pb^{4+}$ , (at)  $^{[3]}Bi^{3+}$ , (au)  $^{[4]}Bi^{3+}$ , (av)  $^{[5]}Bi^{3+}$ , (aw)  $^{[6]}Bi^{3+}$ , (ax)  $^{[7]}Bi^{3+}$ , (ay)  $^{[8]}Bi^{3+}$ , (az)  $^{[9]}Bi^{3+}$ , (ba)  $^{[10]}Bi^{3+}$ , (bb)  $^{[12]}Bi^{3+}$ , (bc)  $^{[4]}Bi^{5+}$ , (bd)  $^{[6]}Bi^{5+}$ .

