



STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

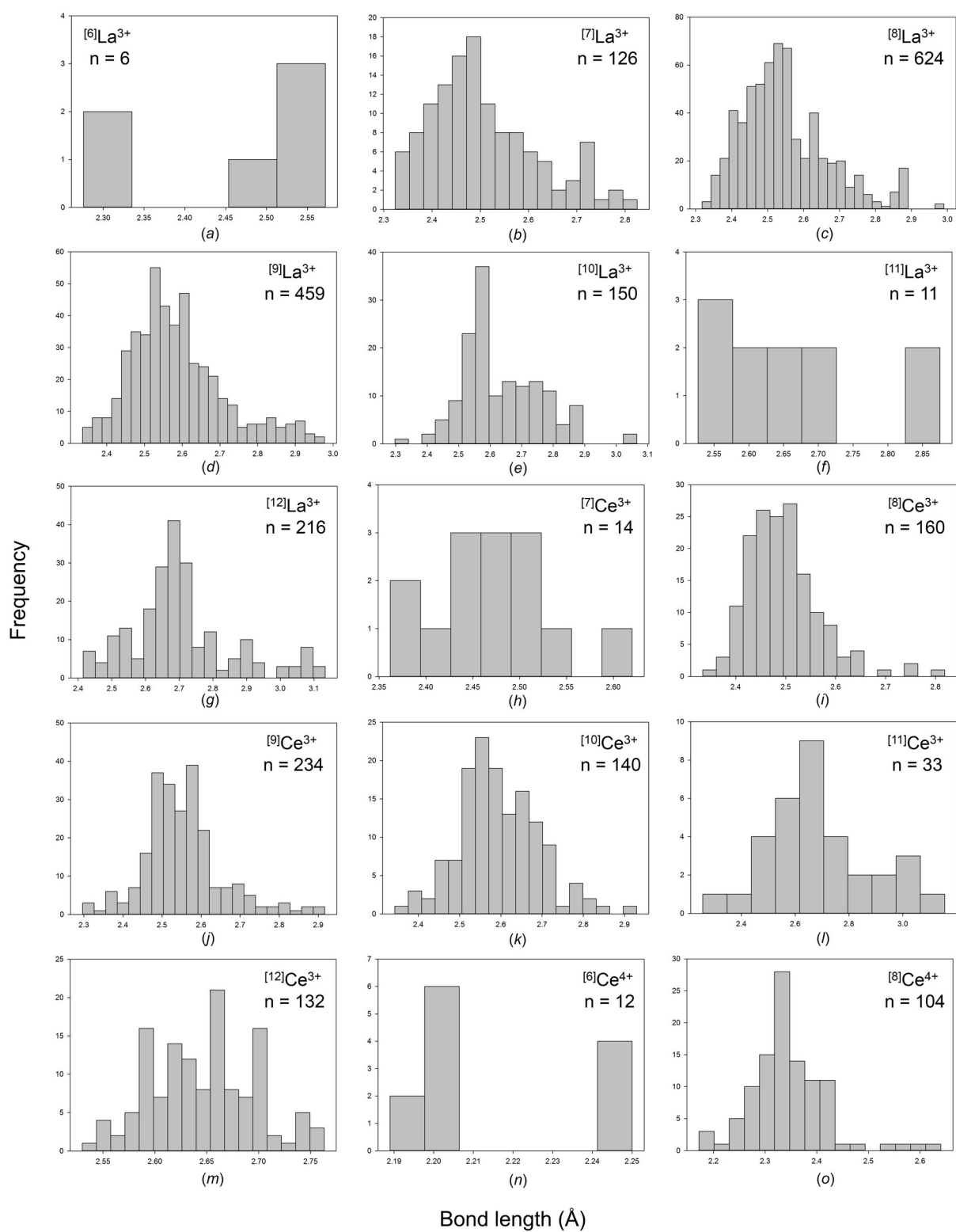
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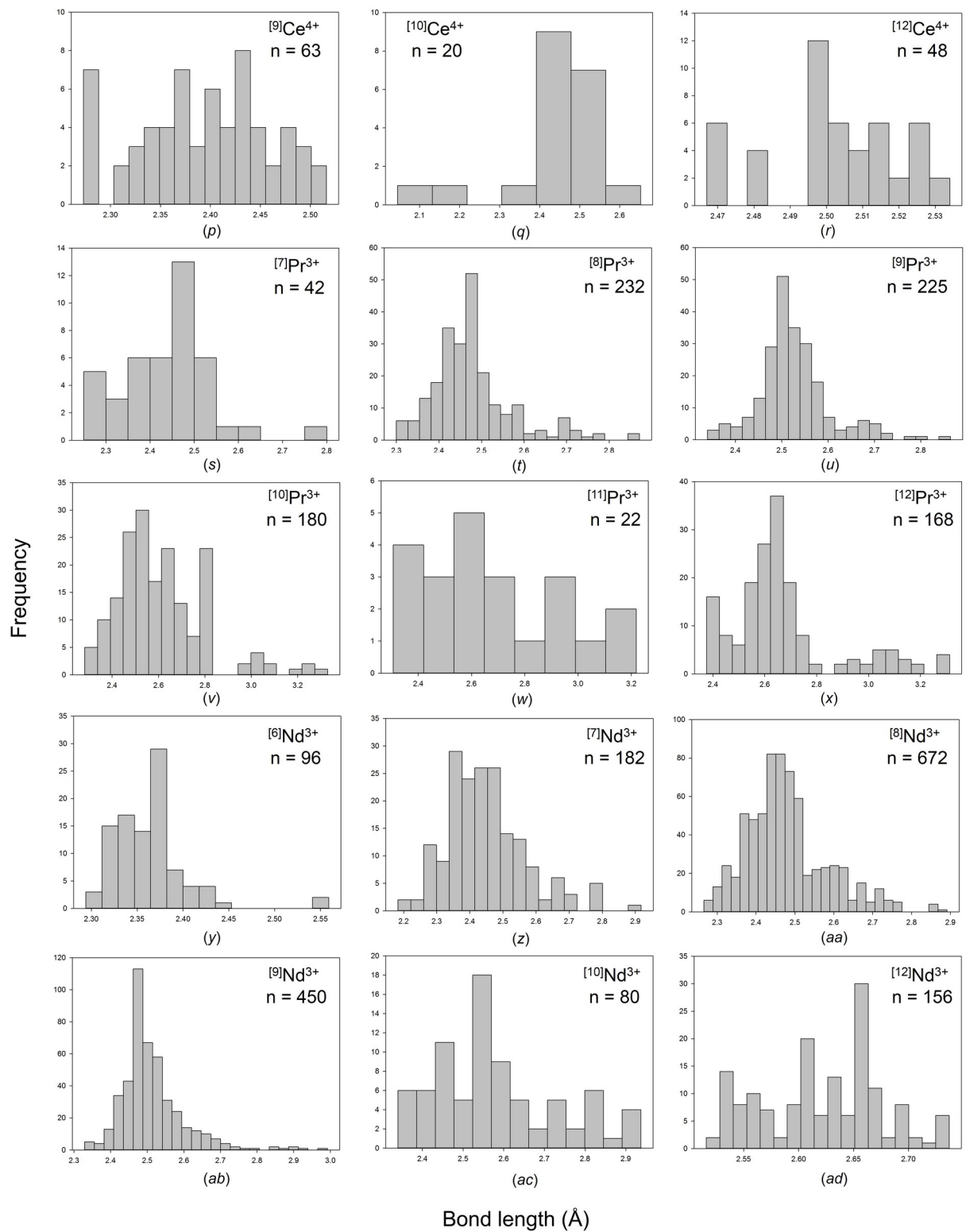
Supporting information for article:

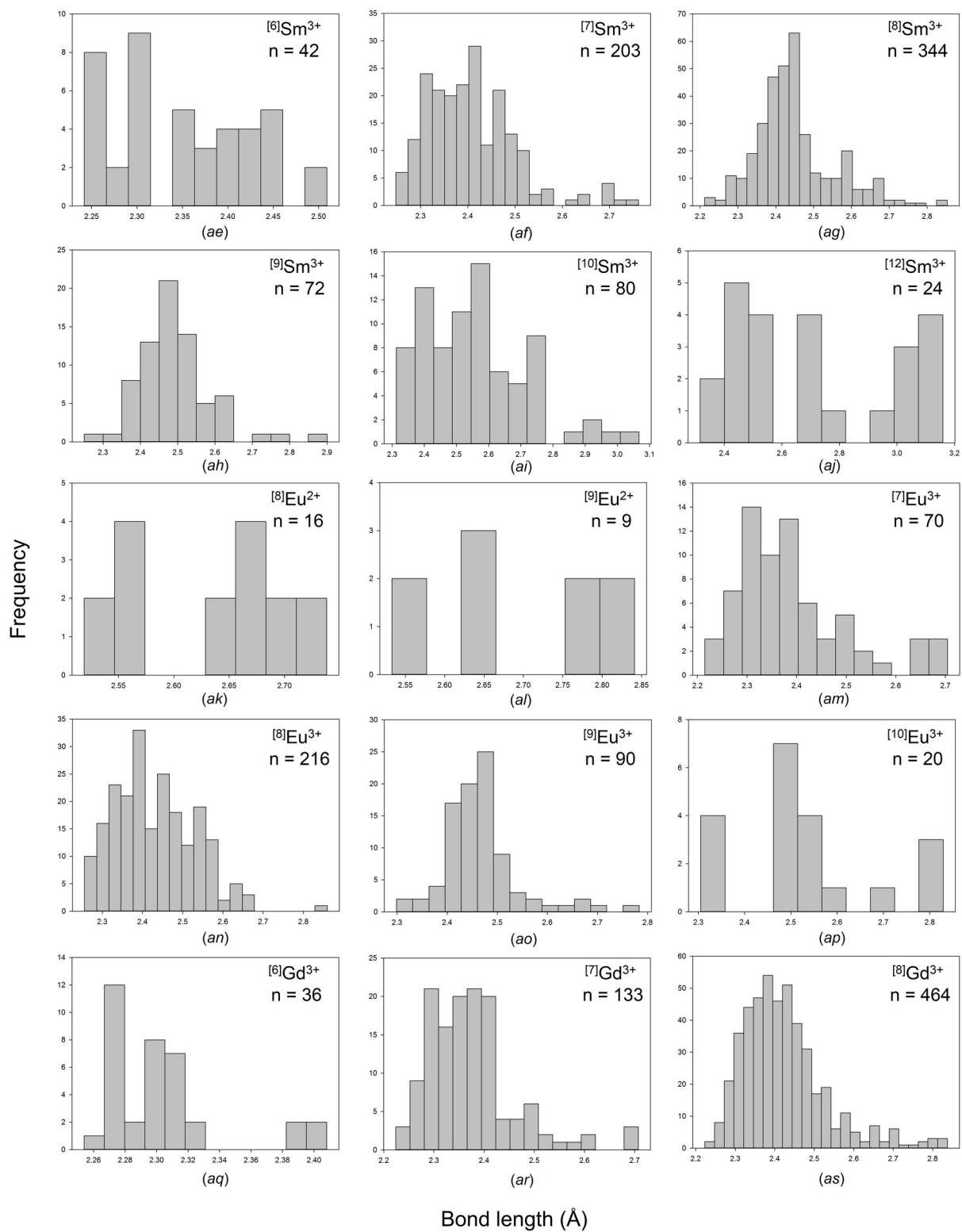
Bond-length distributions for ions bonded to oxygen: results for the lanthanides and actinides and discussion of the f-block contraction

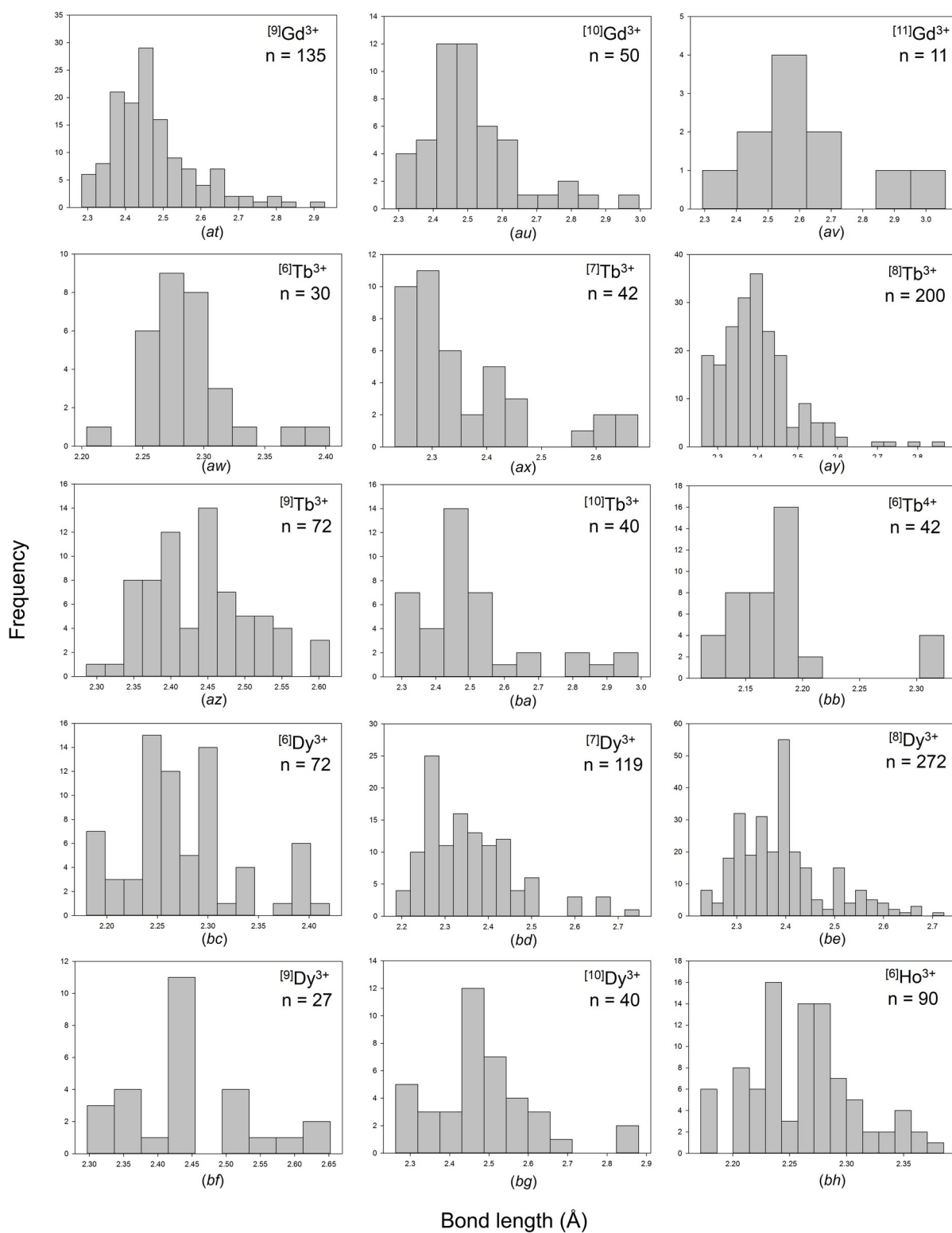
Olivier Charles Gagné

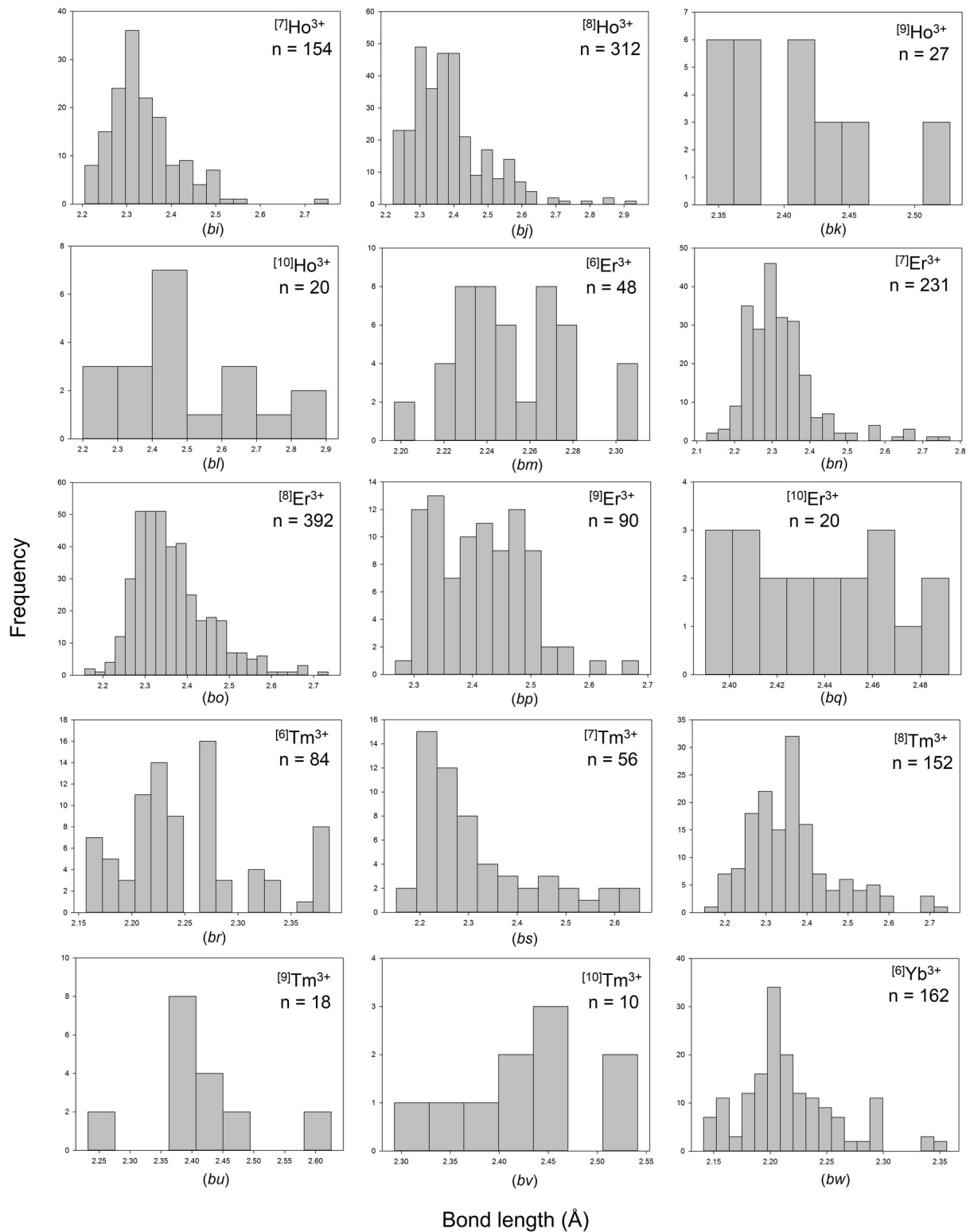
Figure S1 Bond-length distributions for all configurations of the lanthanide ions bonded to O²⁻: (a) ⁶La³⁺, (b) ⁷La³⁺, (c) ⁸La³⁺, (d) ⁹La³⁺, (e) ¹⁰La³⁺, (f) ¹¹La³⁺, (g) ¹²La³⁺, (h) ⁷Ce³⁺, (i) ⁸Ce³⁺, (j) ⁹Ce³⁺, (k) ¹⁰Ce³⁺, (l) ¹¹Ce³⁺, (m) ¹²Ce³⁺, (n) ⁶Ce⁴⁺, (o) ⁸Ce⁴⁺, (p) ⁹Ce⁴⁺, (q) ¹⁰Ce⁴⁺, (r) ¹²Ce⁴⁺, (s) ⁷Pr³⁺, (t) ⁸Pr³⁺, (u) ⁹Pr³⁺, (v) ¹⁰Pr³⁺, (w) ¹¹Pr³⁺, (x) ¹²Pr³⁺, (y) ⁶Nd³⁺, (z) ⁷Nd³⁺, (aa) ⁸Nd³⁺, (ab) ⁹Nd³⁺, (ac) ¹⁰Nd³⁺, (ad) ¹²Nd³⁺, (ae) ⁶Sm³⁺, (af) ⁷Sm³⁺, (ag) ⁸Sm³⁺, (ah) ⁹Sm³⁺, (ai) ¹⁰Sm³⁺, (aj) ¹²Sm³⁺, (ak) ⁸Eu²⁺, (al) ⁹Eu²⁺, (am) ⁷Eu³⁺, (an) ⁸Eu³⁺, (ao) ⁹Eu³⁺, (ap) ¹⁰Eu³⁺, (aq) ⁶Gd³⁺, (ar) ⁷Gd³⁺, (as) ⁸Gd³⁺, (at) ⁹Gd³⁺, (au) ¹⁰Gd³⁺, (av) ¹¹Gd³⁺, (aw) ⁶Tb³⁺, (ax) ⁷Tb³⁺, (ay) ⁸Tb³⁺, (az) ⁹Tb³⁺, (ba) ¹⁰Tb³⁺, (bb) ⁶Tb⁴⁺, (bc) ⁶Dy³⁺, (bd) ⁷Dy³⁺, (be) ⁸Dy³⁺, (bf) ⁹Dy³⁺, (bg) ¹⁰Dy³⁺, (bh) ⁶Ho³⁺, (bi) ⁷Ho³⁺, (bj) ⁸Ho³⁺, (bk) ⁹Ho³⁺, (bl) ¹⁰Ho³⁺, (bm) ⁶Er³⁺, (bn) ⁷Er³⁺, (bo) ⁸Er³⁺, (bp) ⁹Er³⁺, (bq) ¹⁰Er³⁺, (br) ⁶Tm³⁺, (bs) ⁷Tm³⁺, (bt) ⁸Tm³⁺, (bu) ⁹Tm³⁺, (bv) ¹⁰Tm³⁺, (bw) ⁶Yb³⁺, (bx) ⁷Yb³⁺, (by) ⁸Yb³⁺, (bz) ⁹Yb³⁺, (ca) ¹⁰Yb³⁺, (cb) ⁶Lu³⁺, (cc) ⁷Lu³⁺, (cd) ⁸Lu³⁺, (ce) ⁹Lu³⁺, (cf) ¹⁰Lu³⁺.











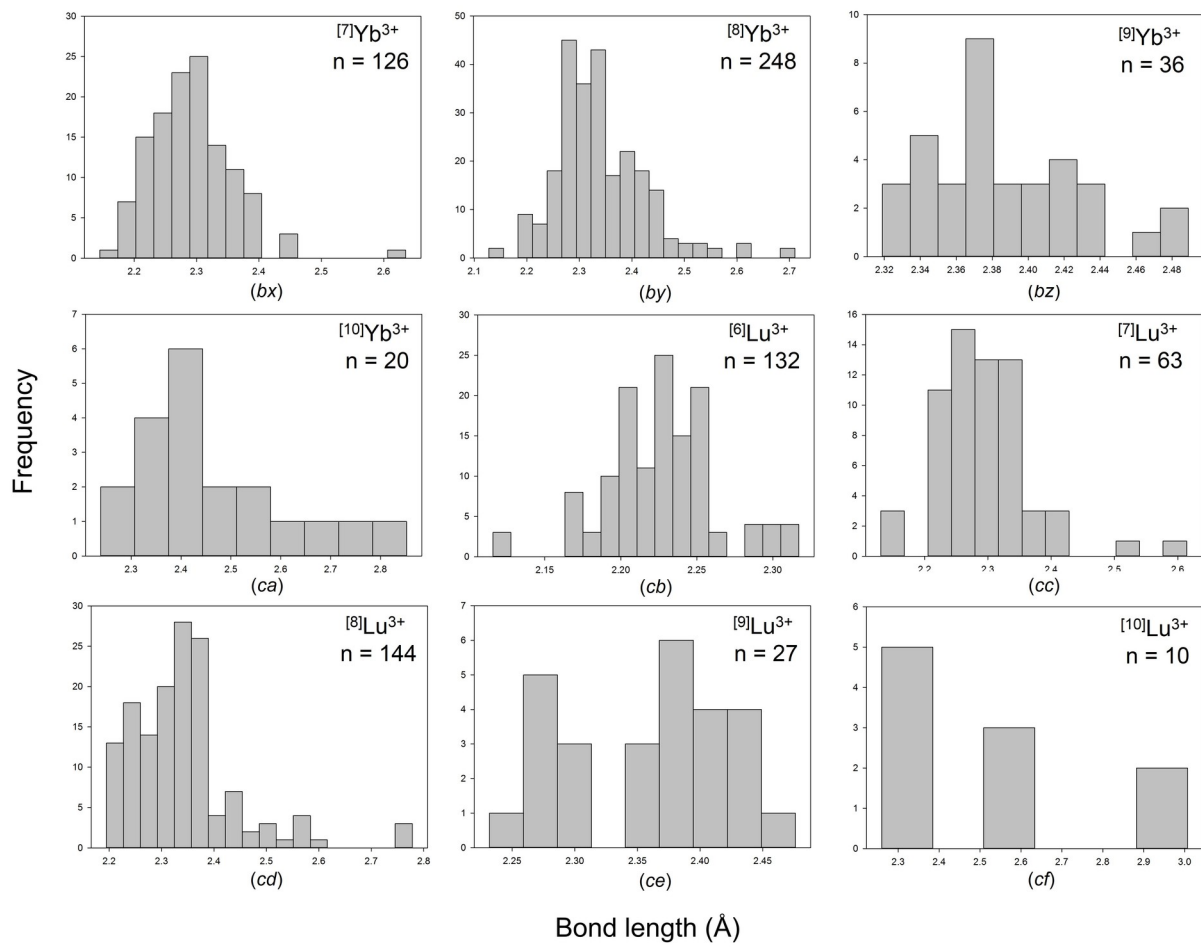
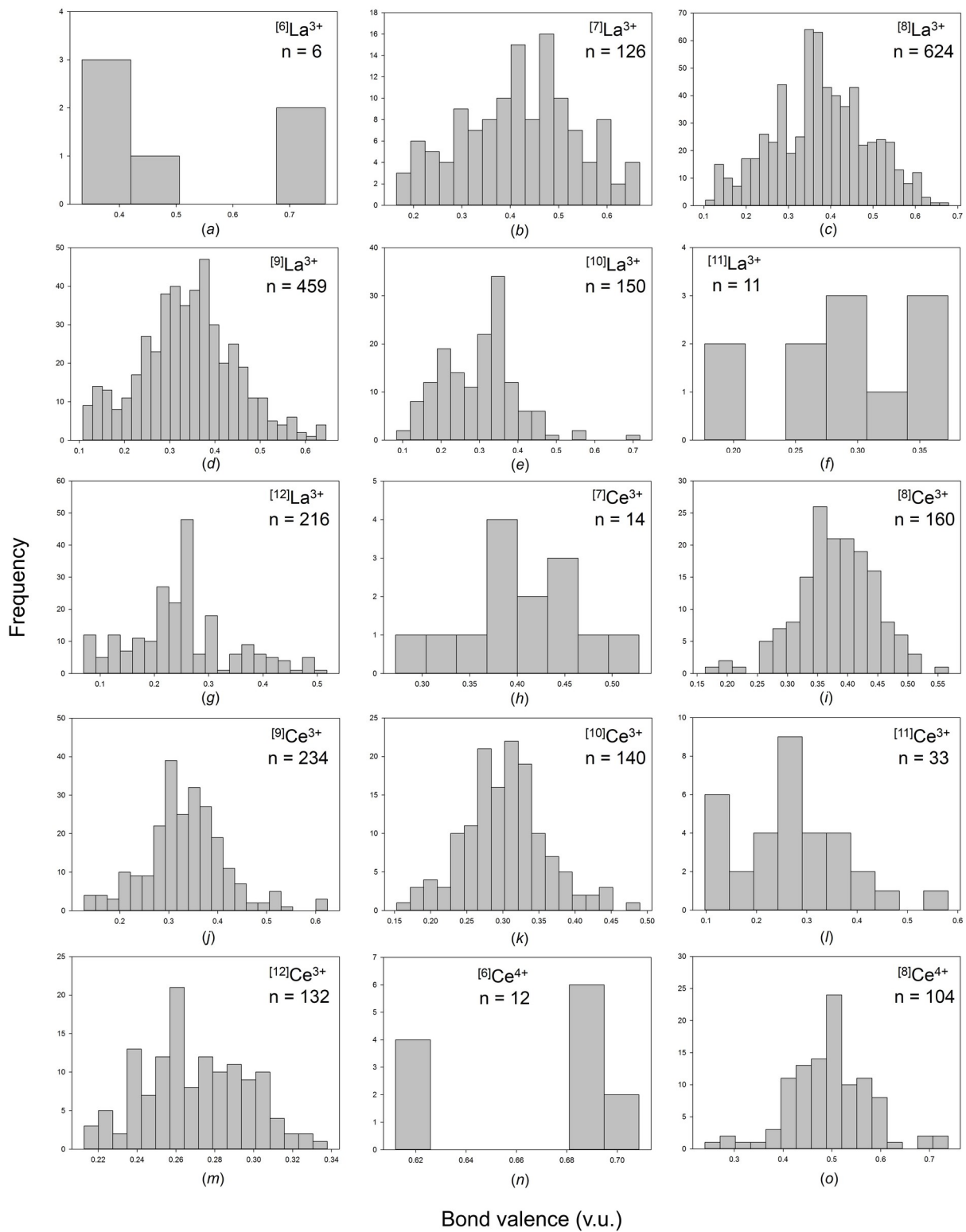
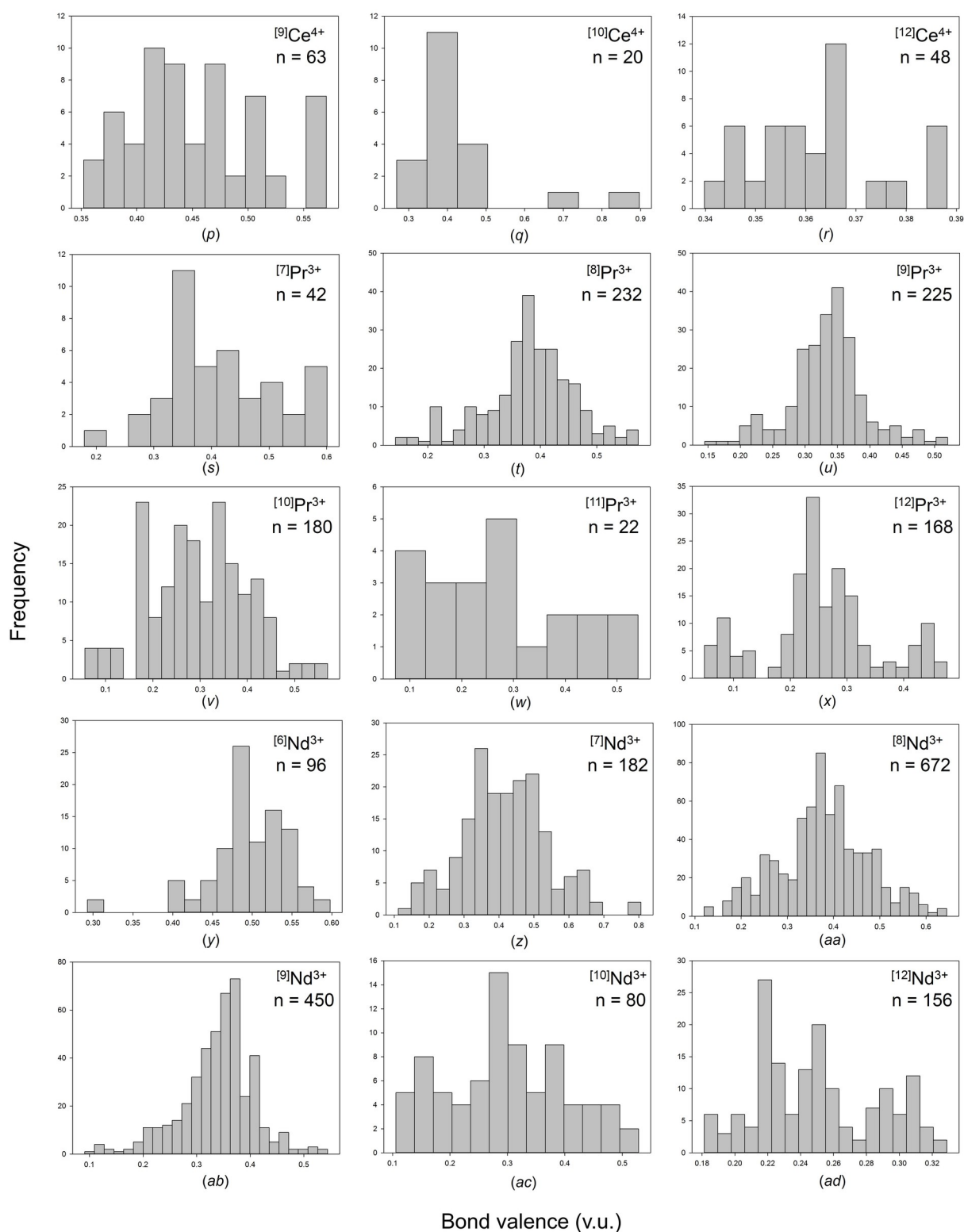
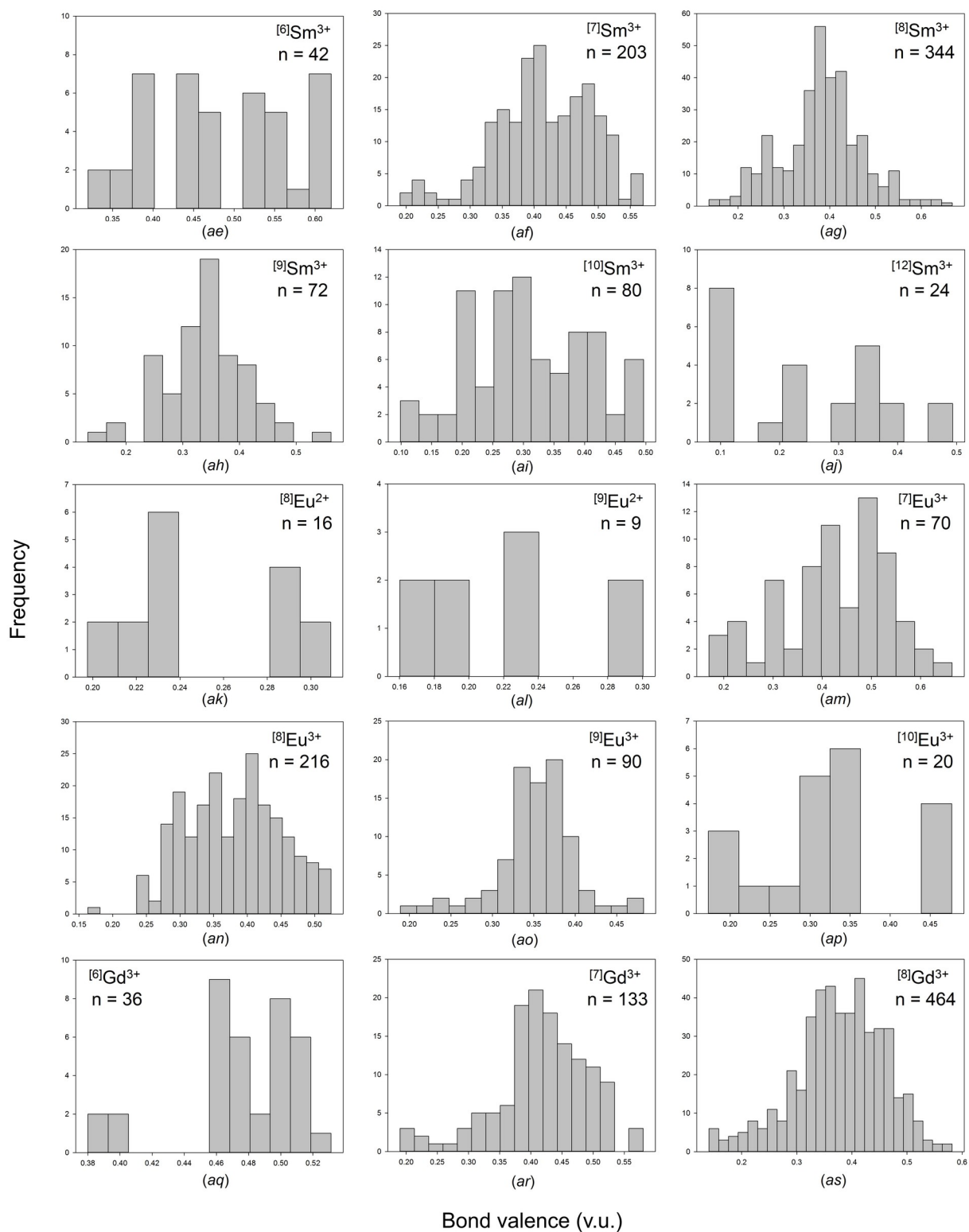


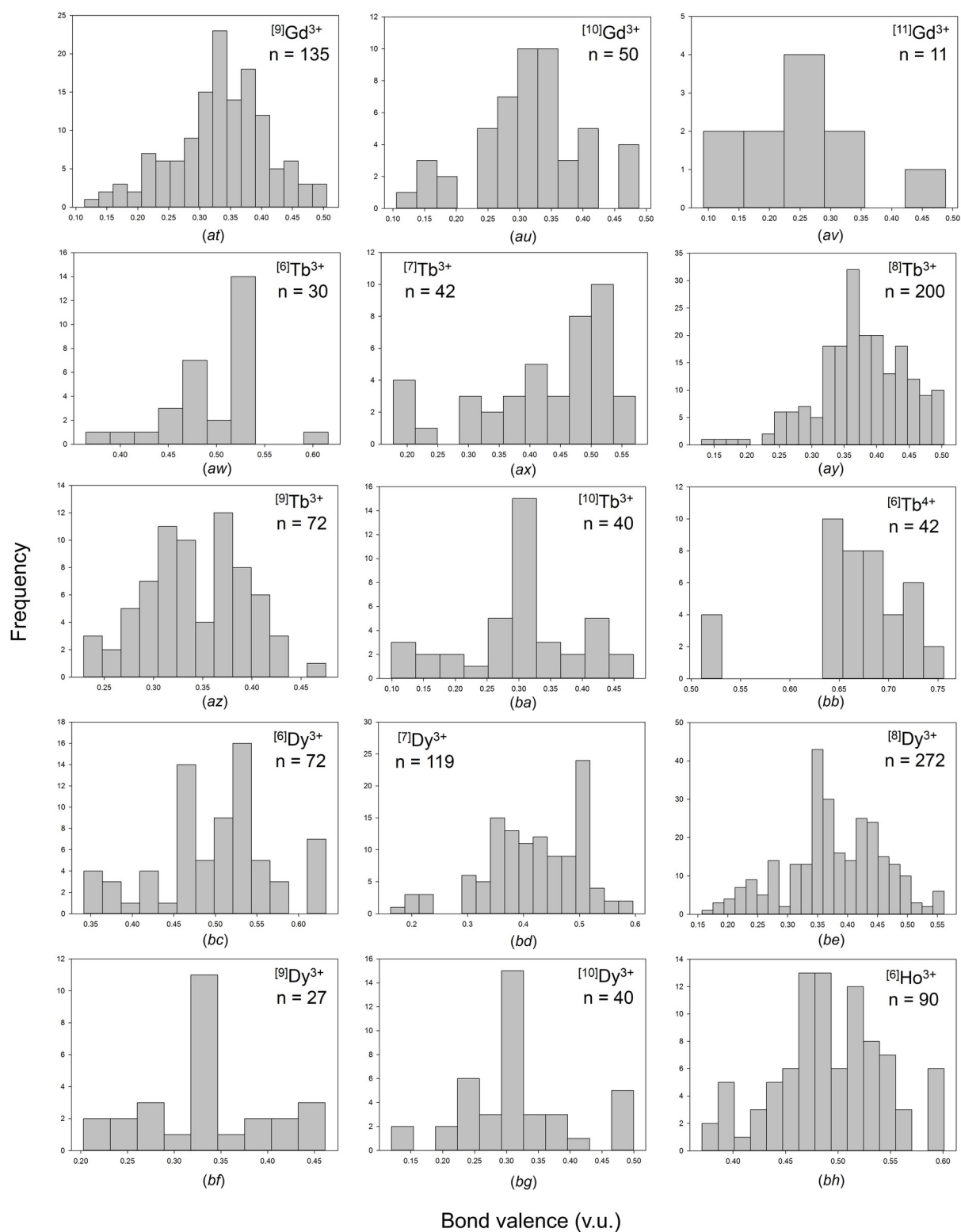
Figure S2 Bond-valence distributions for all configurations of the lanthanide ions bonded to O²⁻: (a)

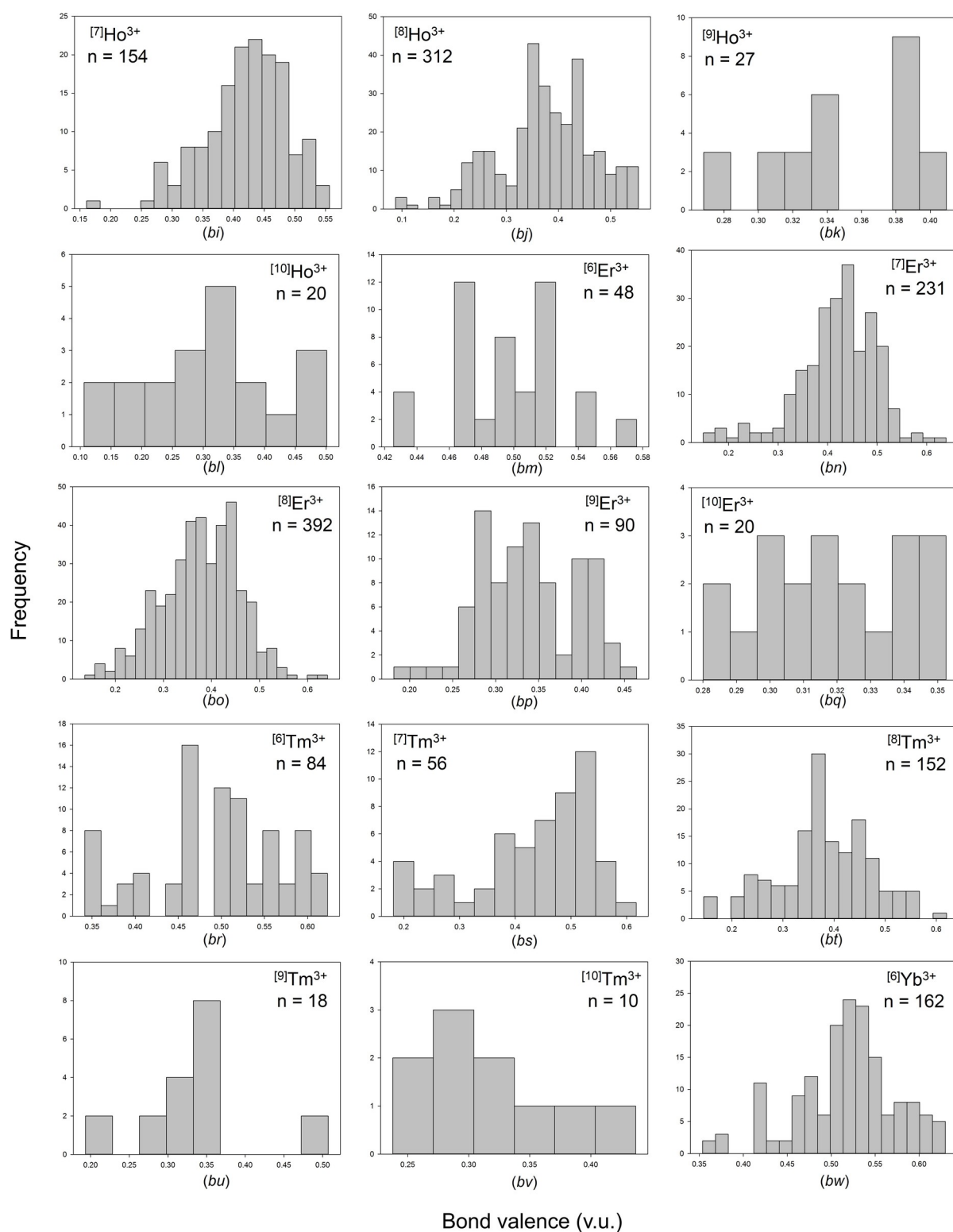
[⁶]La³⁺, (b) [⁷]La³⁺, (c) [⁸]La³⁺, (d) [⁹]La³⁺, (e) [¹⁰]La³⁺, (f) [¹¹]La³⁺, (g) [¹²]La³⁺, (h) [⁷]Ce³⁺, (i) [⁸]Ce³⁺, (j) [⁹]Ce³⁺, (k) [¹⁰]Ce³⁺, (l) [¹¹]Ce³⁺, (m) [¹²]Ce³⁺, (n) [⁶]Ce⁴⁺, (o) [⁸]Ce⁴⁺, (p) [⁹]Ce⁴⁺, (q) [¹⁰]Ce⁴⁺, (r) [¹²]Ce⁴⁺, (s) [⁷]Pr³⁺, (t) [⁸]Pr³⁺, (u) [⁹]Pr³⁺, (v) [¹⁰]Pr³⁺, (w) [¹¹]Pr³⁺, (x) [¹²]Pr³⁺, (y) [⁶]Nd³⁺, (z) [⁷]Nd³⁺, (aa) [⁸]Nd³⁺, (ab) [⁹]Nd³⁺, (ac) [¹⁰]Nd³⁺, (ad) [¹²]Nd³⁺, (ae) [⁶]Sm³⁺, (af) [⁷]Sm³⁺, (ag) [⁸]Sm³⁺, (ah) [⁹]Sm³⁺, (ai) [¹⁰]Sm³⁺, (aj) [¹²]Sm³⁺, (ak) [⁸]Eu²⁺, (al) [⁹]Eu²⁺, (am) [⁷]Eu³⁺, (an) [⁸]Eu³⁺, (ao) [⁹]Eu³⁺, (ap) [¹⁰]Eu³⁺, (aq) [⁶]Gd³⁺, (ar) [⁷]Gd³⁺, (as) [⁸]Gd³⁺, (at) [⁹]Gd³⁺, (au) [¹⁰]Gd³⁺, (av) [¹¹]Gd³⁺, (aw) [⁶]Tb³⁺, (ax) [⁷]Tb³⁺, (ay) [⁸]Tb³⁺, (az) [⁹]Tb³⁺, (ba) [¹⁰]Tb³⁺, (bb) [⁶]Tb⁴⁺, (bc) [⁶]Dy³⁺, (bd) [⁷]Dy³⁺, (be) [⁸]Dy³⁺, (bf) [⁹]Dy³⁺, (bg) [¹⁰]Dy³⁺, (bh) [⁶]Ho³⁺, (bi) [⁷]Ho³⁺, (bj) [⁸]Ho³⁺, (bk) [⁹]Ho³⁺, (bl) [¹⁰]Ho³⁺, (bm) [⁶]Er³⁺, (bn) [⁷]Er³⁺, (bo) [⁸]Er³⁺, (bp) [⁹]Er³⁺, (bq) [¹⁰]Er³⁺, (br) [⁶]Tm³⁺, (bs) [⁷]Tm³⁺, (bt) [⁸]Tm³⁺, (bu) [⁹]Tm³⁺, (bv) [¹⁰]Tm³⁺, (bw) [⁶]Yb³⁺, (bx) [⁷]Yb³⁺, (by) [⁸]Yb³⁺, (bz) [⁹]Yb³⁺, (ca) [¹⁰]Yb³⁺, (cb) [⁶]Lu³⁺, (cc) [⁷]Lu³⁺, (cd) [⁸]Lu³⁺, (ce) [⁹]Lu³⁺, (cf) [¹⁰]Lu³⁺.











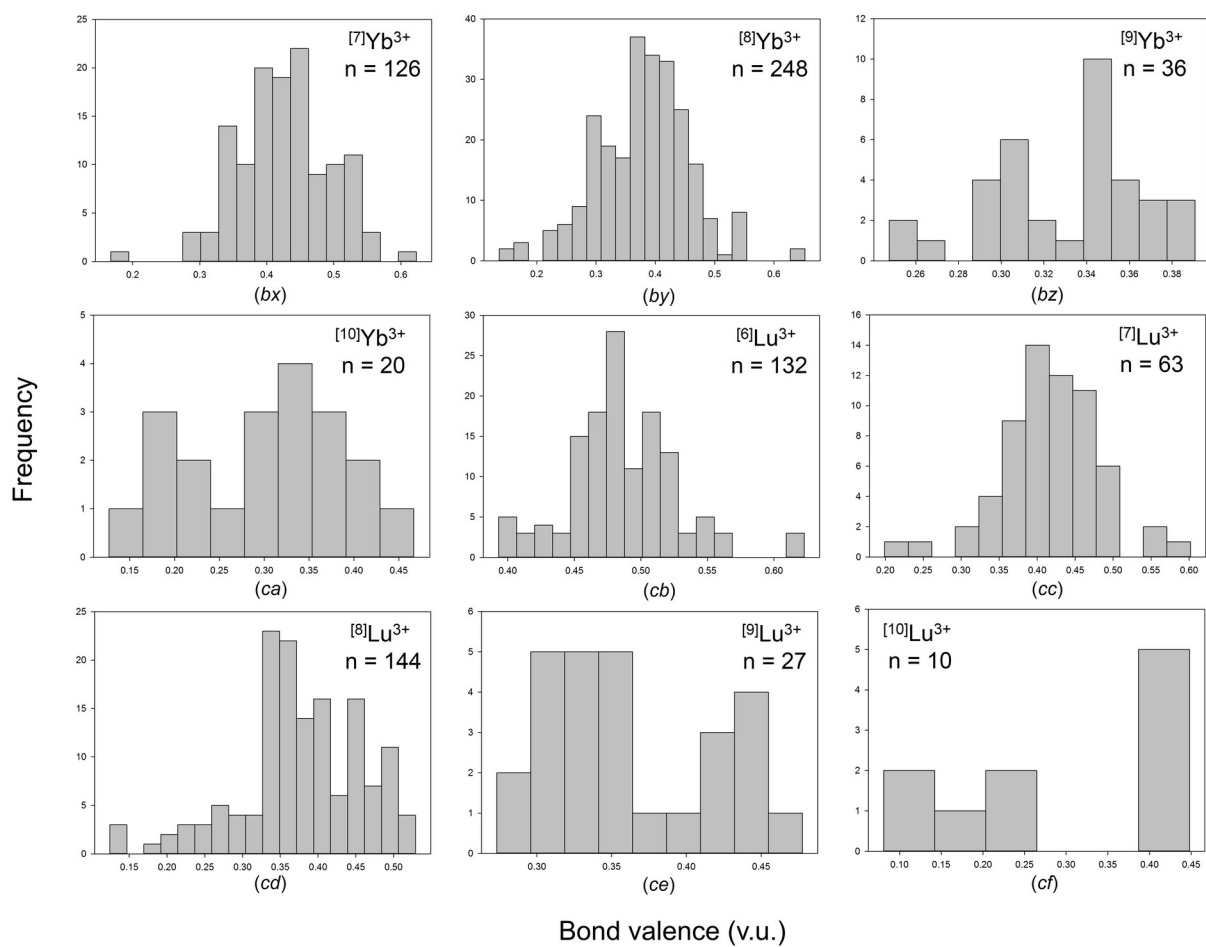
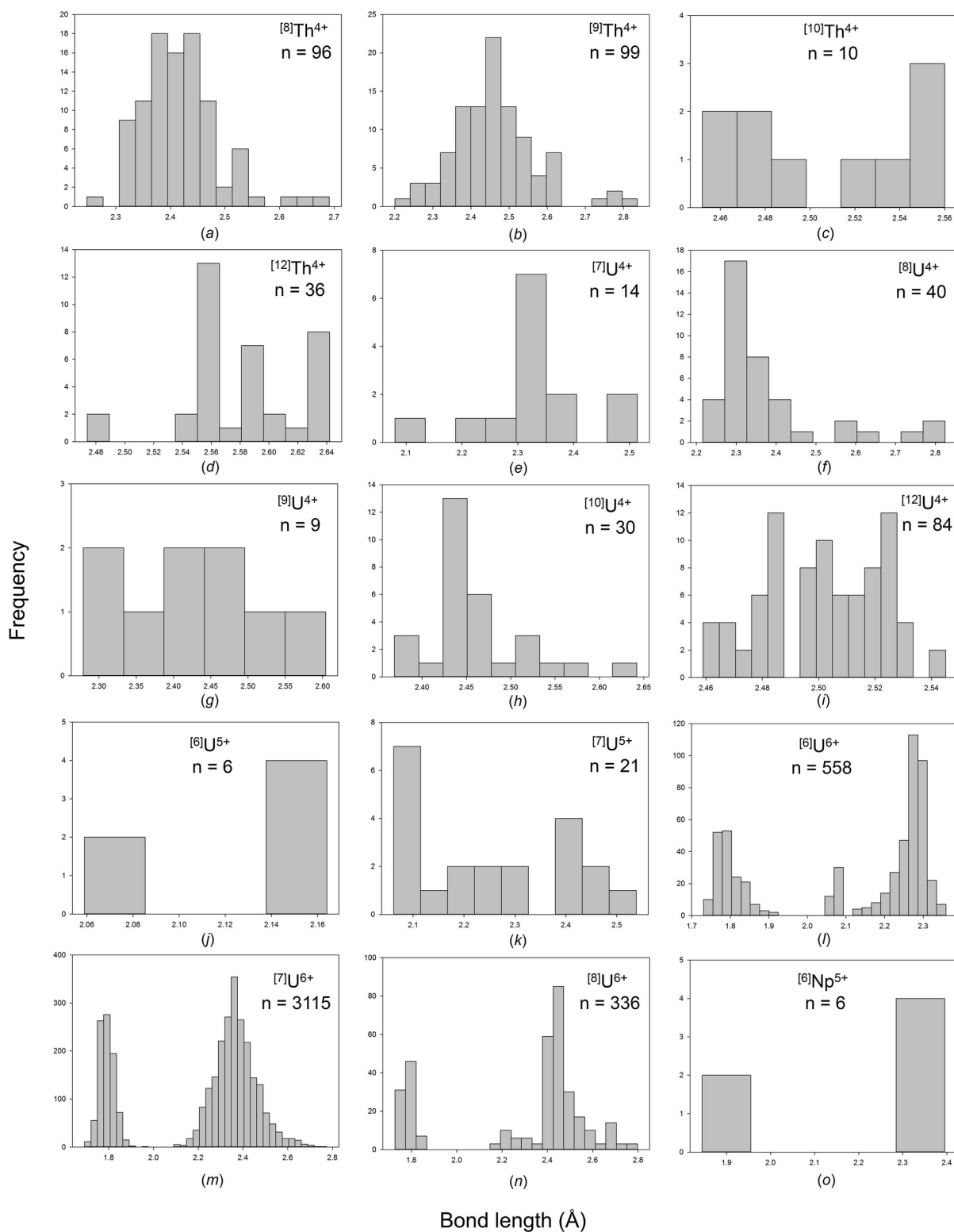


Figure S3 Bond-length distributions for all configurations of the actinide ions bonded to O^{2-} : (a) $^{[8]}Th^{4+}$, (b) $^{[9]}Th^{4+}$, (c) $^{[10]}Th^{4+}$, (d) $^{[12]}Th^{4+}$, (e) $^{[7]}U^{4+}$, (f) $^{[8]}U^{4+}$, (g) $^{[9]}U^{4+}$, (h) $^{[10]}U^{4+}$, (i) $^{[12]}U^{4+}$, (j) $^{[6]}U^{5+}$, (k) $^{[7]}U^{5+}$, (l) $^{[6]}U^{6+}$, (m) $^{[7]}U^{6+}$, (n) $^{[8]}U^{6+}$, (o) $^{[6]}Np^{5+}$, (p) $^{[7]}Np^{5+}$, (q) $^{[8]}Np^{5+}$, (r) $^{[7]}Np^{6+}$, (s) $^{[8]}Np^{6+}$, (t) $^{[6]}Np^{7+}$, (u) $^{[9]}Am^{3+}$, (v) $^{[9]}Cm^{3+}$.



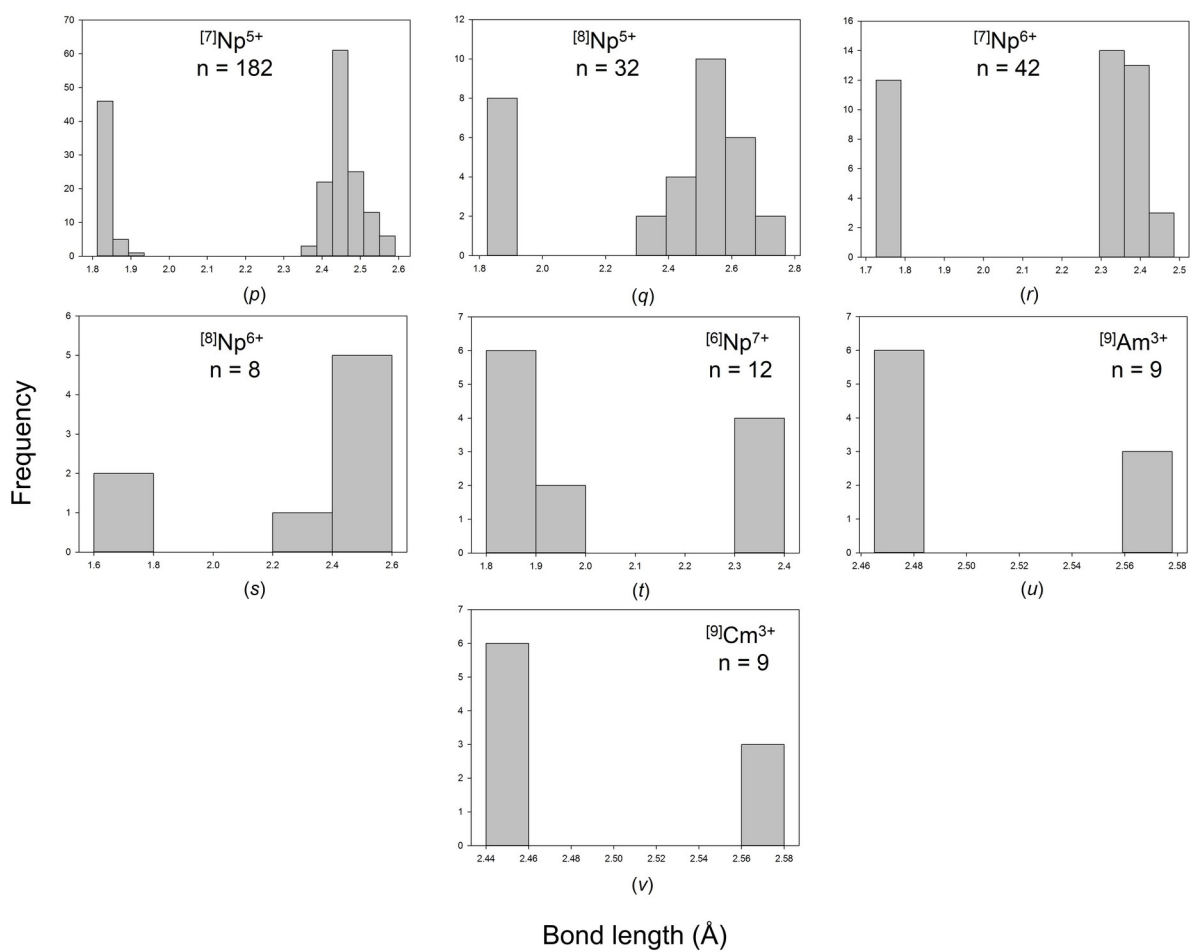
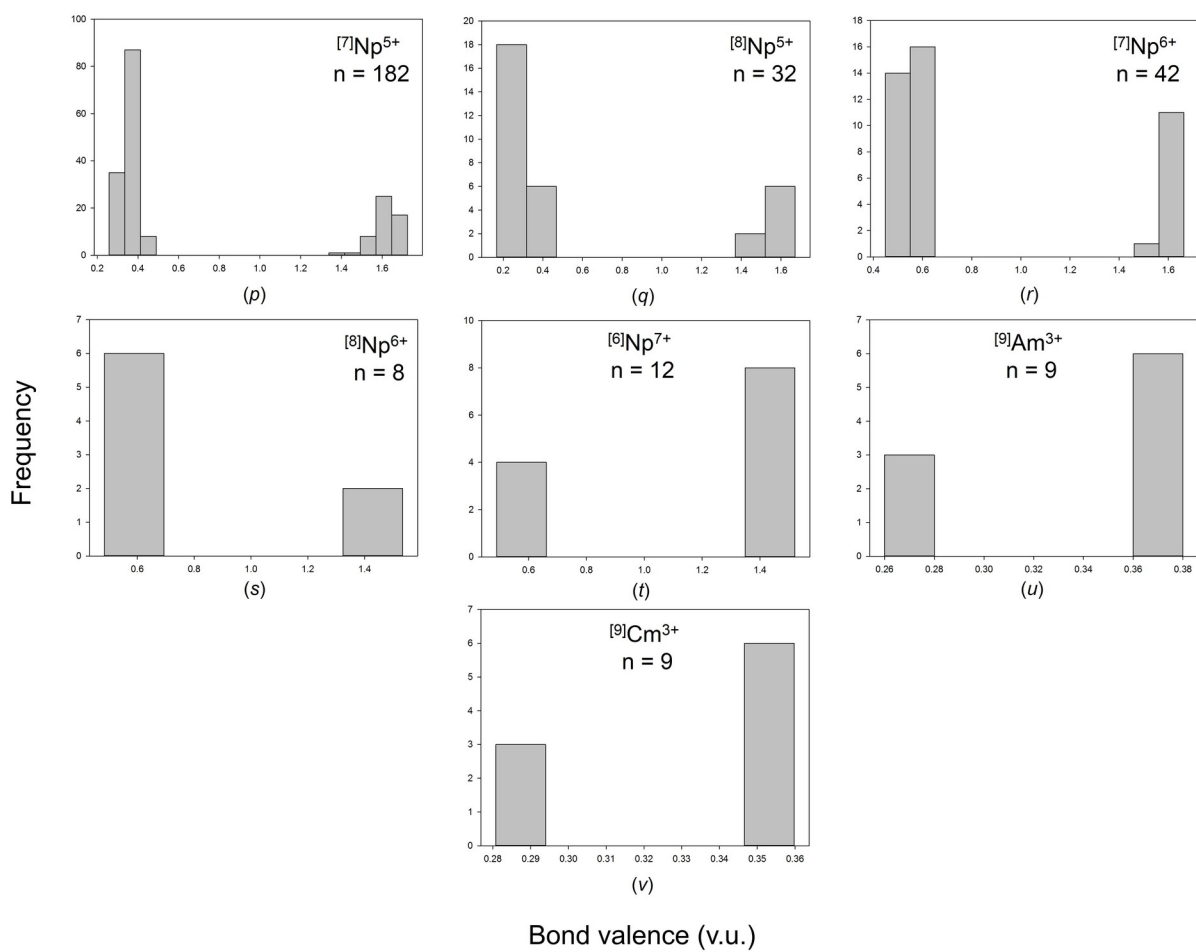
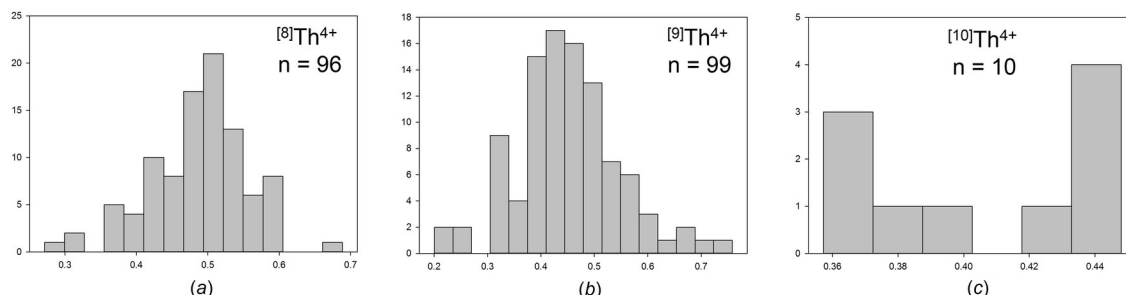


Figure S4 Bond-valence distributions for all configurations of the actinide ions bonded to O^{2-} : (a) $^{[8]}Th^{4+}$, (b) $^{[9]}Th^{4+}$, (c) $^{[10]}Th^{4+}$, (d) $^{[12]}Th^{4+}$, (e) $^{[7]}U^{4+}$, (f) $^{[8]}U^{4+}$, (g) $^{[9]}U^{4+}$, (h) $^{[10]}U^{4+}$, (i) $^{[12]}U^{4+}$, (j) $^{[6]}U^{5+}$, (k) $^{[7]}U^{5+}$, (l) $^{[6]}U^{6+}$, (m) $^{[7]}U^{6+}$, (n) $^{[8]}U^{6+}$, (o) $^{[6]}Np^{5+}$, (p) $^{[7]}Np^{5+}$, (q) $^{[8]}Np^{5+}$, (r) $^{[7]}Np^{6+}$, (s) $^{[8]}Np^{6+}$, (t) $^{[6]}Np^{7+}$, (u) $^{[9]}Am^{3+}$, (v) $^{[9]}Cm^{3+}$.



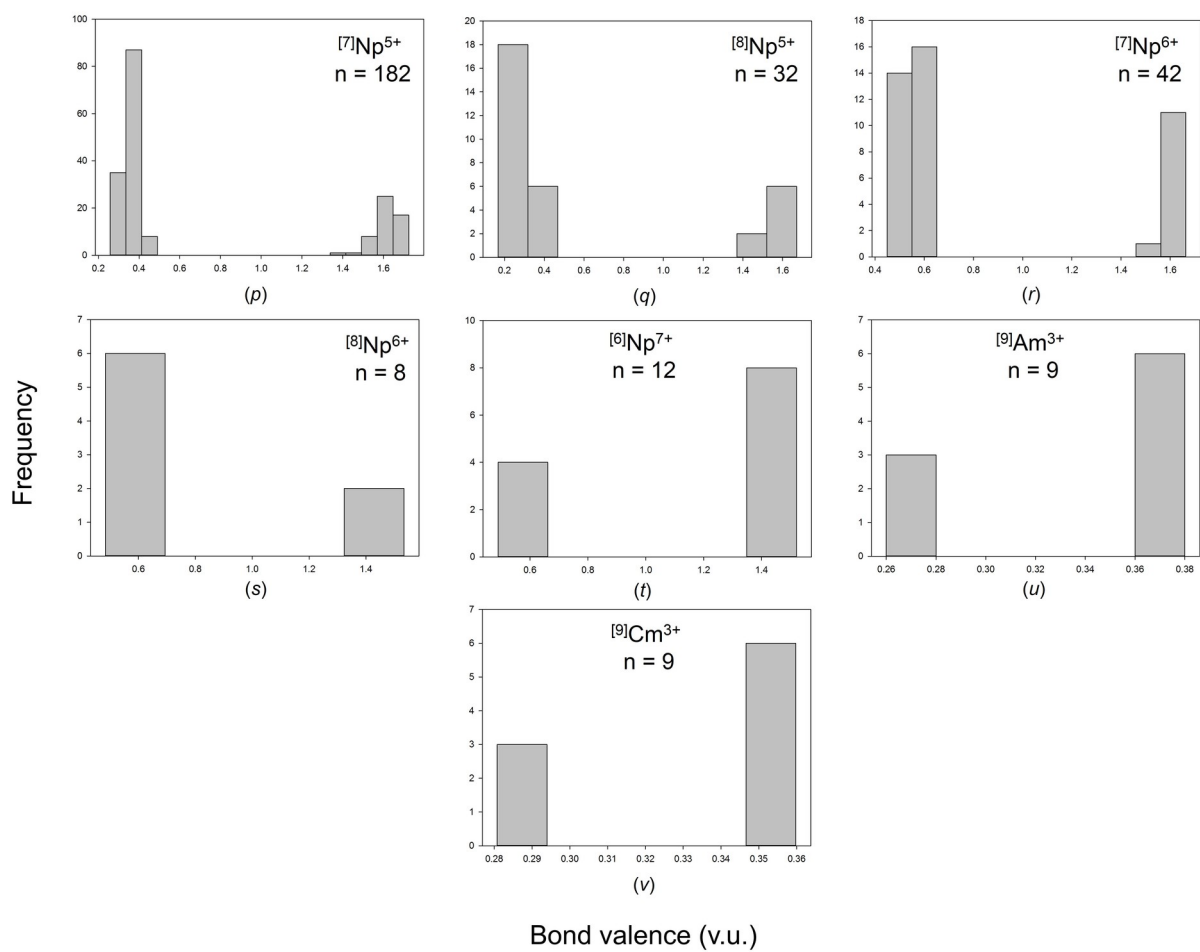
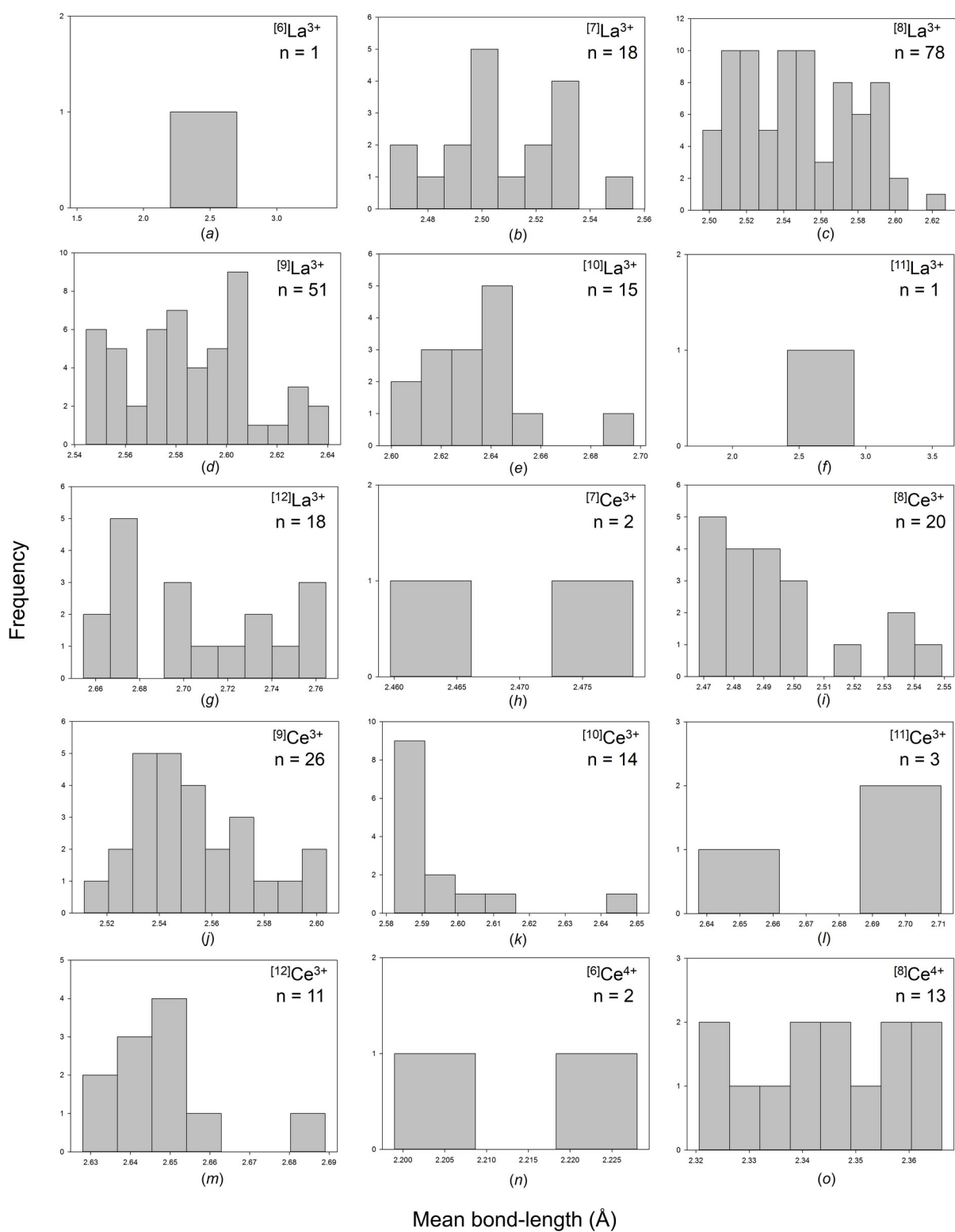
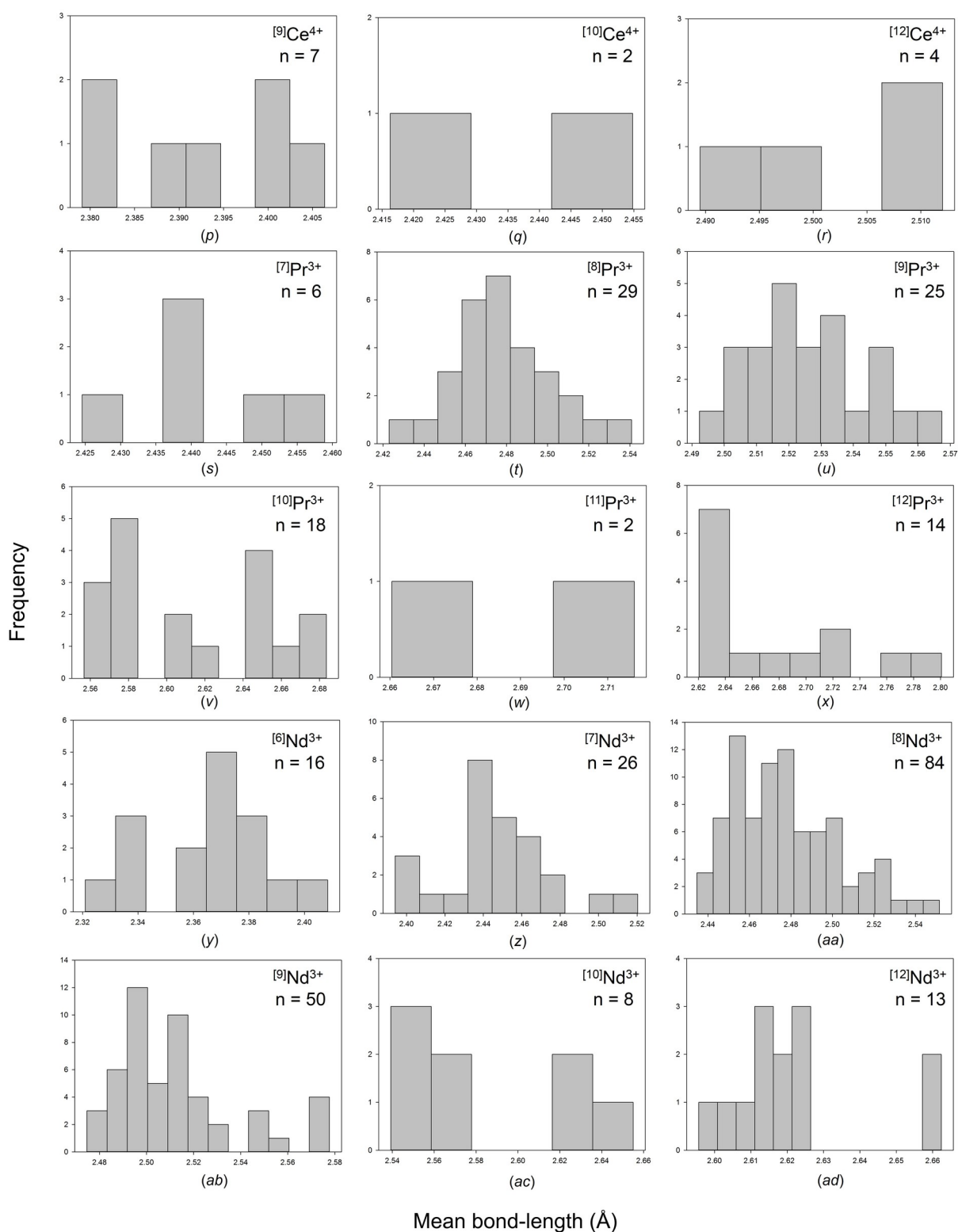
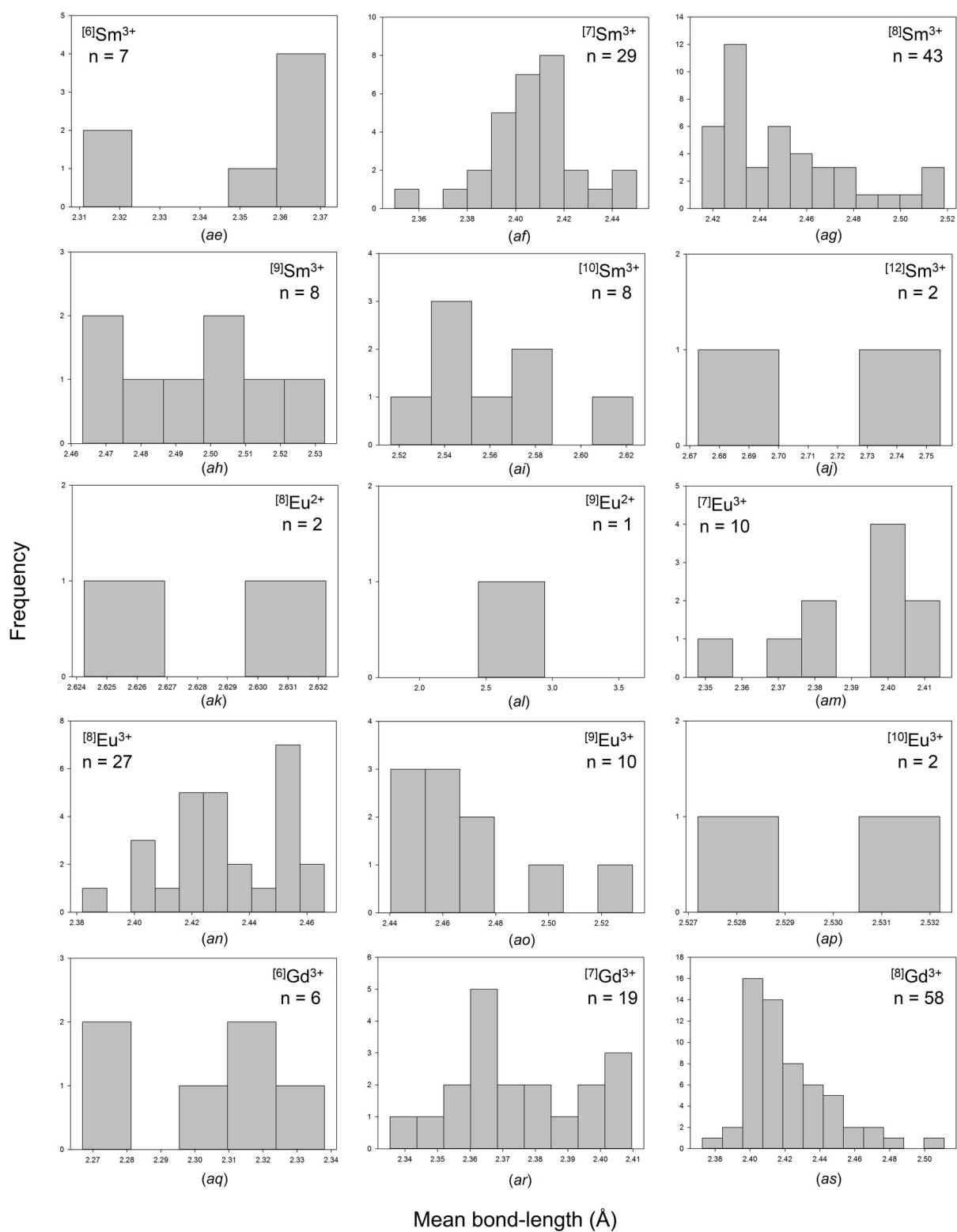
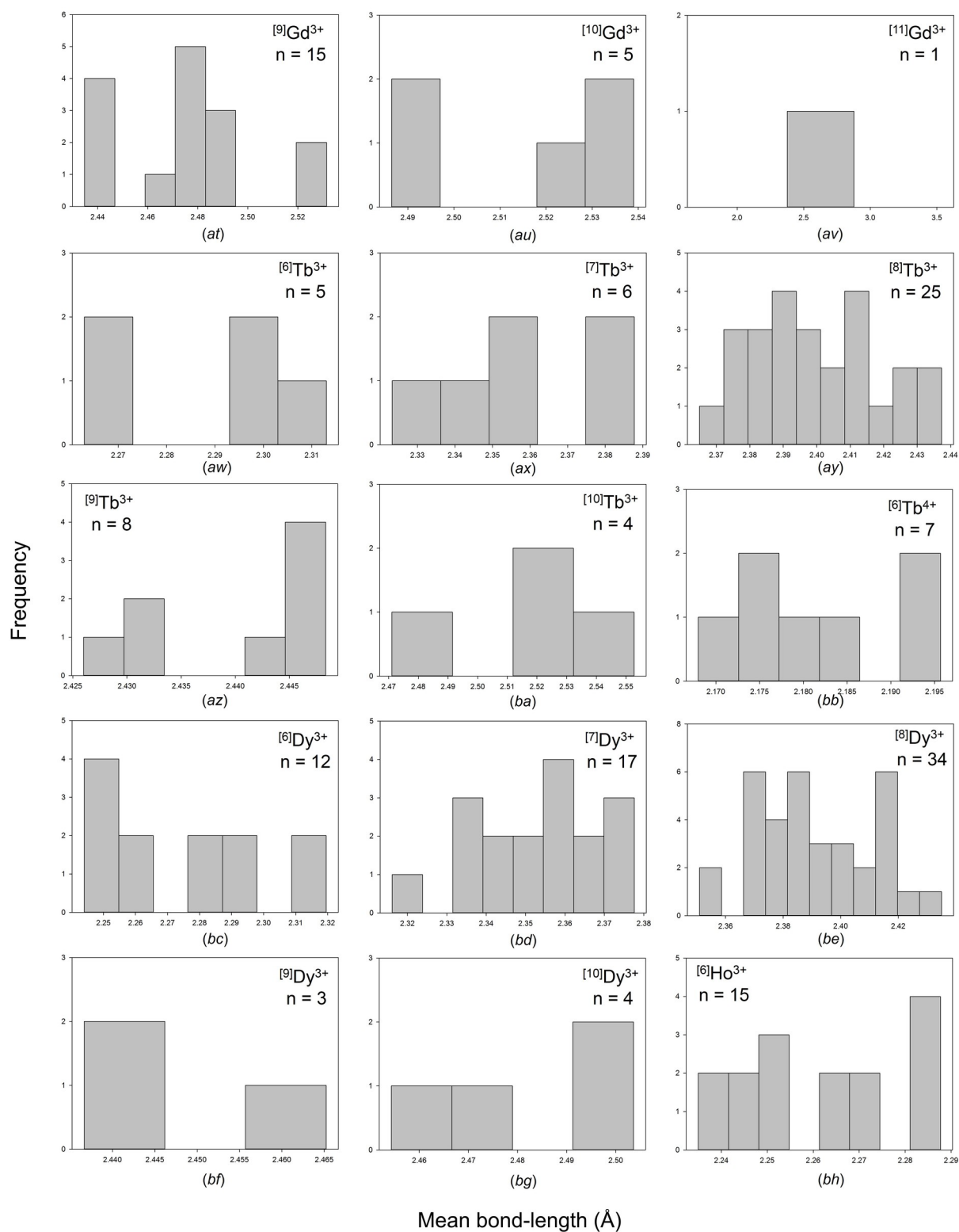


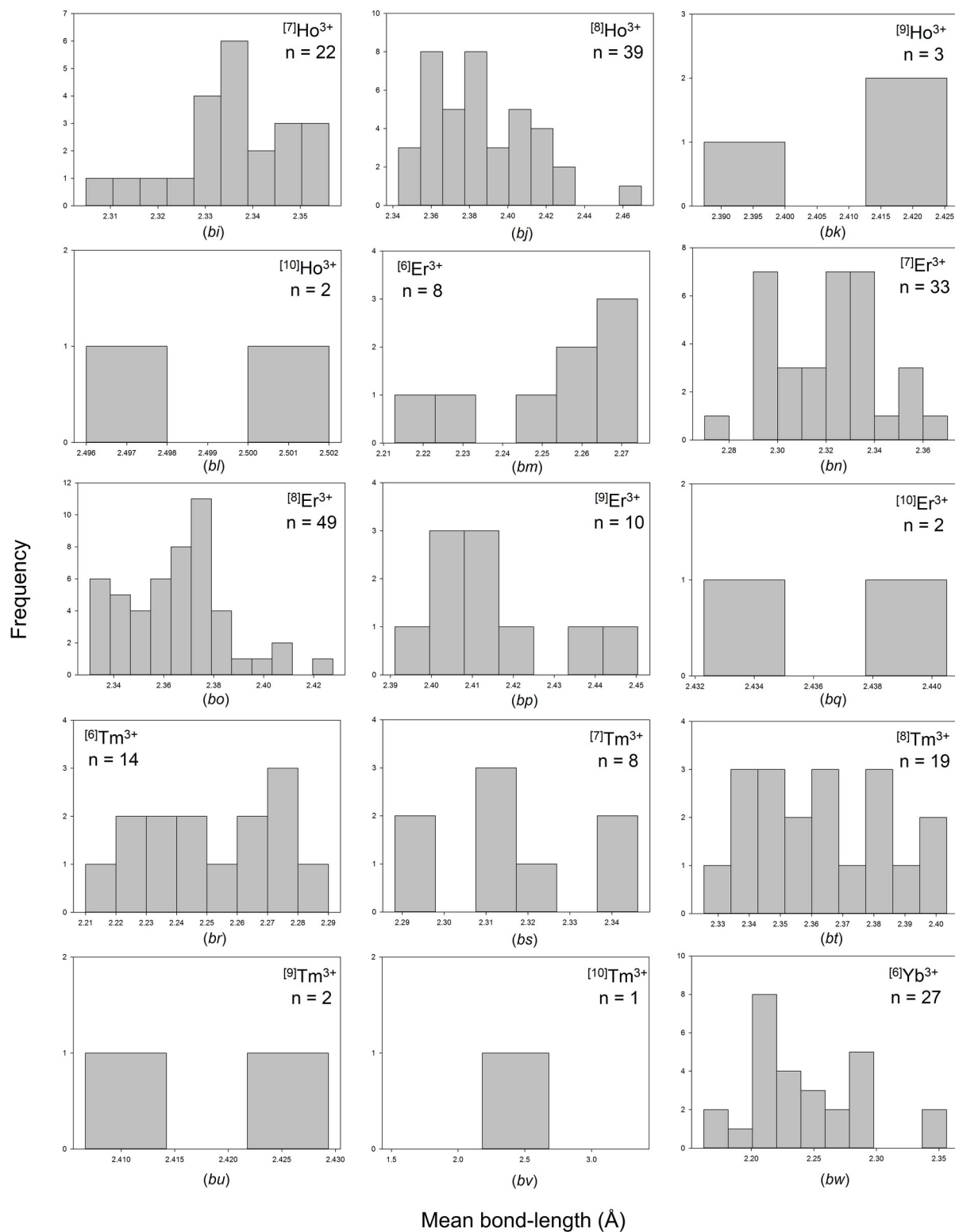
Figure S5 Mean-bond-length distributions for all configurations of the lanthanide ions bonded to O^{2-} : (a) $^{[6]}La^{3+}$, (b) $^{[7]}La^{3+}$, (c) $^{[8]}La^{3+}$, (d) $^{[9]}La^{3+}$, (e) $^{[10]}La^{3+}$, (f) $^{[11]}La^{3+}$, (g) $^{[12]}La^{3+}$, (h) $^{[7]}Ce^{3+}$, (i) $^{[8]}Ce^{3+}$, (j) $^{[9]}Ce^{3+}$, (k) $^{[10]}Ce^{3+}$, (l) $^{[11]}Ce^{3+}$, (m) $^{[12]}Ce^{3+}$, (n) $^{[6]}Ce^{4+}$, (o) $^{[8]}Ce^{4+}$, (p) $^{[9]}Ce^{4+}$, (q) $^{[10]}Ce^{4+}$, (r) $^{[12]}Ce^{4+}$, (s) $^{[7]}Pr^{3+}$, (t) $^{[8]}Pr^{3+}$, (u) $^{[9]}Pr^{3+}$, (v) $^{[10]}Pr^{3+}$, (w) $^{[11]}Pr^{3+}$, (x) $^{[12]}Pr^{3+}$, (y) $^{[6]}Nd^{3+}$, (z) $^{[7]}Nd^{3+}$, (aa) $^{[8]}Nd^{3+}$, (ab) $^{[9]}Nd^{3+}$, (ac) $^{[10]}Nd^{3+}$, (ad) $^{[12]}Nd^{3+}$, (ae) $^{[6]}Sm^{3+}$, (af) $^{[7]}Sm^{3+}$, (ag) $^{[8]}Sm^{3+}$, (ah) $^{[9]}Sm^{3+}$, (ai) $^{[10]}Sm^{3+}$, (aj) $^{[12]}Sm^{3+}$, (ak) $^{[8]}Eu^{2+}$, (al) $^{[9]}Eu^{2+}$, (am) $^{[7]}Eu^{3+}$, (an) $^{[8]}Eu^{3+}$, (ao) $^{[9]}Eu^{3+}$, (ap) $^{[10]}Eu^{3+}$, (aq) $^{[6]}Gd^{3+}$, (ar) $^{[7]}Gd^{3+}$, (as) $^{[8]}Gd^{3+}$, (at) $^{[9]}Gd^{3+}$, (au) $^{[10]}Gd^{3+}$, (av) $^{[11]}Gd^{3+}$, (aw) $^{[6]}Tb^{3+}$, (ax) $^{[7]}Tb^{3+}$, (ay) $^{[8]}Tb^{3+}$, (az) $^{[9]}Tb^{3+}$, (ba) $^{[10]}Tb^{3+}$, (bb) $^{[6]}Tb^{4+}$, (bc) $^{[6]}Dy^{3+}$, (bd) $^{[7]}Dy^{3+}$, (be) $^{[8]}Dy^{3+}$, (bf) $^{[9]}Dy^{3+}$, (bg) $^{[10]}Dy^{3+}$, (bh) $^{[6]}Ho^{3+}$, (bi) $^{[7]}Ho^{3+}$, (bj) $^{[8]}Ho^{3+}$, (bk) $^{[9]}Ho^{3+}$, (bl) $^{[10]}Ho^{3+}$, (bm) $^{[6]}Er^{3+}$, (bn) $^{[7]}Er^{3+}$, (bo) $^{[8]}Er^{3+}$, (bp) $^{[9]}Er^{3+}$, (bq) $^{[10]}Er^{3+}$, (br) $^{[6]}Tm^{3+}$, (bs) $^{[7]}Tm^{3+}$, (bt) $^{[8]}Tm^{3+}$, (bu) $^{[9]}Tm^{3+}$, (bv) $^{[10]}Tm^{3+}$, (bw) $^{[6]}Yb^{3+}$, (bx) $^{[7]}Yb^{3+}$, (by) $^{[8]}Yb^{3+}$, (bz) $^{[9]}Yb^{3+}$, (ca) $^{[10]}Yb^{3+}$, (cb) $^{[6]}Lu^{3+}$, (cc) $^{[7]}Lu^{3+}$, (cd) $^{[8]}Lu^{3+}$, (ce) $^{[9]}Lu^{3+}$, (cf) $^{[10]}Lu^{3+}$.











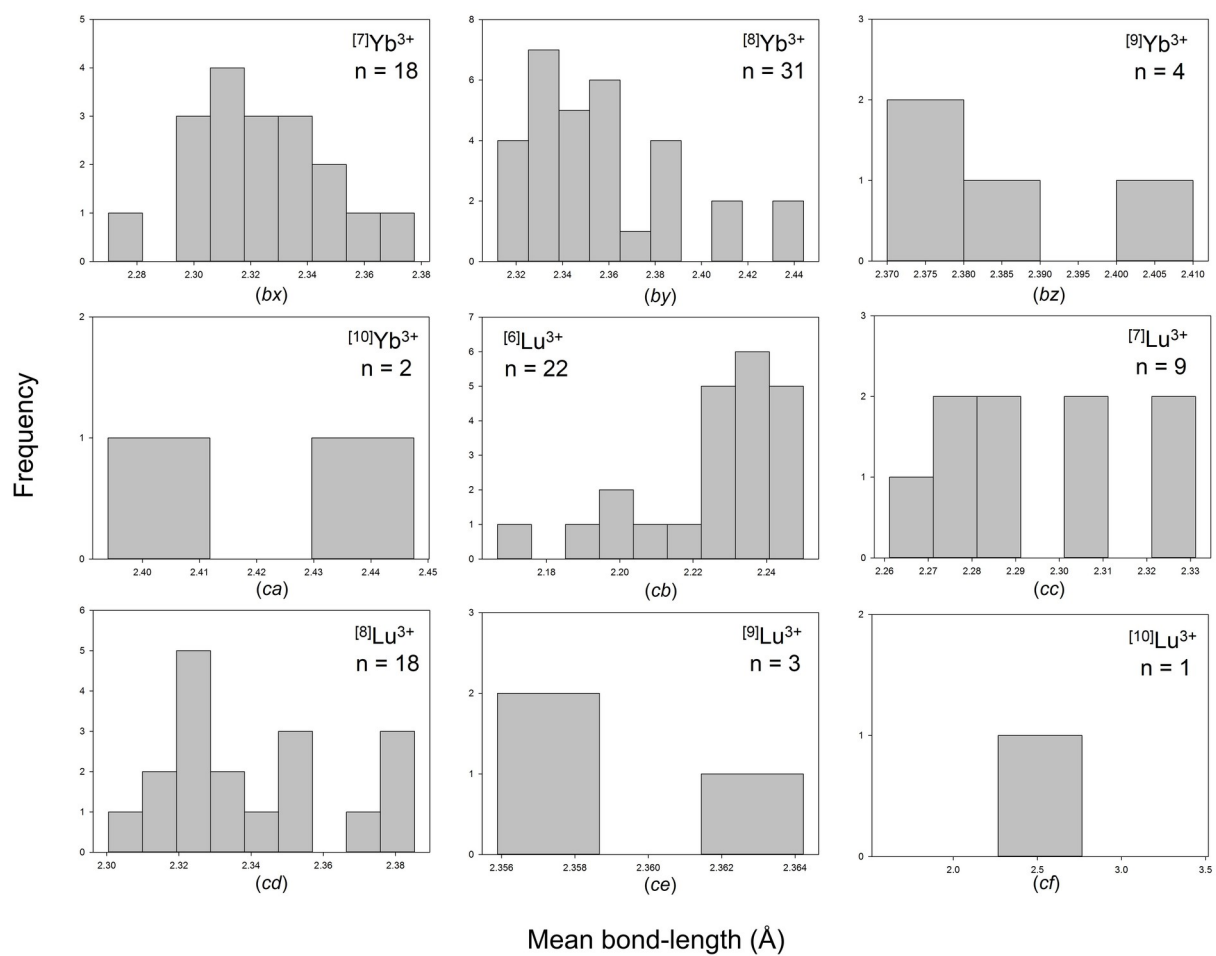
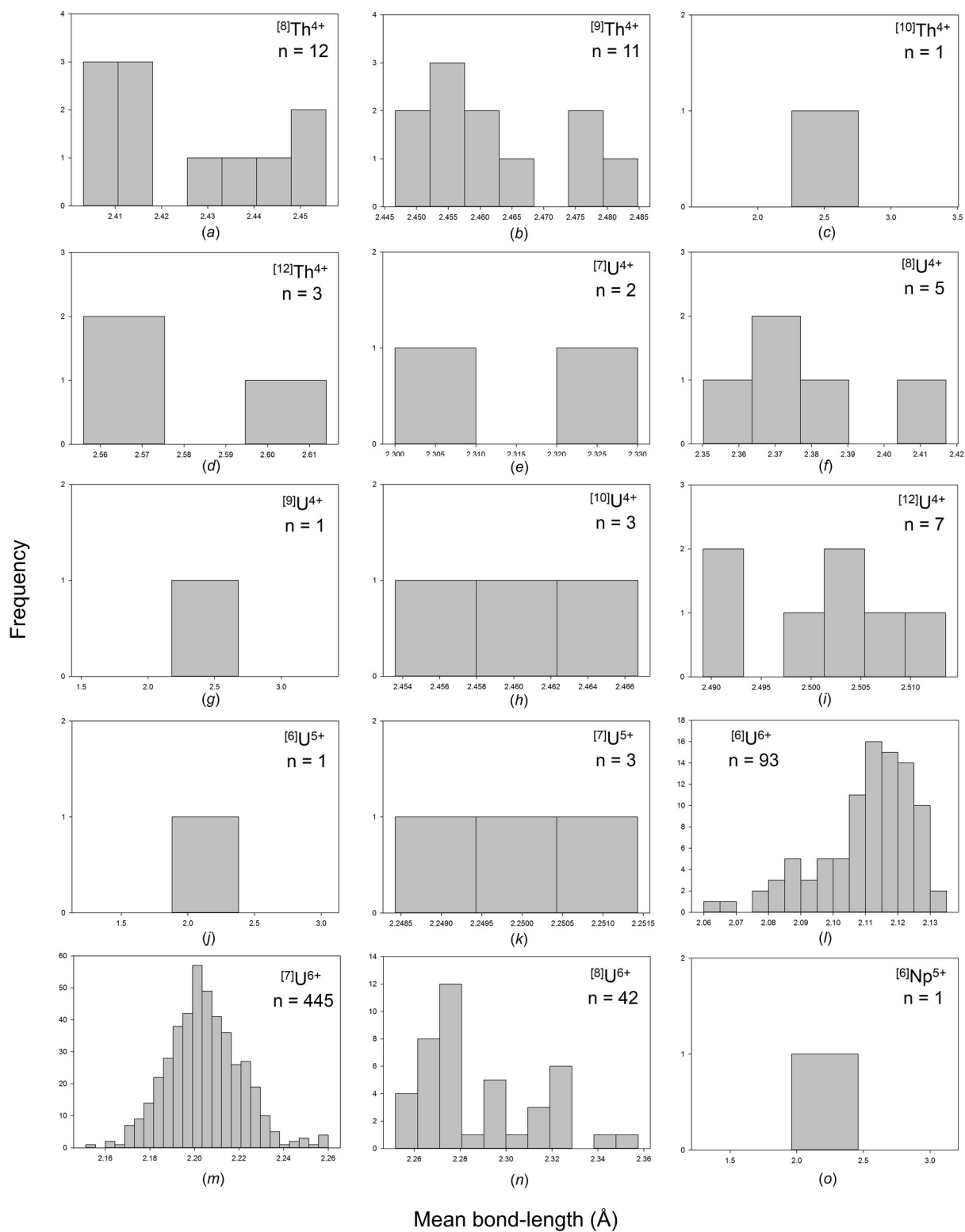


Figure S6 Mean-bond-length distributions for all configurations of the actinide ions bonded to O²⁻:

(a) ^[8]Th⁴⁺, (b) ^[9]Th⁴⁺, (c) ^[10]Th⁴⁺, (d) ^[12]Th⁴⁺, (e) ^[7]U⁴⁺, (f) ^[8]U⁴⁺, (g) ^[9]U⁴⁺, (h) ^[10]U⁴⁺, (i) ^[12]U⁴⁺, (j) ^[6]U⁵⁺, (k) ^[7]U⁵⁺, (l) ^[6]U⁶⁺, (m) ^[7]U⁶⁺, (n) ^[8]U⁶⁺, (o) ^[6]Np⁵⁺, (p) ^[7]Np⁵⁺, (q) ^[8]Np⁵⁺, (r) ^[7]Np⁶⁺, (s) ^[8]Np⁶⁺, (t) ^[6]Np⁷⁺, (u) ^[9]Am³⁺, (v) ^[9]Cm³⁺.



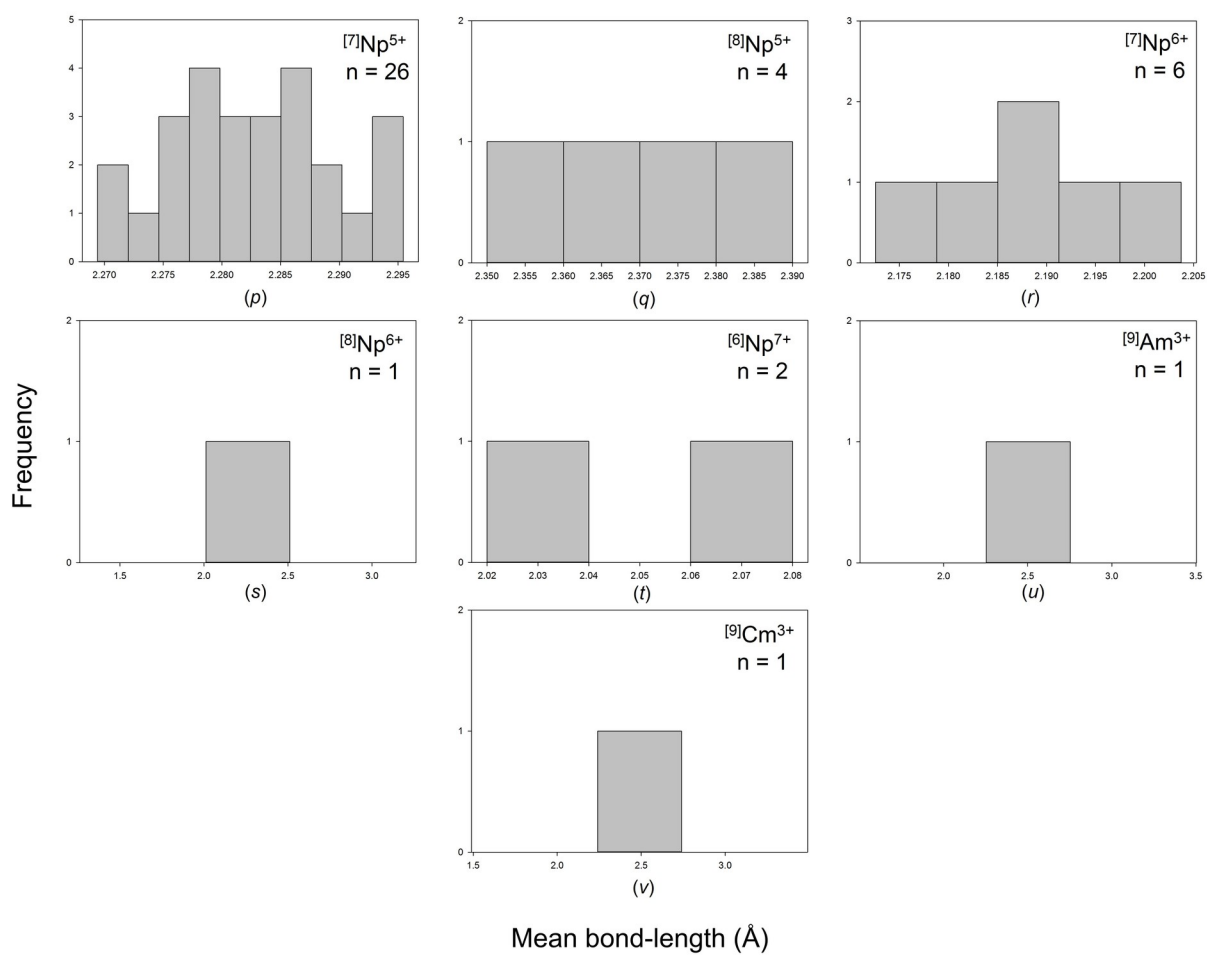
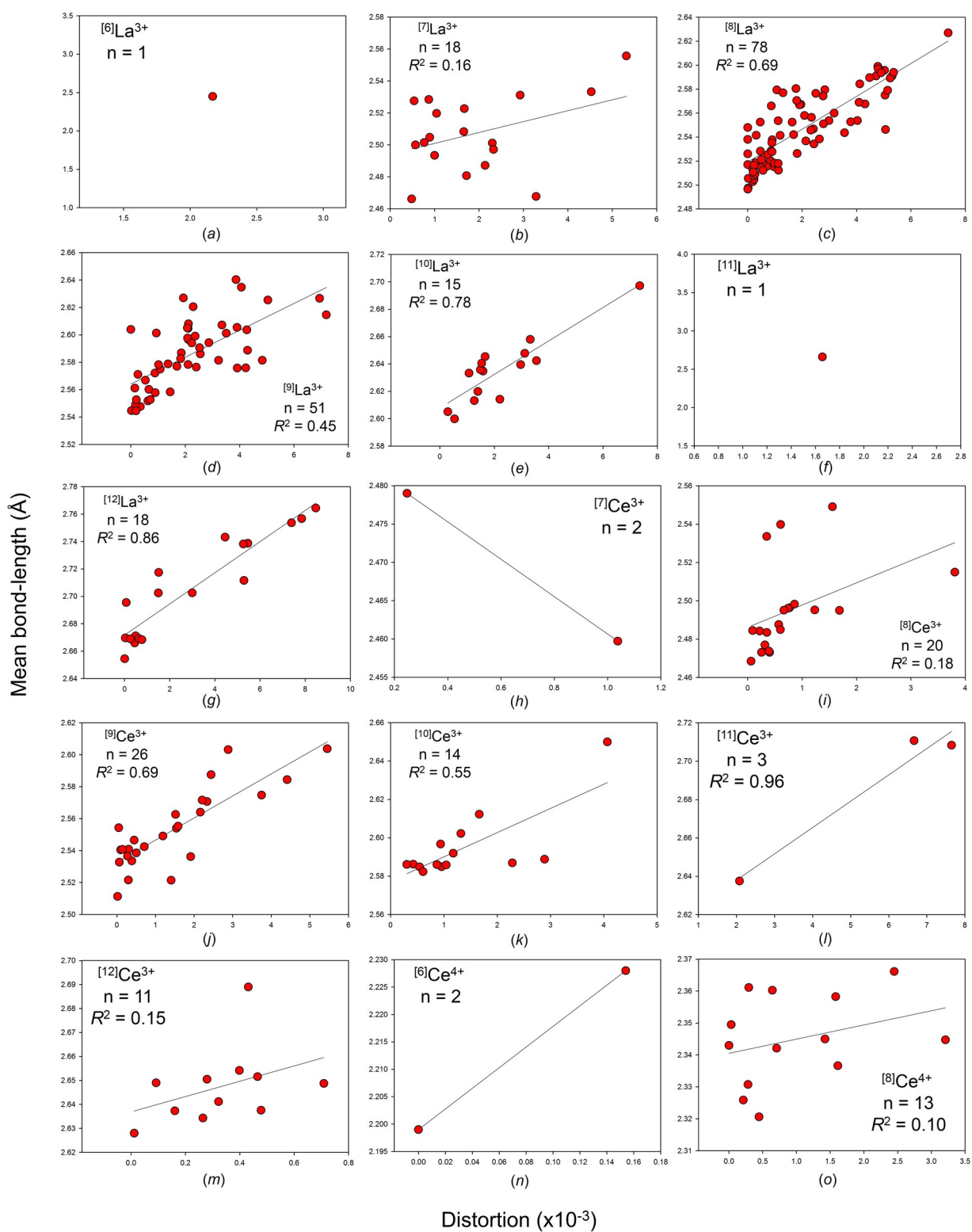
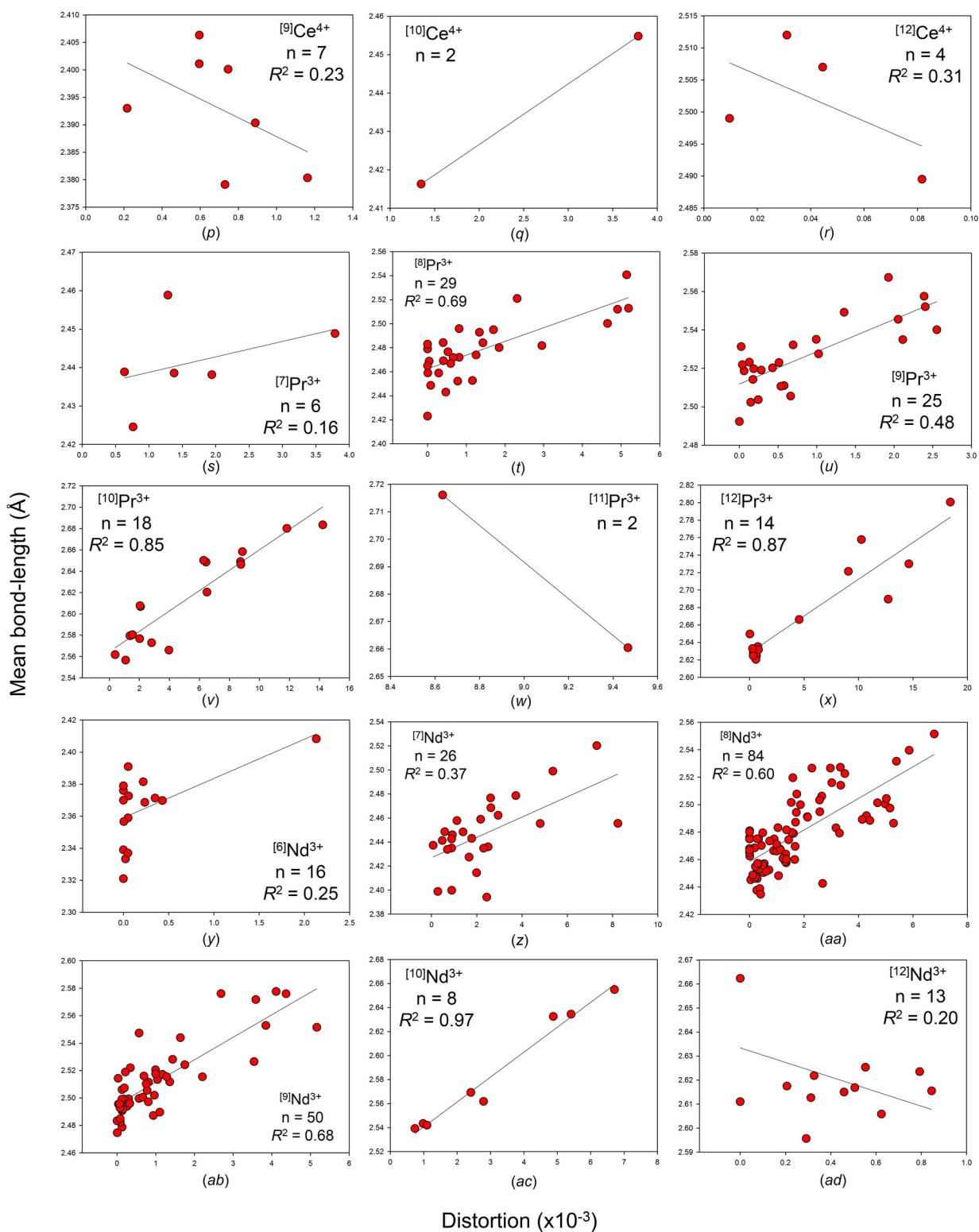
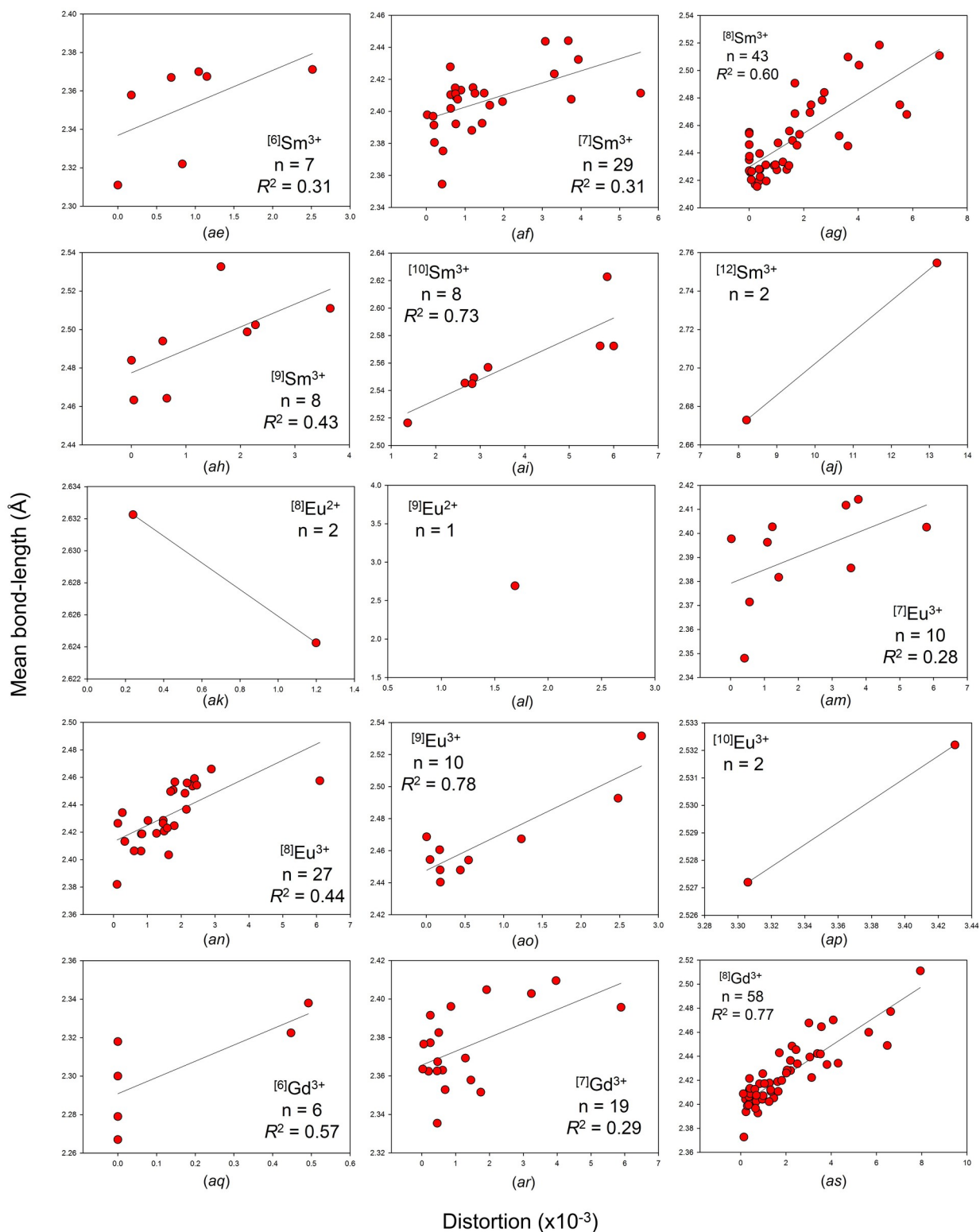
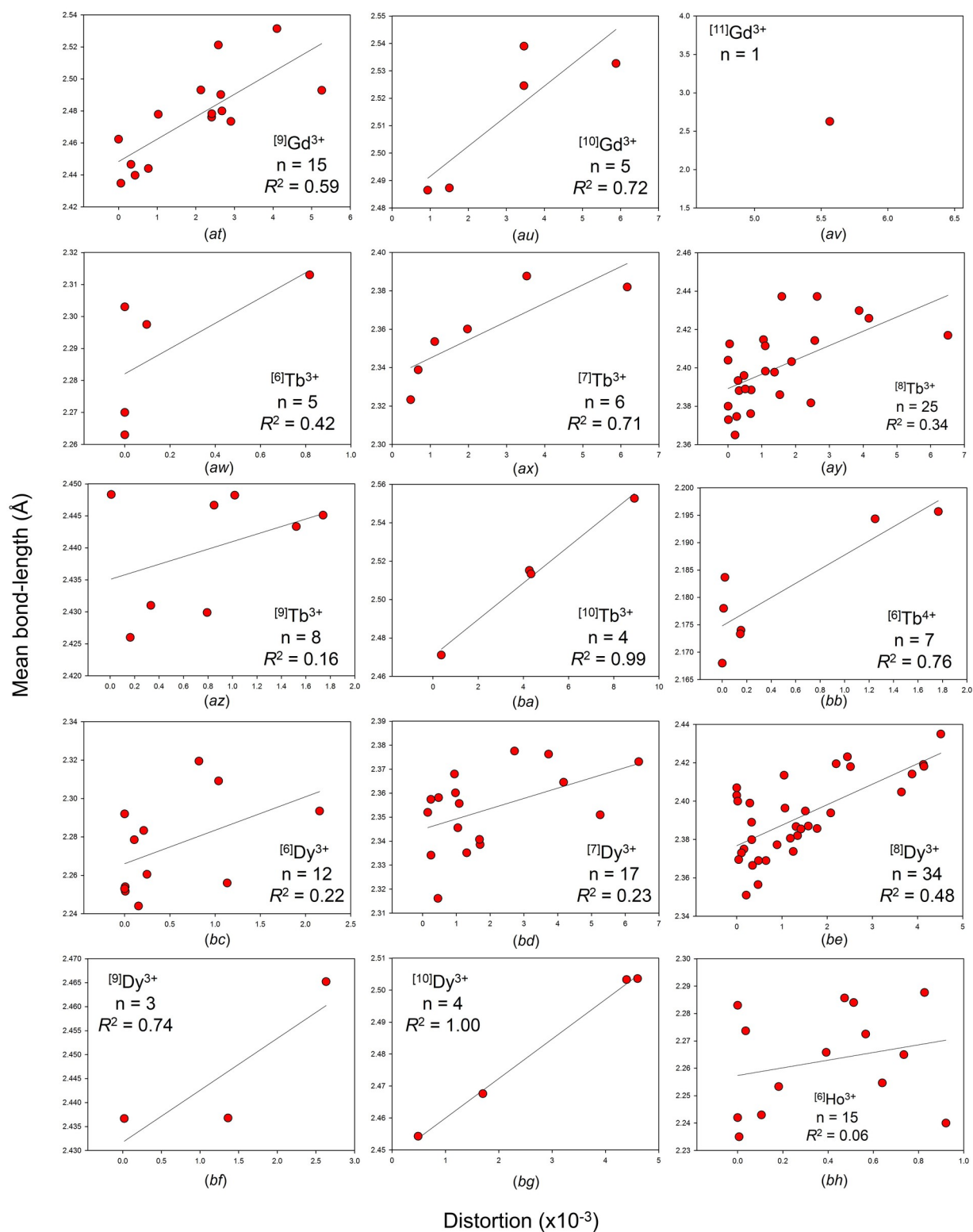


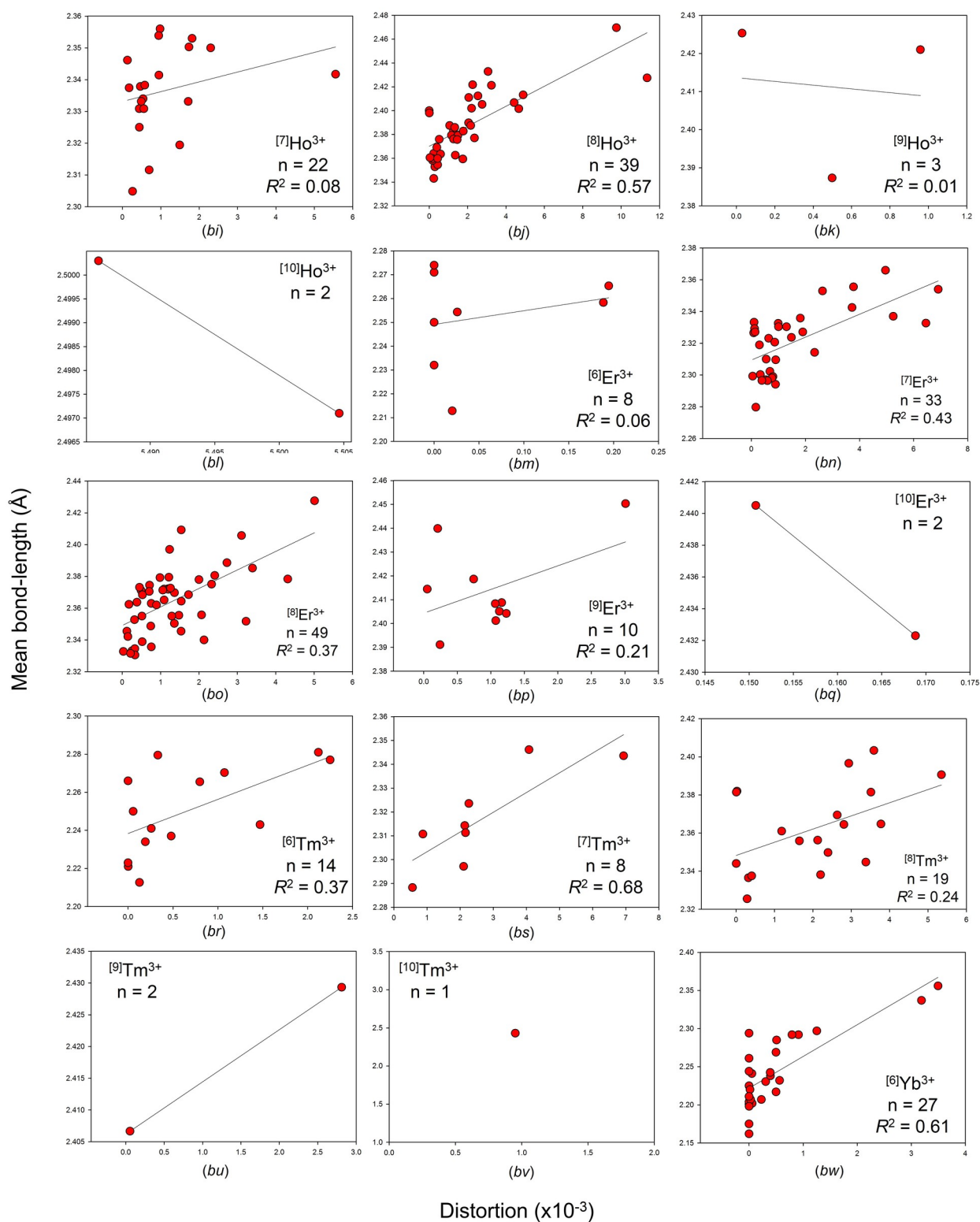
Figure S7 The effect of bond-length distortion on mean bond-length for all configurations of the lanthanide ions bonded to O²⁻: (a) ⁶La³⁺, (b) ⁷La³⁺, (c) ⁸La³⁺, (d) ⁹La³⁺, (e) ¹⁰La³⁺, (f) ¹¹La³⁺, (g) ¹²La³⁺, (h) ⁷Ce³⁺, (i) ⁸Ce³⁺, (j) ⁹Ce³⁺, (k) ¹⁰Ce³⁺, (l) ¹¹Ce³⁺, (m) ¹²Ce³⁺, (n) ⁶Ce⁴⁺, (o) ⁸Ce⁴⁺, (p) ⁹Ce⁴⁺, (q) ¹⁰Ce⁴⁺, (r) ¹²Ce⁴⁺, (s) ⁷Pr³⁺, (t) ⁸Pr³⁺, (u) ⁹Pr³⁺, (v) ¹⁰Pr³⁺, (w) ¹¹Pr³⁺, (x) ¹²Pr³⁺, (y) ⁶Nd³⁺, (z) ⁷Nd³⁺, (aa) ⁸Nd³⁺, (ab) ⁹Nd³⁺, (ac) ¹⁰Nd³⁺, (ad) ¹²Nd³⁺, (ae) ⁶Sm³⁺, (af) ⁷Sm³⁺, (ag) ⁸Sm³⁺, (ah) ⁹Sm³⁺, (ai) ¹⁰Sm³⁺, (aj) ¹²Sm³⁺, (ak) ⁸Eu²⁺, (al) ⁹Eu²⁺, (am) ⁷Eu³⁺, (an) ⁸Eu³⁺, (ao) ⁹Eu³⁺, (ap) ¹⁰Eu³⁺, (aq) ⁶Gd³⁺, (ar) ⁷Gd³⁺, (as) ⁸Gd³⁺, (at) ⁹Gd³⁺, (au) ¹⁰Gd³⁺, (av) ¹¹Gd³⁺, (aw) ⁶Tb³⁺, (ax) ⁷Tb³⁺, (ay) ⁸Tb³⁺, (az) ⁹Tb³⁺, (ba) ¹⁰Tb³⁺, (bb) ⁶Tb⁴⁺, (bc) ⁶Dy³⁺, (bd) ⁷Dy³⁺, (be) ⁸Dy³⁺, (bf) ⁹Dy³⁺, (bg) ¹⁰Dy³⁺, (bh) ⁶Ho³⁺, (bi) ⁷Ho³⁺, (bj) ⁸Ho³⁺, (bk) ⁹Ho³⁺, (bl) ¹⁰Ho³⁺, (bm) ⁶Er³⁺, (bn) ⁷Er³⁺, (bo) ⁸Er³⁺, (bp) ⁹Er³⁺, (bq) ¹⁰Er³⁺, (br) ⁶Tm³⁺, (bs) ⁷Tm³⁺, (bt) ⁸Tm³⁺, (bu) ⁹Tm³⁺, (bv) ¹⁰Tm³⁺, (bw) ⁶Yb³⁺, (bx) ⁷Yb³⁺, (by) ⁸Yb³⁺, (bz) ⁹Yb³⁺, (ca) ¹⁰Yb³⁺, (cb) ⁶Lu³⁺, (cc) ⁷Lu³⁺, (cd) ⁸Lu³⁺, (ce) ⁹Lu³⁺, (cf) ¹⁰Lu³⁺.











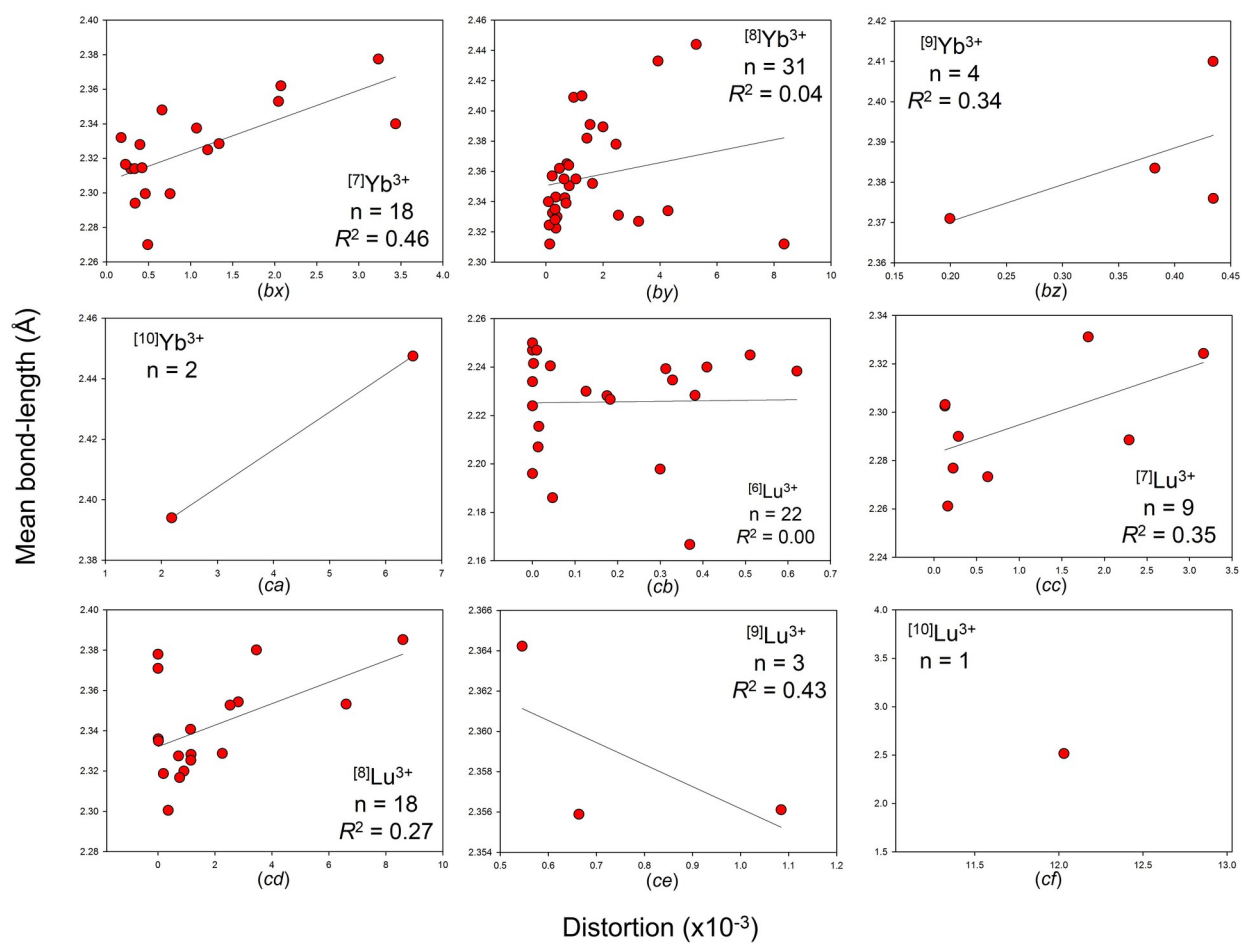


Figure S8 The effect of bond-length distortion on mean bond-length for all configurations of the actinide ions bonded to O²⁻: (a) ^[8]Th⁴⁺, (b) ^[9]Th⁴⁺, (c) ^[10]Th⁴⁺, (d) ^[12]Th⁴⁺, (e) ^[7]U⁴⁺, (f) ^[8]U⁴⁺, (g) ^[9]U⁴⁺, (h) ^[10]U⁴⁺, (i) ^[12]U⁴⁺, (j) ^[6]U⁵⁺, (k) ^[7]U⁵⁺, (l) ^[6]U⁶⁺, (m) ^[7]U⁶⁺, (n) ^[8]U⁶⁺, (o) ^[6]Np⁵⁺, (p) ^[7]Np⁵⁺, (q) ^[8]Np⁵⁺, (r) ^[7]Np⁶⁺, (s) ^[8]Np⁶⁺, (t) ^[6]Np⁷⁺, (u) ^[9]Am³⁺, (v) ^[9]Cm³⁺.

