



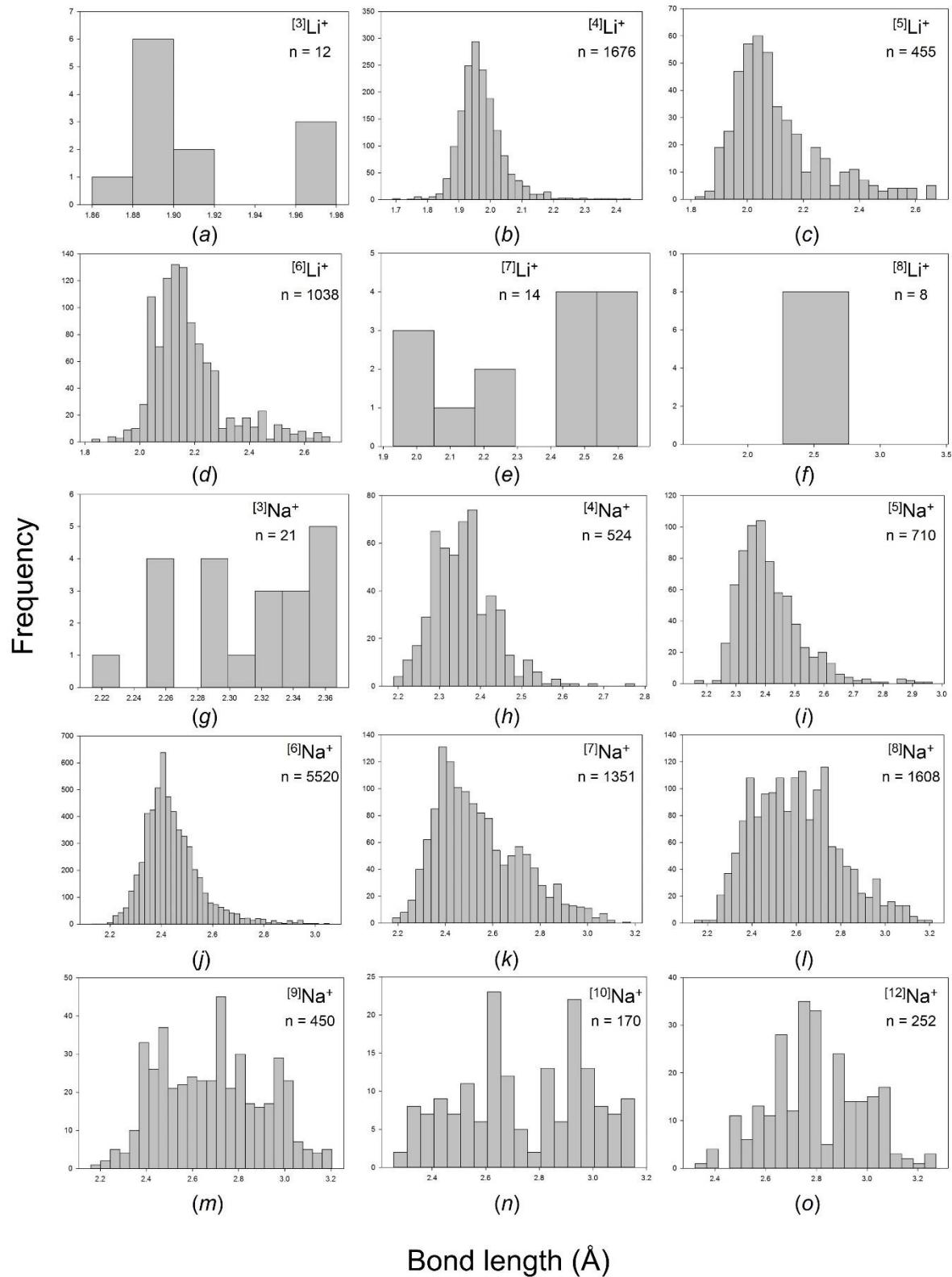
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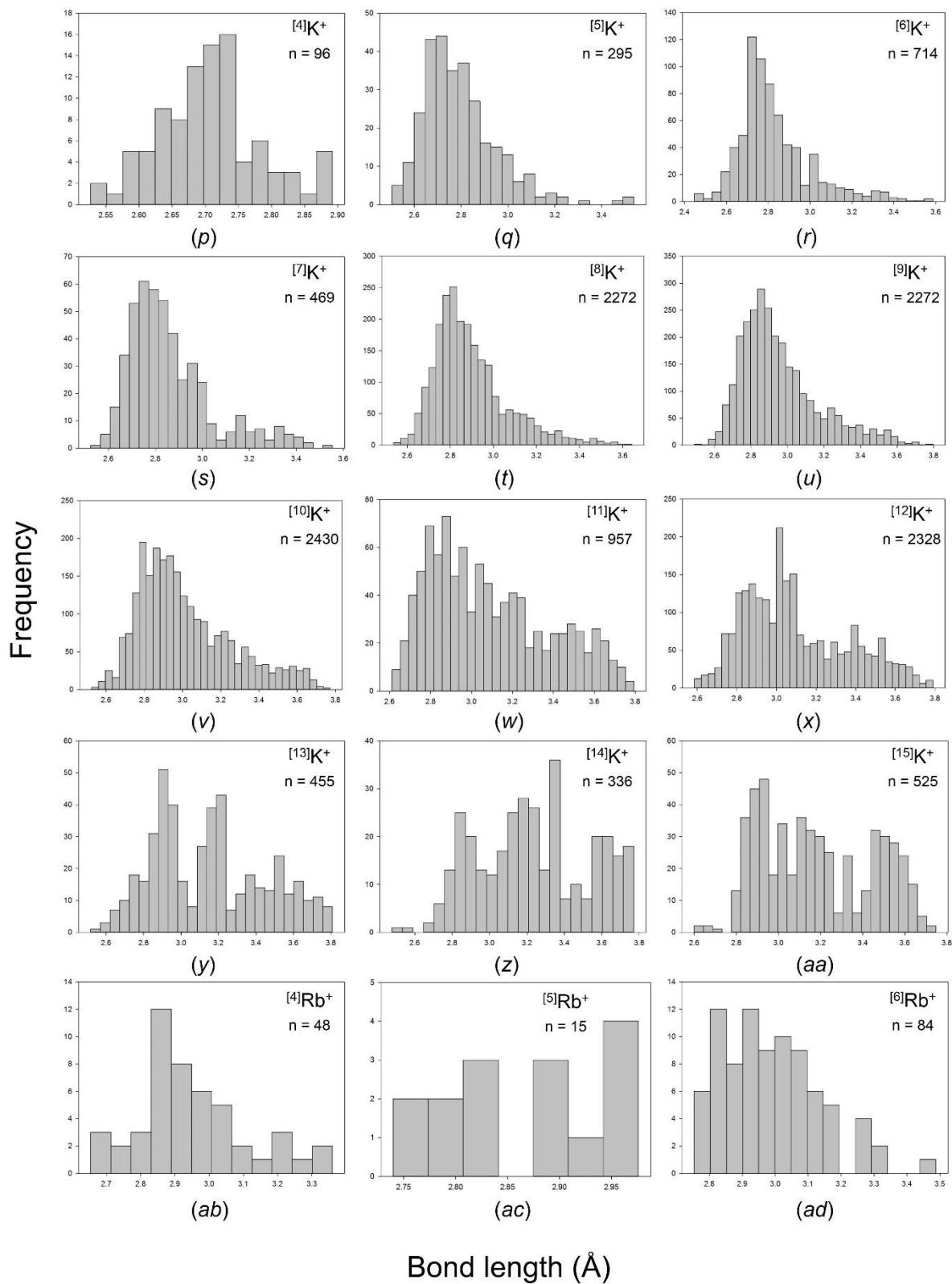
**Volume 72 (2016)**

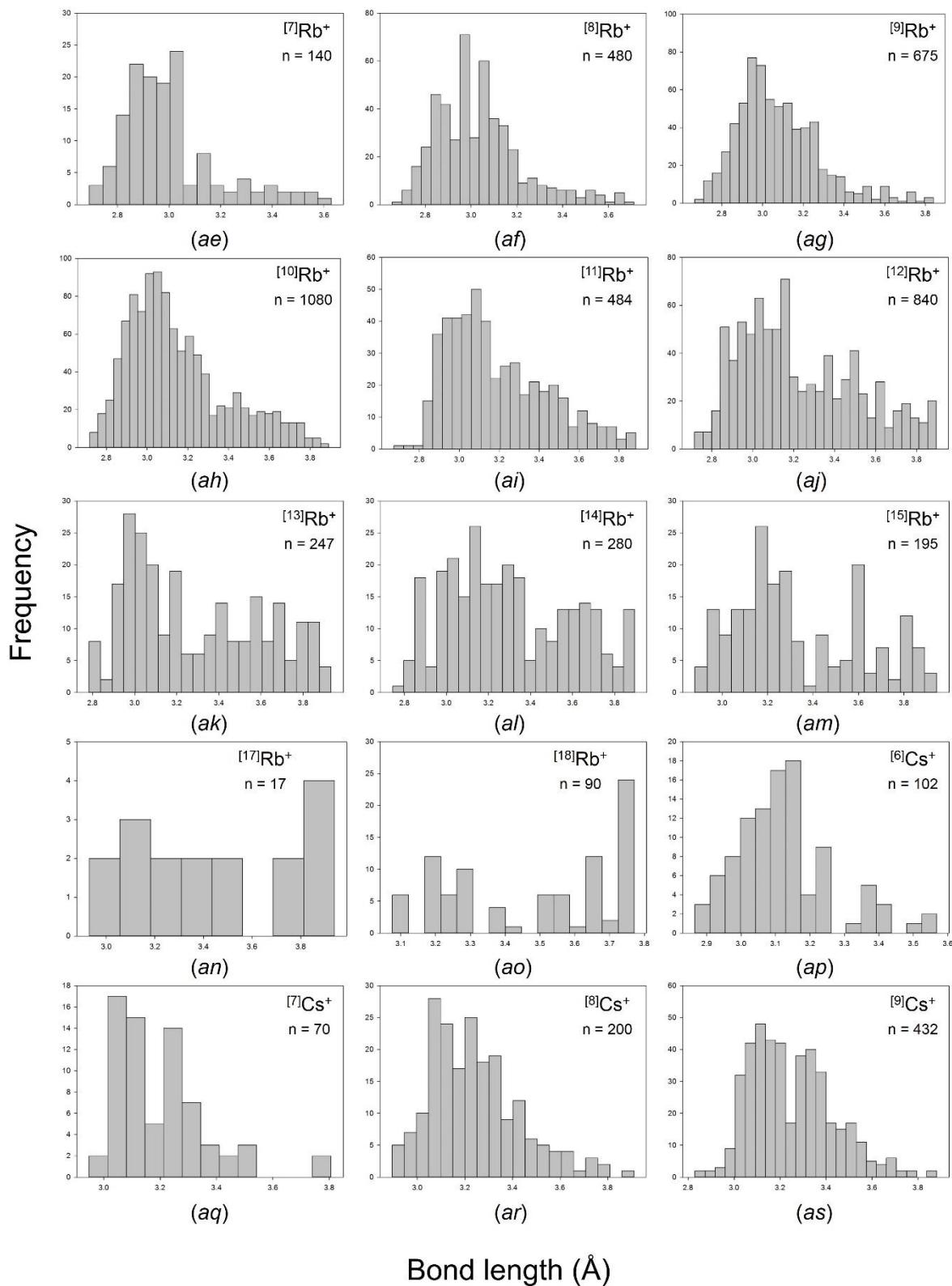
**Supporting information for article:**

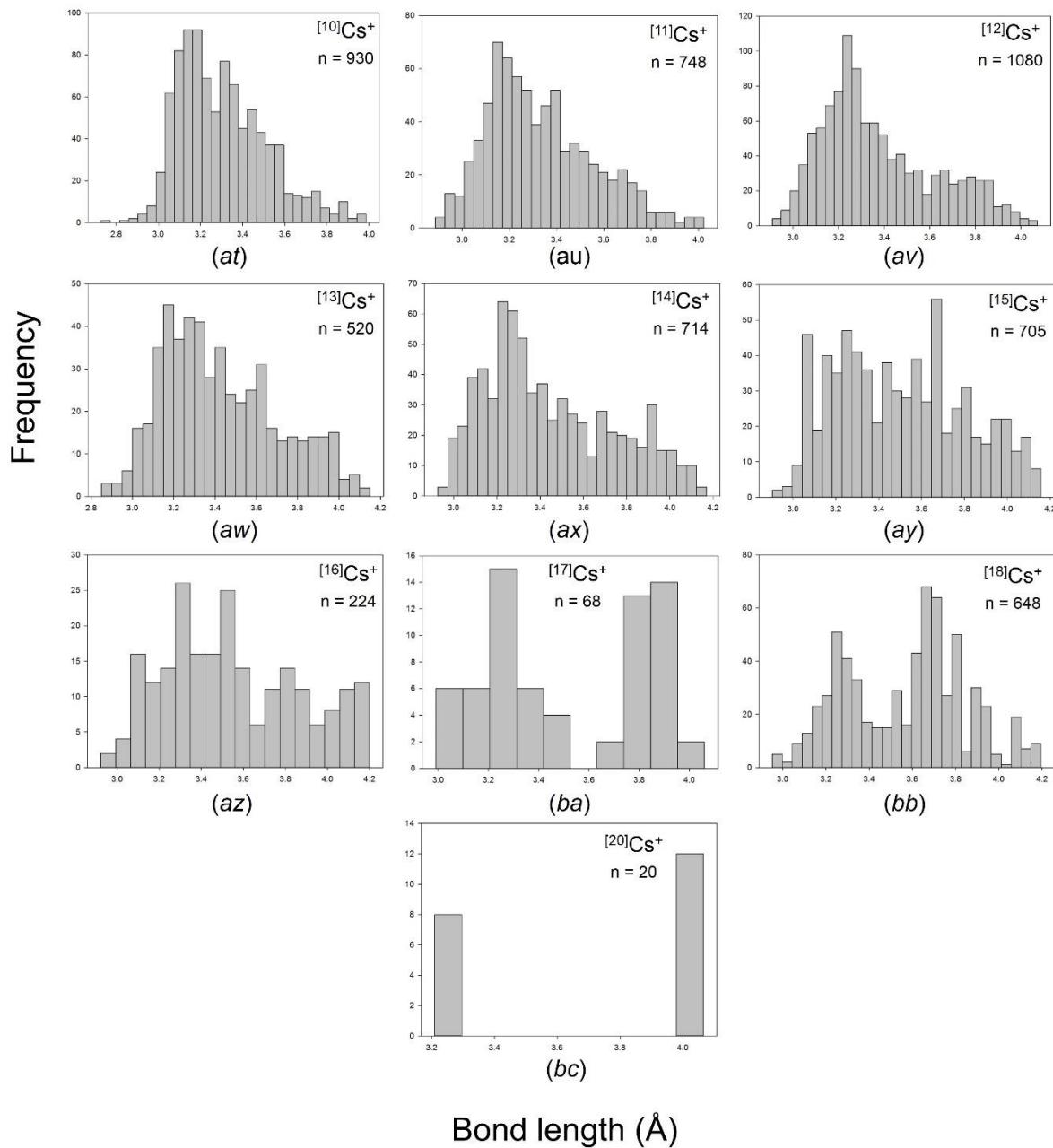
**Bond-length distributions for ions bonded to oxygen: Alkali and alkaline-earth metals**

**Olivier Charles Gagné and Frank Christopher Hawthorne**

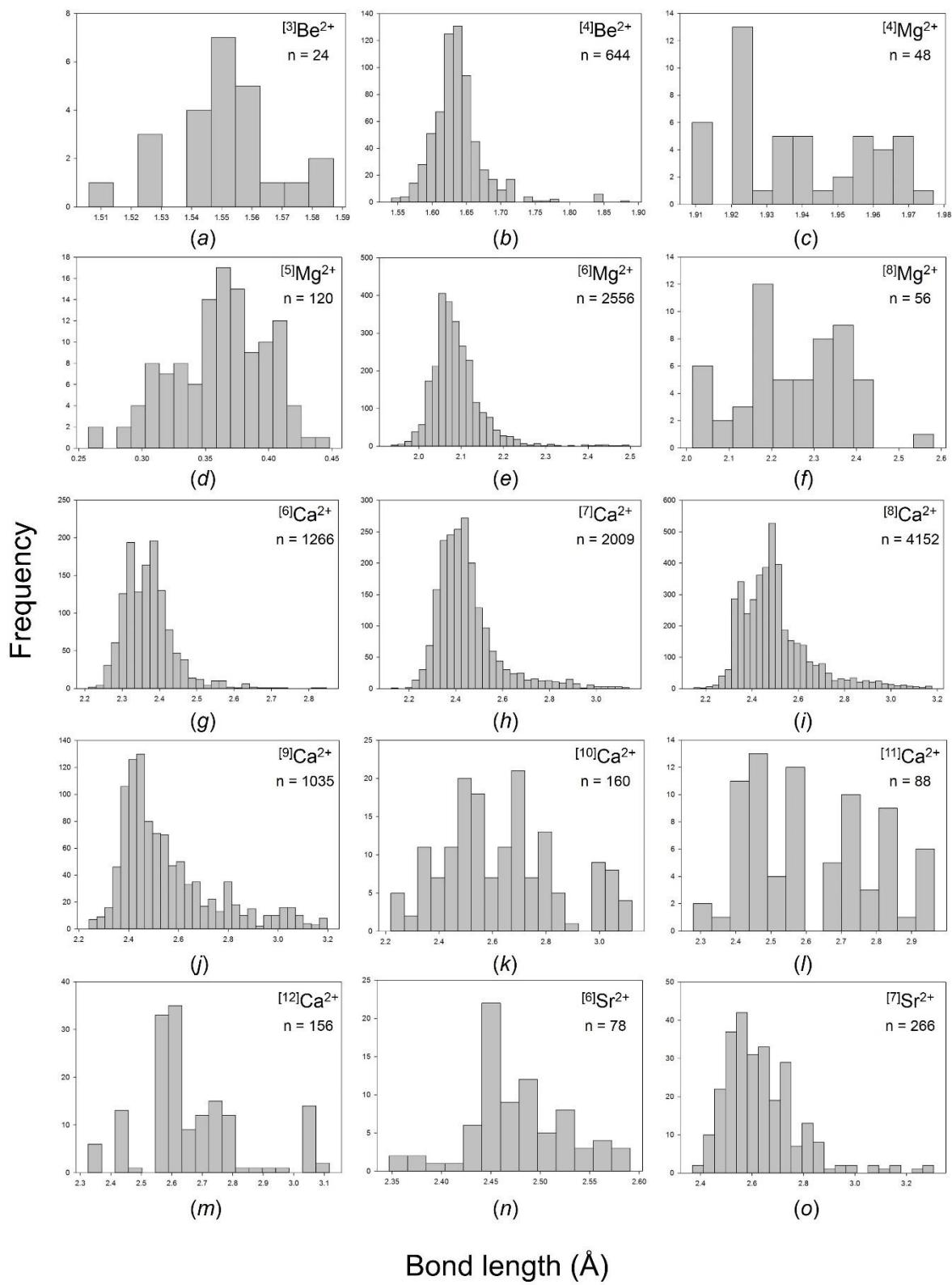


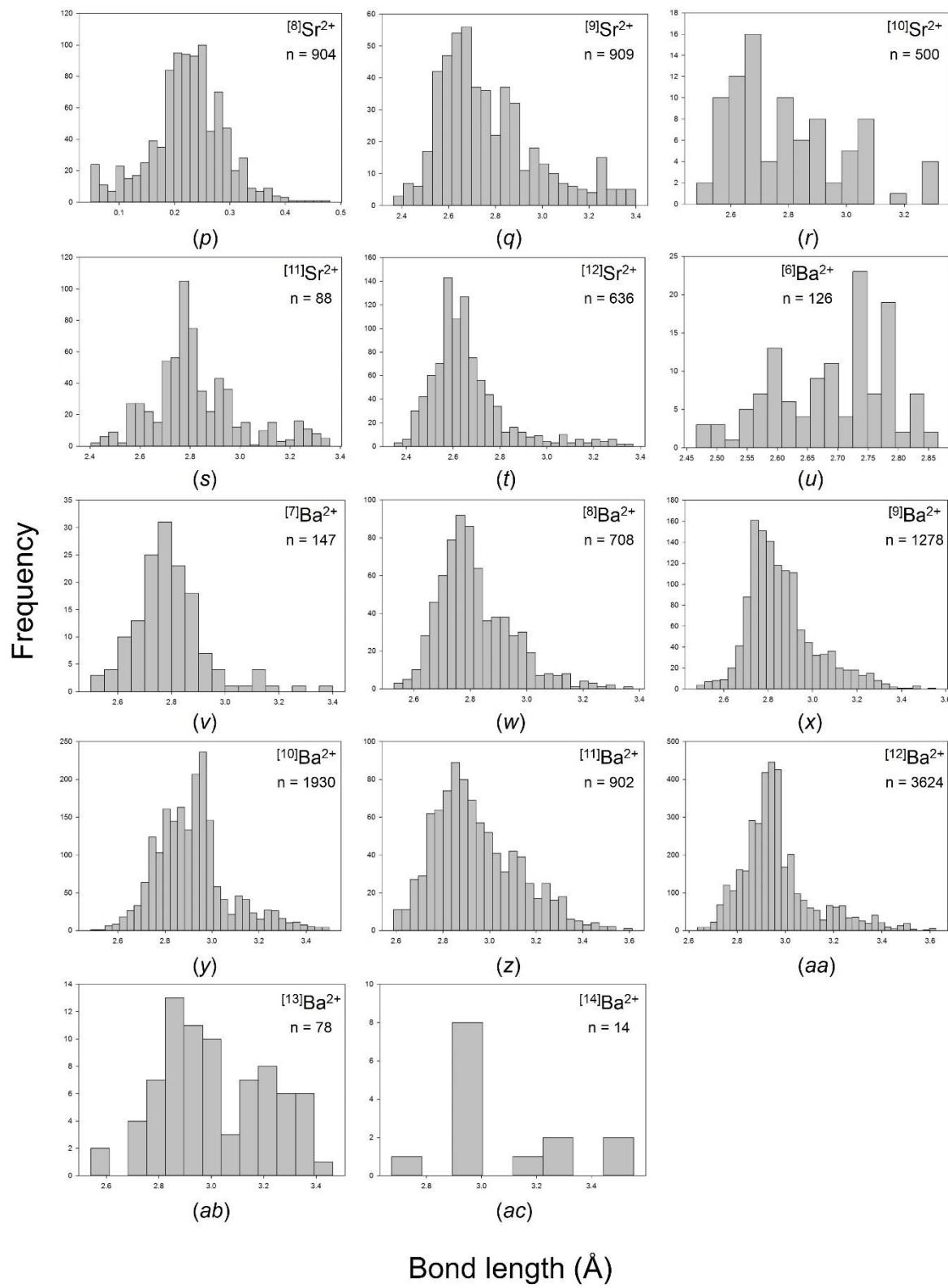






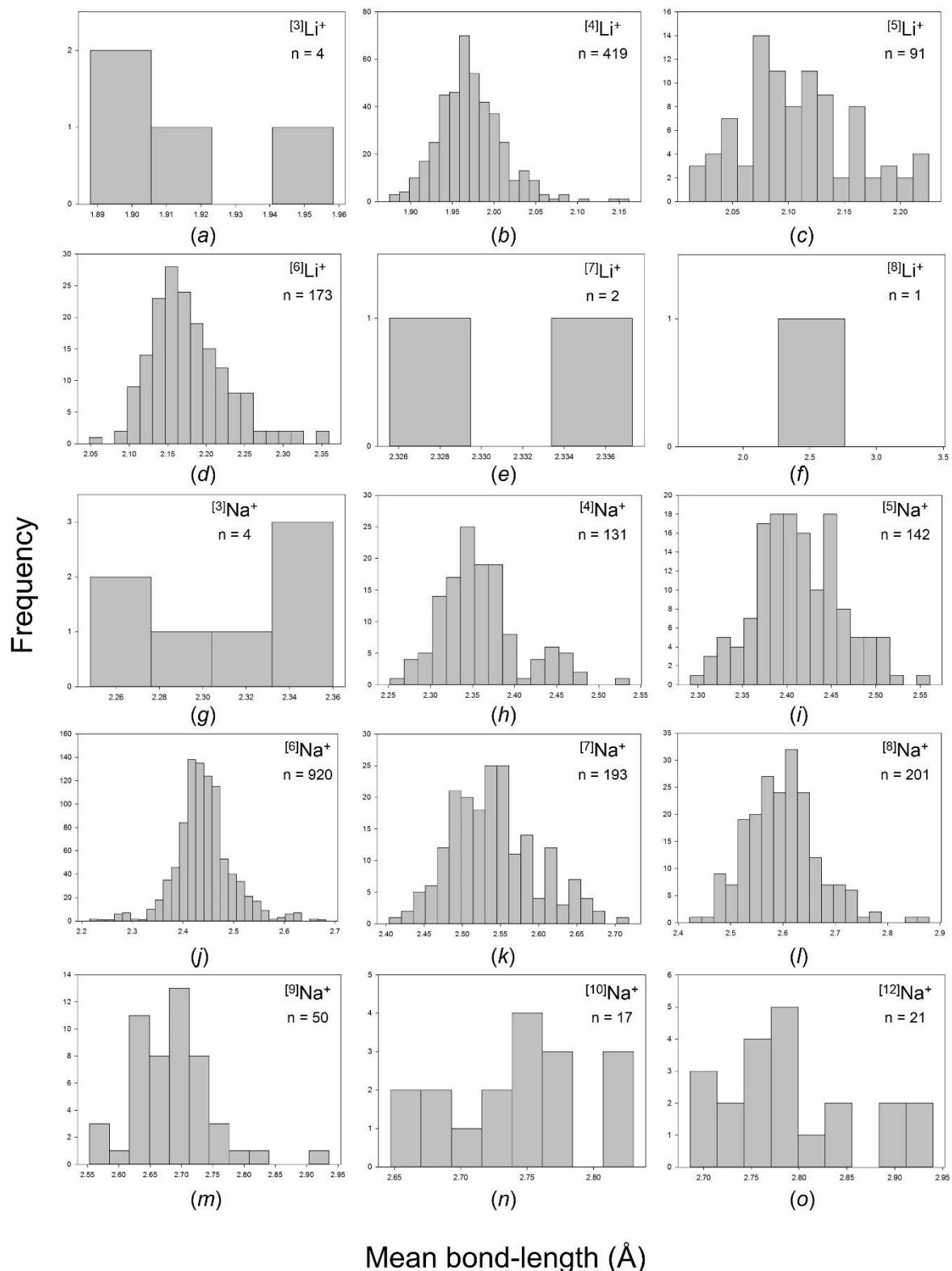
**Figure S1** Bond-length distributions for all configurations of the alkali-metal ions bonded to  $\text{O}^{2-}$ : (a)  ${}^3\text{Li}^+$ , (b)  ${}^4\text{Li}^+$ , (c)  ${}^5\text{Li}^+$ , (d)  ${}^6\text{Li}^+$ , (e)  ${}^7\text{Li}^+$ , (f)  ${}^8\text{Li}^+$ , (g)  ${}^3\text{Na}^+$ , (h)  ${}^4\text{Na}^+$ , (i)  ${}^5\text{Na}^+$ , (j)  ${}^6\text{Na}^+$ , (k)  ${}^7\text{Na}^+$ , (l)  ${}^8\text{Na}^+$ , (m)  ${}^9\text{Na}^+$ , (n)  ${}^{10}\text{Na}^+$ , (o)  ${}^{12}\text{Na}^+$ , (p)  ${}^4\text{K}^+$ , (q)  ${}^5\text{K}^+$ , (r)  ${}^6\text{K}^+$ , (s)  ${}^7\text{K}^+$ , (t)  ${}^8\text{K}^+$ , (u)  ${}^9\text{K}^+$ , (v)  ${}^{10}\text{K}^+$ , (w)  ${}^{11}\text{K}^+$ , (x)  ${}^{12}\text{K}^+$ , (y)  ${}^{13}\text{K}^+$ , (aa)  ${}^{15}\text{K}^+$ , (ab)  ${}^4\text{Rb}^+$ , (ac)  ${}^5\text{Rb}^+$ , (ad)  ${}^6\text{Rb}^+$ , (ae)  ${}^7\text{Rb}^+$ , (af)  ${}^8\text{Rb}^+$ , (ag)  ${}^9\text{Rb}^+$ , (ah)  ${}^{10}\text{Rb}^+$ , (ai)  ${}^{11}\text{Rb}^+$ , (aj)  ${}^{12}\text{Rb}^+$ , (ak)  ${}^{13}\text{Rb}^+$ , (al)  ${}^{14}\text{Rb}^+$ , (am)  ${}^{15}\text{Rb}^+$ , (an)  ${}^{17}\text{Rb}^+$ , (ao)  ${}^{18}\text{Rb}^+$ , (ap)  ${}^6\text{Cs}^+$ , (aq)  ${}^7\text{Cs}^+$ , (ar)  ${}^8\text{Cs}^+$ , (as)  ${}^9\text{Cs}^+$ , (at)  ${}^{10}\text{Cs}^+$ , (au)  ${}^{11}\text{Cs}^+$ , (av)  ${}^{12}\text{Cs}^+$ , (aw)  ${}^{13}\text{Cs}^+$ , (ax)  ${}^{14}\text{Cs}^+$ , (ay)  ${}^{15}\text{Cs}^+$ , (az)  ${}^{16}\text{Cs}^+$ , (ba)  ${}^{17}\text{Cs}^+$ , (bb)  ${}^{18}\text{Cs}^+$ , (bc)  ${}^{20}\text{Cs}^+$ .

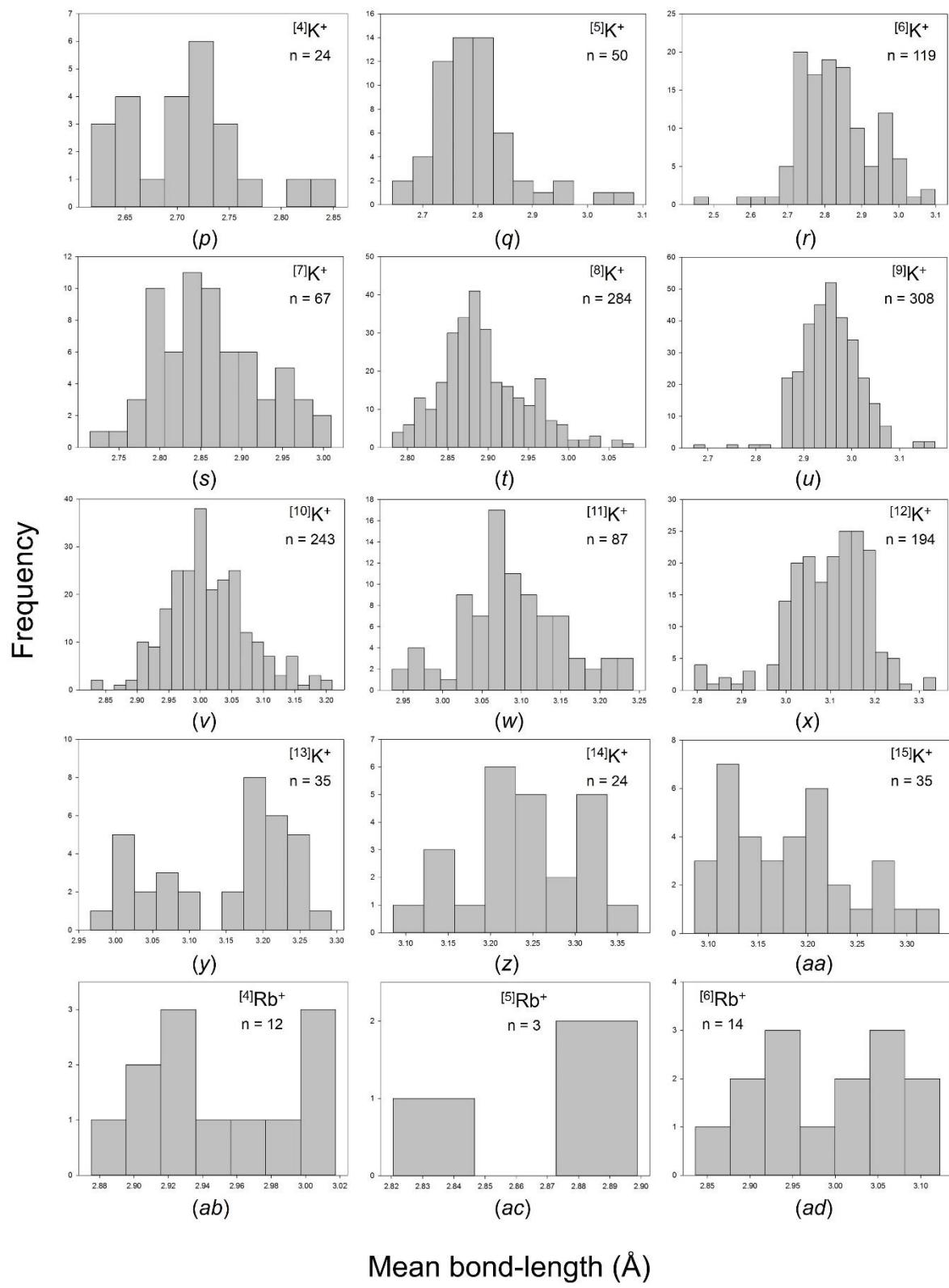


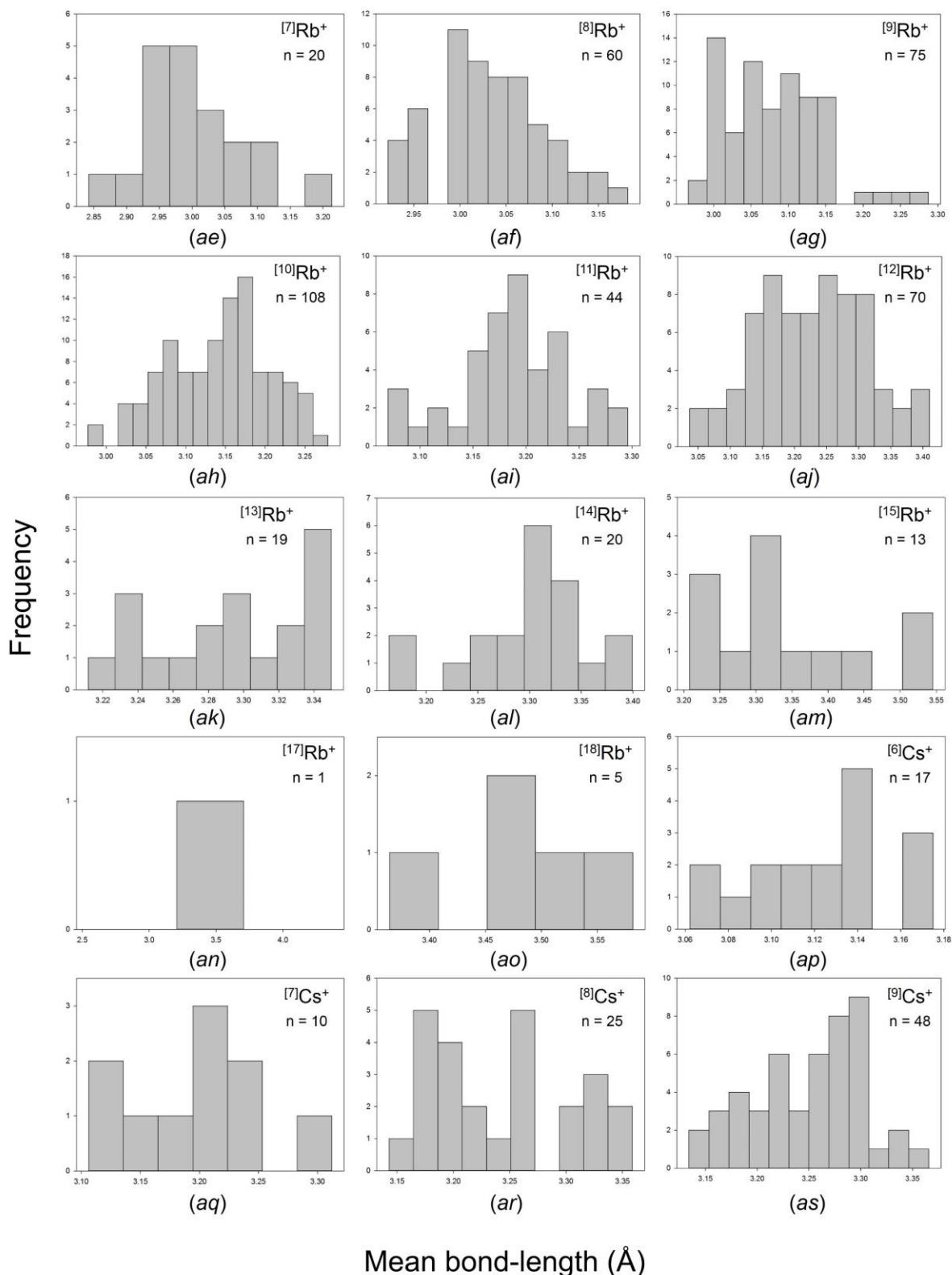


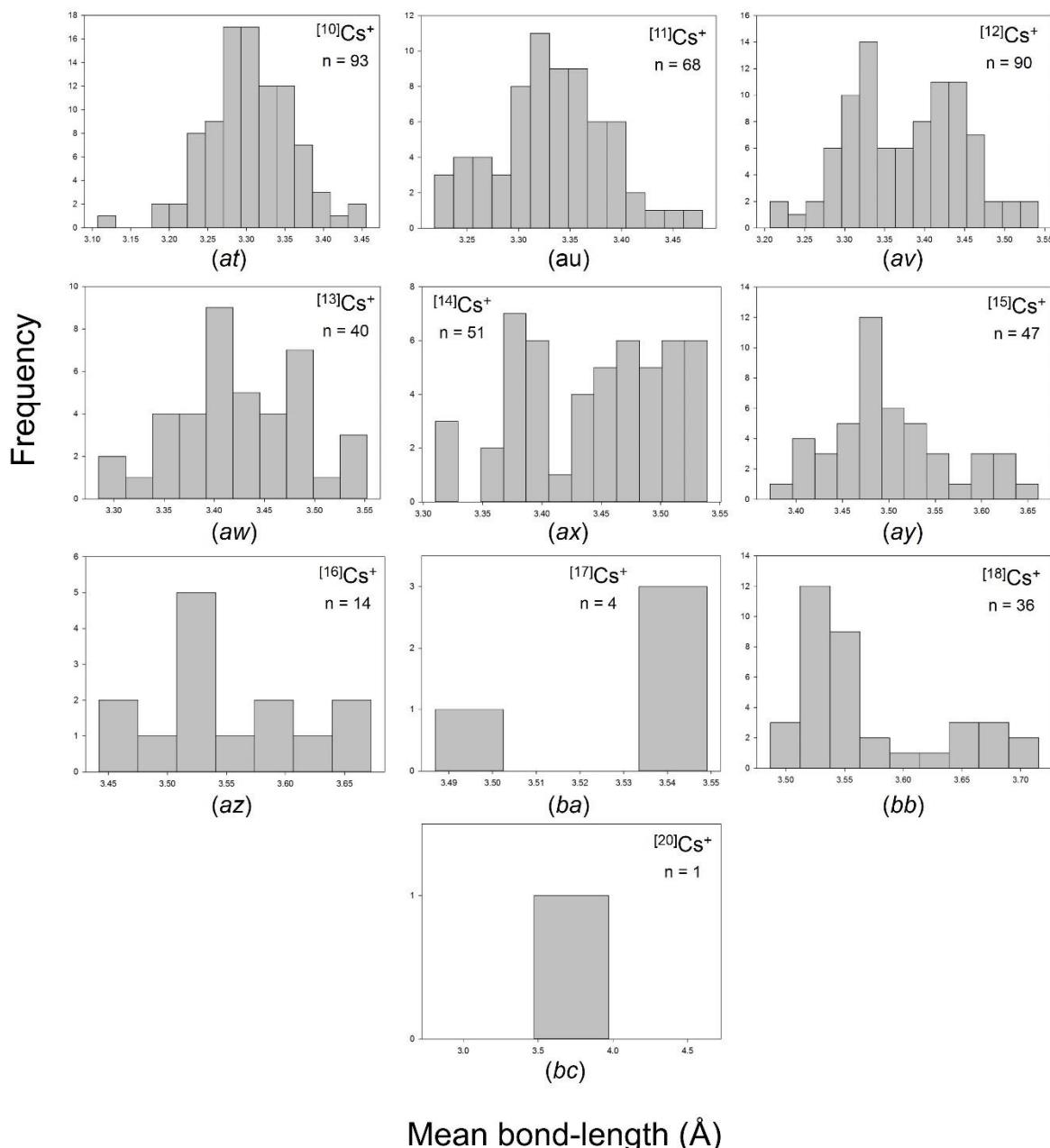
**Figure S2** Bond-length distributions for all configurations of the alkaline-earth-metal ions bonded to  $\text{O}^{2-}$ : (a)  ${}^{[3]}\text{Be}^{2+}$ , (b)  ${}^{[4]}\text{Be}^{2+}$ , (c)  ${}^{[4]}\text{Mg}^{2+}$ , (d)  ${}^{[5]}\text{Mg}^{2+}$ , (e)  ${}^{[6]}\text{Mg}^{2+}$ , (f)  ${}^{[8]}\text{Mg}^{2+}$ , (g)  ${}^{[6]}\text{Ca}^{2+}$ , (h)  ${}^{[7]}\text{Ca}^{2+}$ , (i)  ${}^{[8]}\text{Ca}^{2+}$ , (j)  ${}^{[9]}\text{Ca}^{2+}$ , (k)  ${}^{[10]}\text{Ca}^{2+}$ , (l)  ${}^{[11]}\text{Ca}^{2+}$ , (m)  ${}^{[12]}\text{Ca}^{2+}$ , (n)  ${}^{[6]}\text{Sr}^{2+}$ , (o)  ${}^{[7]}\text{Sr}^{2+}$ , (p)  ${}^{[8]}\text{Sr}^{2+}$ , (q)  ${}^{[9]}\text{Sr}^{2+}$ , (r)

$[^{10}]\text{Sr}^{2+}$ , (*s*)  $[^{11}]\text{Sr}^{2+}$ , (*t*)  $[^{12}]\text{Sr}^{2+}$ , (*u*)  $[^6]\text{Ba}^{2+}$ , (*v*)  $[^7]\text{Ba}^{2+}$ , (*w*)  $[^8]\text{Ba}^{2+}$ , (*x*)  $[^9]\text{Ba}^{2+}$ , (*y*)  $[^{10}]\text{Ba}^{2+}$ , (*z*)  $[^{11}]\text{Ba}^{2+}$ , (*aa*)  $[^{12}]\text{Ba}^{2+}$ , (*ab*)  $[^{13}]\text{Ba}^{2+}$ , (*ac*)  $[^{14}]\text{Ba}^{2+}$ .

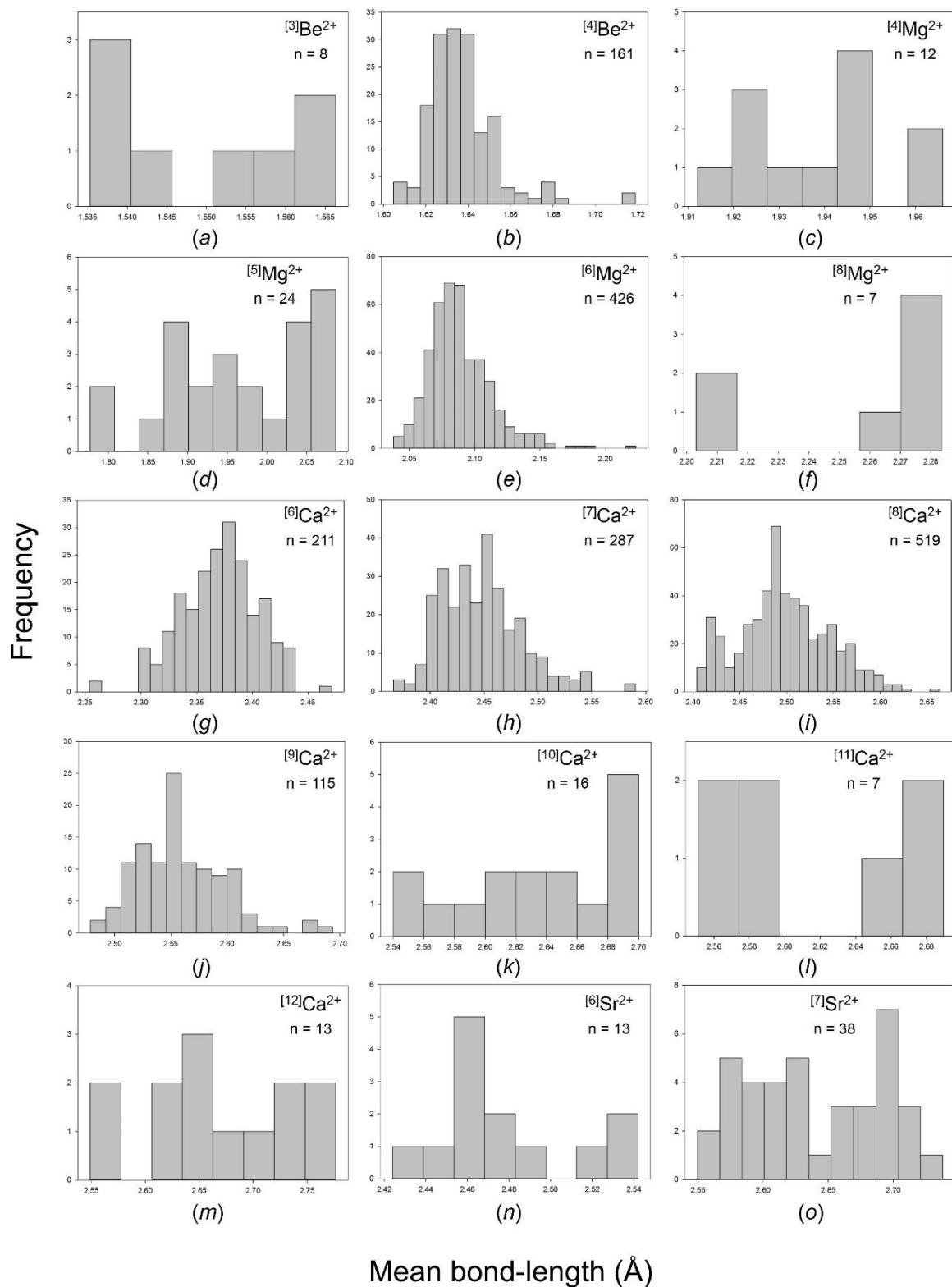


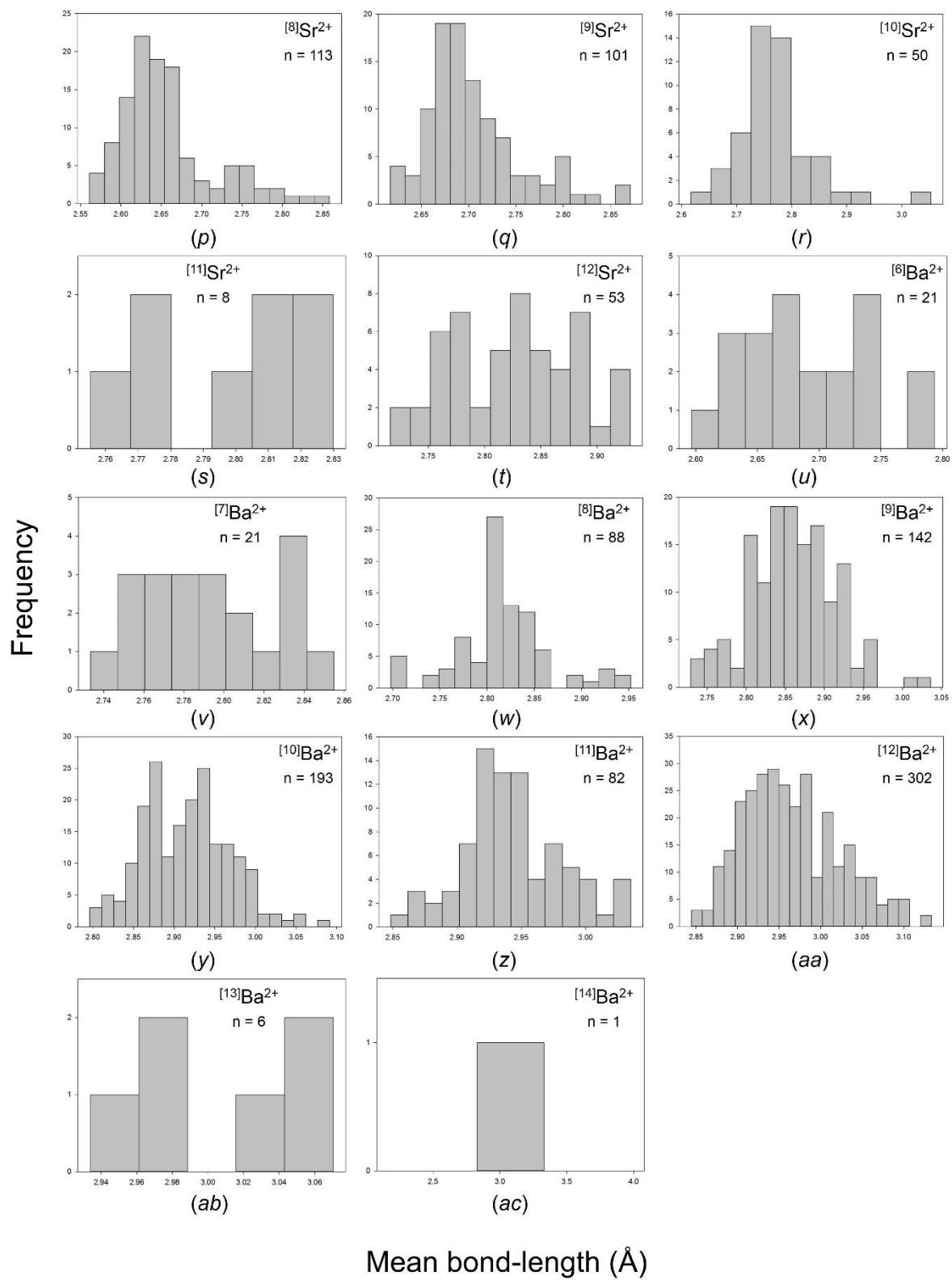




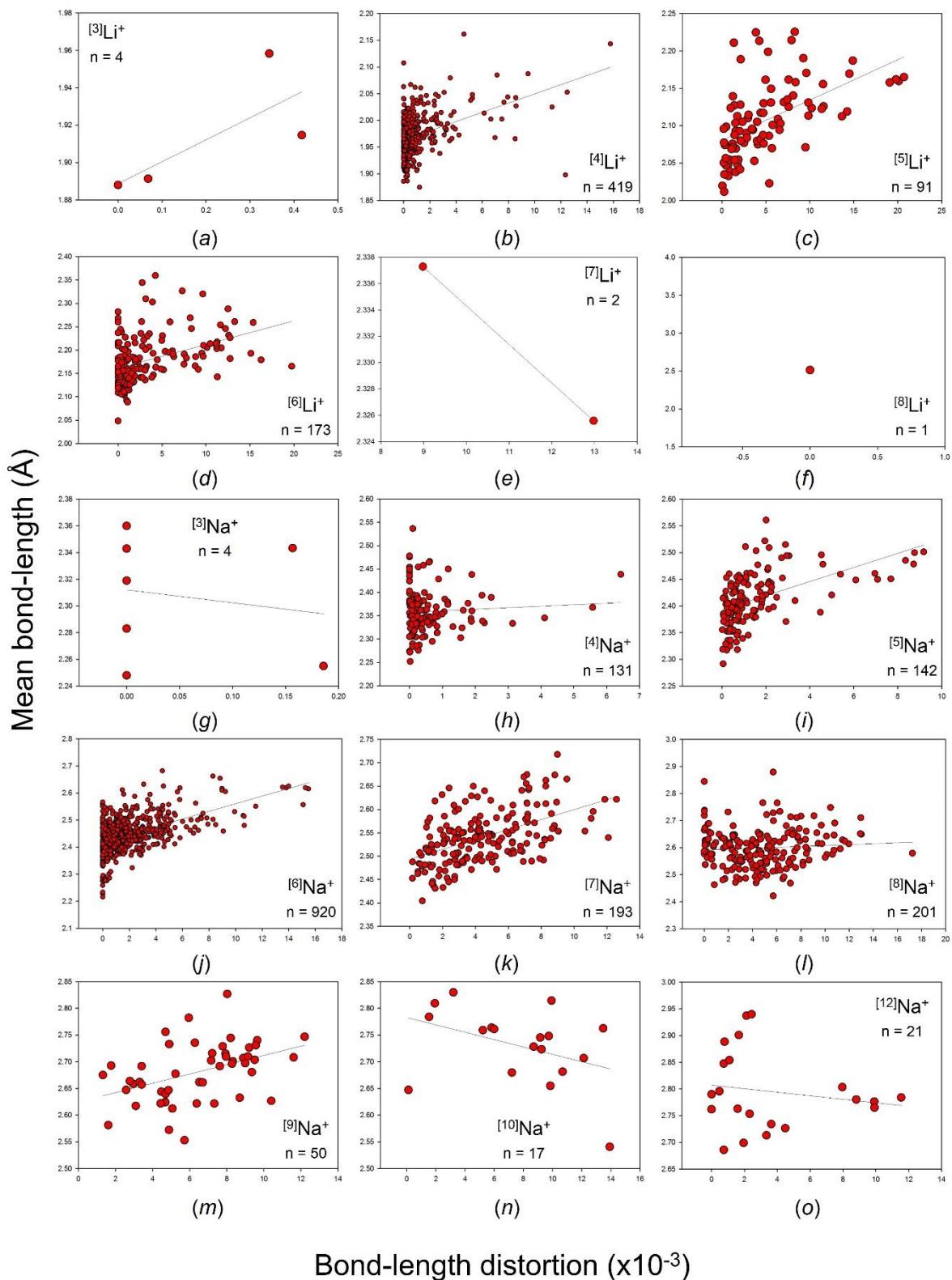


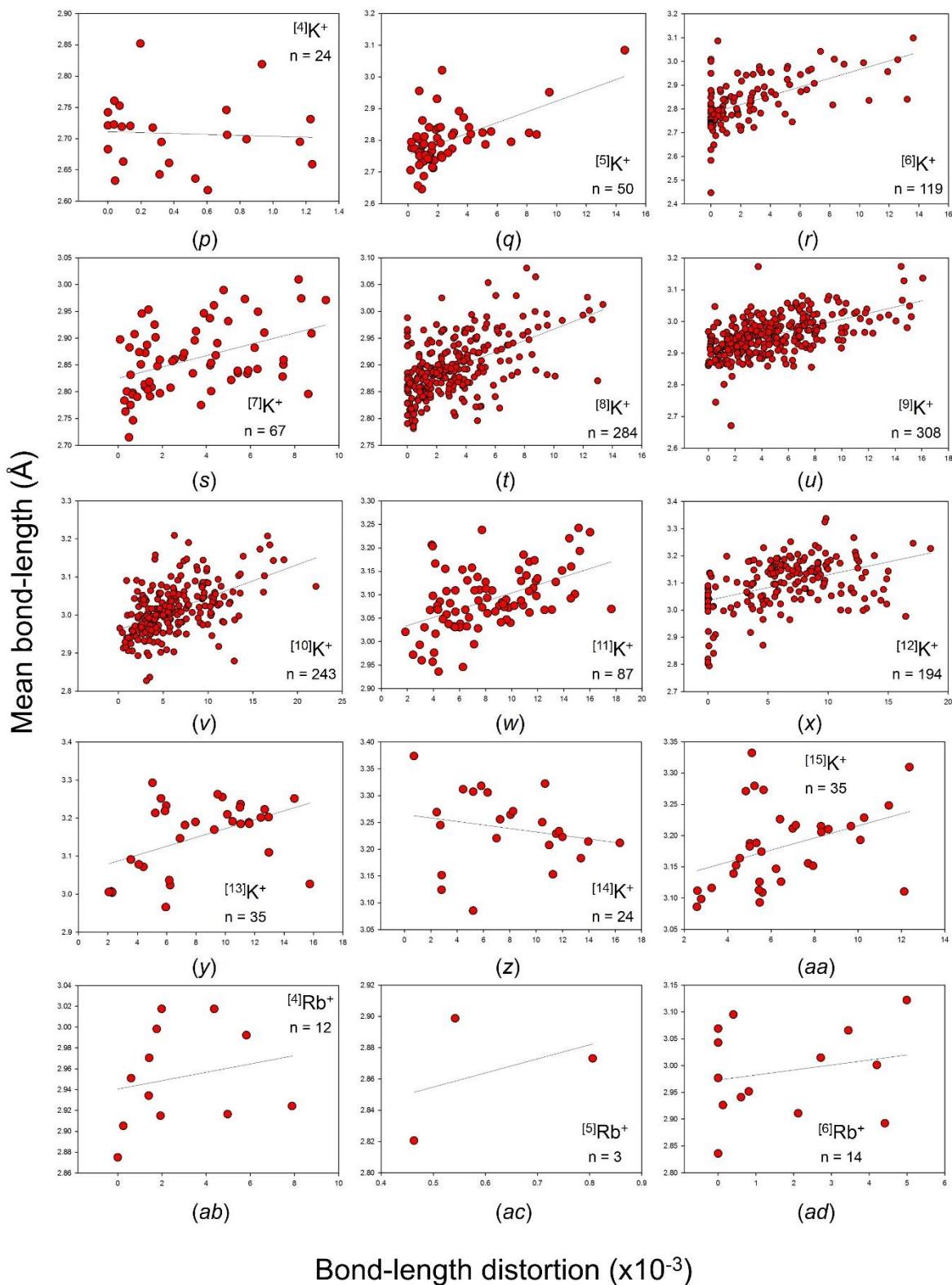
**Figure S3** Mean bond-length distributions for all configurations of the alkali-metal ions bonded to  $\text{O}_2^-$ : (a)  ${}^{[3]}\text{Li}^+$ , (b)  ${}^{[4]}\text{Li}^+$ , (c)  ${}^{[5]}\text{Li}^+$ , (d)  ${}^{[6]}\text{Li}^+$ , (e)  ${}^{[7]}\text{Li}^+$ , (f)  ${}^{[8]}\text{Li}^+$ , (g)  ${}^{[3]}\text{Na}^+$ , (h)  ${}^{[4]}\text{Na}^+$ , (i)  ${}^{[5]}\text{Na}^+$ , (j)  ${}^{[6]}\text{Na}^+$ , (k)  ${}^{[7]}\text{Na}^+$ , (l)  ${}^{[8]}\text{Na}^+$ , (m)  ${}^{[9]}\text{Na}^+$ , (n)  ${}^{[10]}\text{Na}^+$ , (o)  ${}^{[12]}\text{Na}^+$ , (p)  ${}^{[4]}\text{K}^+$ , (q)  ${}^{[5]}\text{K}^+$ , (r)  ${}^{[6]}\text{K}^+$ , (s)  ${}^{[7]}\text{K}^+$ , (t)  ${}^{[8]}\text{K}^+$ , (u)  ${}^{[9]}\text{K}^+$ , (v)  ${}^{[10]}\text{K}^+$ , (w)  ${}^{[11]}\text{K}^+$ , (x)  ${}^{[12]}\text{K}^+$ , (y)  ${}^{[13]}\text{K}^+$ , (z)  ${}^{[14]}\text{K}^+$ , (aa)  ${}^{[15]}\text{K}^+$ , (ab)  ${}^{[4]}\text{Rb}^+$ , (ac)  ${}^{[5]}\text{Rb}^+$ , (ad)  ${}^{[6]}\text{Rb}^+$ , (ae)  ${}^{[7]}\text{Rb}^+$ , (af)  ${}^{[8]}\text{Rb}^+$ , (ag)  ${}^{[9]}\text{Rb}^+$ , (ah)  ${}^{[10]}\text{Rb}^+$ , (ai)  ${}^{[11]}\text{Rb}^+$ , (aj)  ${}^{[12]}\text{Rb}^+$ , (ak)  ${}^{[13]}\text{Rb}^+$ , (al)  ${}^{[14]}\text{Rb}^+$ , (am)  ${}^{[15]}\text{Rb}^+$ , (an)  ${}^{[17]}\text{Rb}^+$ , (ao)  ${}^{[18]}\text{Rb}^+$ , (ap)  ${}^{[6]}\text{Cs}^+$ , (aq)  ${}^{[7]}\text{Cs}^+$ , (ar)  ${}^{[8]}\text{Cs}^+$ , (as)  ${}^{[9]}\text{Cs}^+$ , (at)  ${}^{[10]}\text{Cs}^+$ , (au)  ${}^{[11]}\text{Cs}^+$ , (av)  ${}^{[12]}\text{Cs}^+$ , (aw)  ${}^{[13]}\text{Cs}^+$ , (ax)  ${}^{[14]}\text{Cs}^+$ , (ay)  ${}^{[15]}\text{Cs}^+$ , (az)  ${}^{[16]}\text{Cs}^+$ , (ba)  ${}^{[17]}\text{Cs}^+$ , (bb)  ${}^{[18]}\text{Cs}^+$ , (bc)  ${}^{[20]}\text{Cs}^+$ .

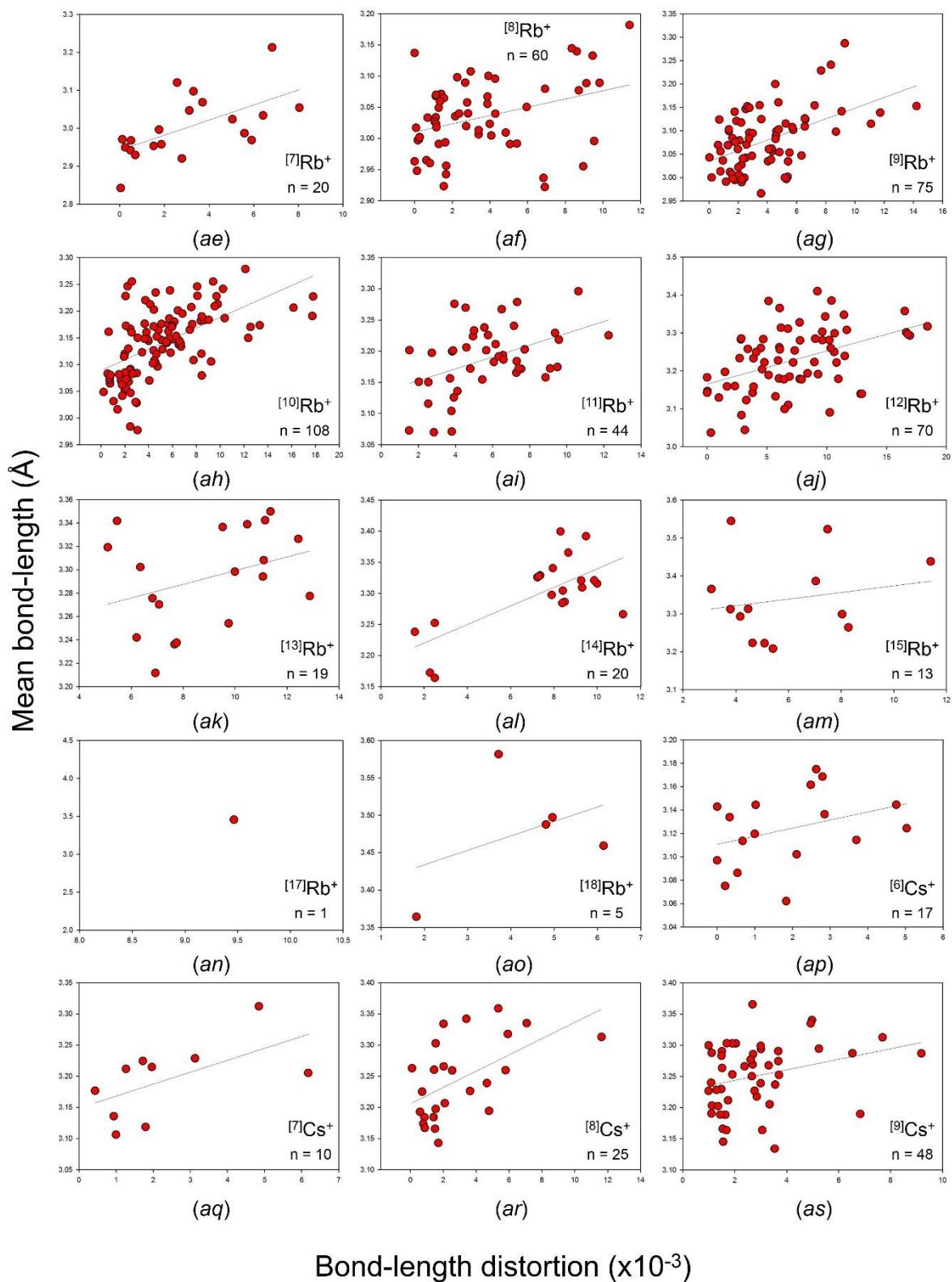


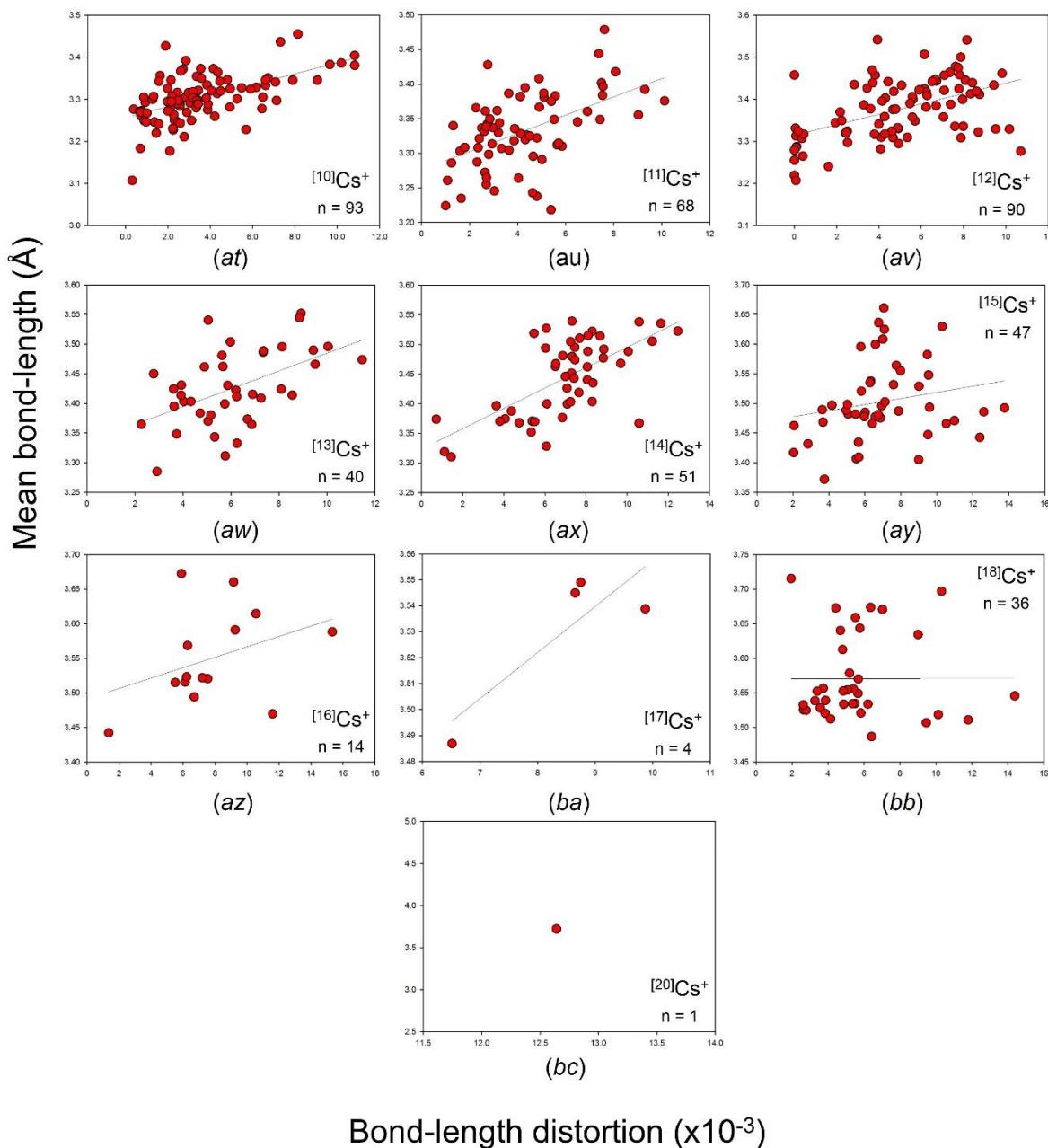


**Figure S4** Mean bond-length distributions for all configurations of the alkaline-earth-metal ions bonded to O<sup>2-</sup>: (a) <sup>[3]</sup>Be<sup>2+</sup>, (b) <sup>[4]</sup>Be<sup>2+</sup>, (c) <sup>[4]</sup>Mg<sup>2+</sup>, (d) <sup>[5]</sup>Mg<sup>2+</sup>, (e) <sup>[6]</sup>Mg<sup>2+</sup>, (f) <sup>[8]</sup>Mg<sup>2+</sup>, (g) <sup>[6]</sup>Ca<sup>2+</sup>, (h) <sup>[7]</sup>Ca<sup>2+</sup>, (i) <sup>[8]</sup>Ca<sup>2+</sup>, (j) <sup>[9]</sup>Ca<sup>2+</sup>, (k) <sup>[10]</sup>Ca<sup>2+</sup>, (l) <sup>[11]</sup>Ca<sup>2+</sup>, (m) <sup>[12]</sup>Ca<sup>2+</sup>, (n) <sup>[6]</sup>Sr<sup>2+</sup>, (o) <sup>[7]</sup>Sr<sup>2+</sup>, (p) <sup>[8]</sup>Sr<sup>2+</sup>, (q) <sup>[9]</sup>Sr<sup>2+</sup>, (r) <sup>[10]</sup>Sr<sup>2+</sup>, (s) <sup>[11]</sup>Sr<sup>2+</sup>, (t) <sup>[12]</sup>Sr<sup>2+</sup>, (u) <sup>[6]</sup>Ba<sup>2+</sup>, (v) <sup>[7]</sup>Ba<sup>2+</sup>, (w) <sup>[8]</sup>Ba<sup>2+</sup>, (x) <sup>[9]</sup>Ba<sup>2+</sup>, (y) <sup>[10]</sup>Ba<sup>2+</sup>, (z) <sup>[11]</sup>Ba<sup>2+</sup>, (aa) <sup>[12]</sup>Ba<sup>2+</sup>, (ab) <sup>[13]</sup>Ba<sup>2+</sup>, (ac) <sup>[14]</sup>Ba<sup>2+</sup>.

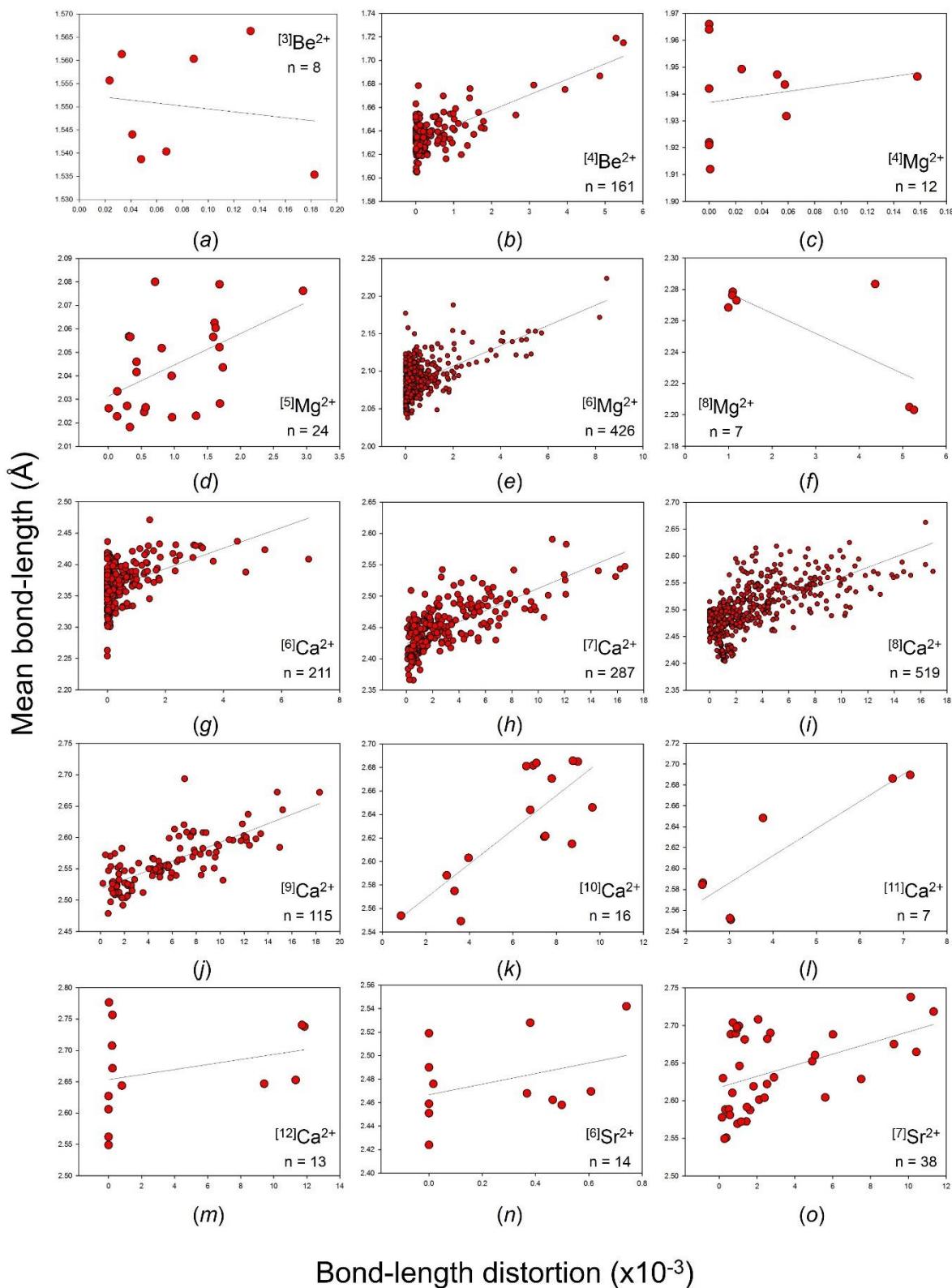


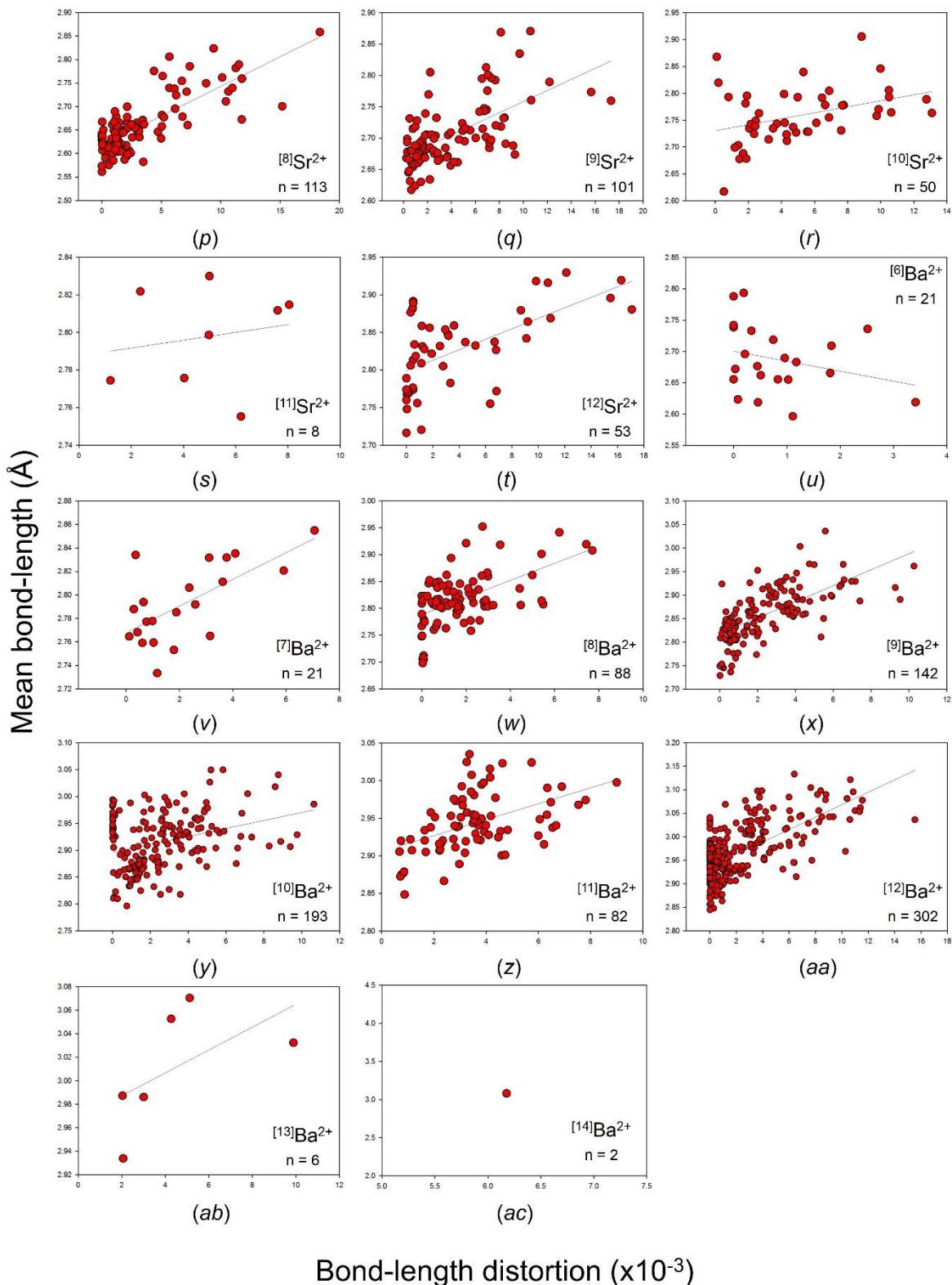






**Figure S5** The effect of bond-length distortion on mean bond-length for all configurations of the alkaline-earth-metal ions bonded to  $\text{O}^{2-}$ : (a)  ${}^{[3]}\text{Li}^+$ , (b)  ${}^{[4]}\text{Li}^+$ , (c)  ${}^{[5]}\text{Li}^+$ , (d)  ${}^{[6]}\text{Li}^+$ , (e)  ${}^{[7]}\text{Li}^+$ , (f)  ${}^{[8]}\text{Li}^+$ , (g)  ${}^{[3]}\text{Na}^+$ , (h)  ${}^{[4]}\text{Na}^+$ , (i)  ${}^{[5]}\text{Na}^+$ , (j)  ${}^{[6]}\text{Na}^+$ , (k)  ${}^{[7]}\text{Na}^+$ , (l)  ${}^{[8]}\text{Na}^+$ , (m)  ${}^{[9]}\text{Na}^+$ , (n)  ${}^{[10]}\text{Na}^+$ , (o)  ${}^{[12]}\text{Na}^+$ , (p)  ${}^{[4]}\text{K}^+$ , (q)  ${}^{[5]}\text{K}^+$ , (r)  ${}^{[6]}\text{K}^+$ , (s)  ${}^{[7]}\text{K}^+$ , (t)  ${}^{[8]}\text{K}^+$ , (u)  ${}^{[9]}\text{K}^+$ , (v)  ${}^{[10]}\text{K}^+$ , (w)  ${}^{[11]}\text{K}^+$ , (x)  ${}^{[12]}\text{K}^+$ , (y)  ${}^{[13]}\text{K}^+$ , (z)  ${}^{[14]}\text{K}^+$ , (aa)  ${}^{[15]}\text{K}^+$ , (ab)  ${}^{[4]}\text{Rb}^+$ , (ac)  ${}^{[5]}\text{Rb}^+$ , (ad)  ${}^{[6]}\text{Rb}^+$ , (ae)  ${}^{[7]}\text{Rb}^+$ , (af)  ${}^{[8]}\text{Rb}^+$ , (ag)  ${}^{[9]}\text{Rb}^+$ , (ah)  ${}^{[10]}\text{Rb}^+$ , (ai)  ${}^{[11]}\text{Rb}^+$ , (aj)  ${}^{[12]}\text{Rb}^+$ , (ak)  ${}^{[13]}\text{Rb}^+$ , (al)  ${}^{[14]}\text{Rb}^+$ , (am)  ${}^{[15]}\text{Rb}^+$ , (an)  ${}^{[17]}\text{Rb}^+$ , (ao)  ${}^{[18]}\text{Rb}^+$ , (ap)  ${}^{[6]}\text{Cs}^+$ , (aq)  ${}^{[7]}\text{Cs}^+$ , (ar)  ${}^{[8]}\text{Cs}^+$ , (as)  ${}^{[9]}\text{Cs}^+$ , (at)  ${}^{[10]}\text{Cs}^+$ , (au)  ${}^{[11]}\text{Cs}^+$ , (av)  ${}^{[12]}\text{Cs}^+$ , (aw)  ${}^{[13]}\text{Cs}^+$ , (ax)  ${}^{[14]}\text{Cs}^+$ , (ay)  ${}^{[15]}\text{Cs}^+$ , (az)  ${}^{[16]}\text{Cs}^+$ , (ba)  ${}^{[17]}\text{Cs}^+$ , (bb)  ${}^{[18]}\text{Cs}^+$ , (bc)  ${}^{[20]}\text{Cs}^+$ .





**Figure S6** The effect of bond-length distortion on mean bond-length for all configurations of the alkaline-earth-metal ions bonded to O<sup>2-</sup>: (a) <sup>[3]</sup>Be<sup>2+</sup>, (b) <sup>[4]</sup>Be<sup>2+</sup>, (c) <sup>[4]</sup>Mg<sup>2+</sup>, (d) <sup>[5]</sup>Mg<sup>2+</sup>, (e) <sup>[6]</sup>Mg<sup>2+</sup>, (f) <sup>[8]</sup>Mg<sup>2+</sup>, (g) <sup>[6]</sup>Ca<sup>2+</sup>, (h) <sup>[7]</sup>Ca<sup>2+</sup>, (i) <sup>[8]</sup>Ca<sup>2+</sup>, (j) <sup>[9]</sup>Ca<sup>2+</sup>, (k) <sup>[10]</sup>Ca<sup>2+</sup>, (l) <sup>[11]</sup>Ca<sup>2+</sup>, (m) <sup>[12]</sup>Ca<sup>2+</sup>, (n) <sup>[6]</sup>Sr<sup>2+</sup>, (o) <sup>[7]</sup>Sr<sup>2+</sup>, (p) <sup>[8]</sup>Sr<sup>2+</sup>, (q) <sup>[9]</sup>Sr<sup>2+</sup>, (r) <sup>[10]</sup>Sr<sup>2+</sup>, (s) <sup>[11]</sup>Sr<sup>2+</sup>, (t) <sup>[12]</sup>Sr<sup>2+</sup>, (u) <sup>[6]</sup>Ba<sup>2+</sup>, (v) <sup>[7]</sup>Ba<sup>2+</sup>, (w) <sup>[8]</sup>Ba<sup>2+</sup>, (x) <sup>[9]</sup>Ba<sup>2+</sup>, (y) <sup>[10]</sup>Ba<sup>2+</sup>, (z) <sup>[11]</sup>Ba<sup>2+</sup>, (aa) <sup>[12]</sup>Ba<sup>2+</sup>, (ab) <sup>[13]</sup>Ba<sup>2+</sup>, (ac) <sup>[14]</sup>Ba<sup>2+</sup>.