



STRUCTURAL SCIENCE  
CRYSTAL ENGINEERING  
MATERIALS

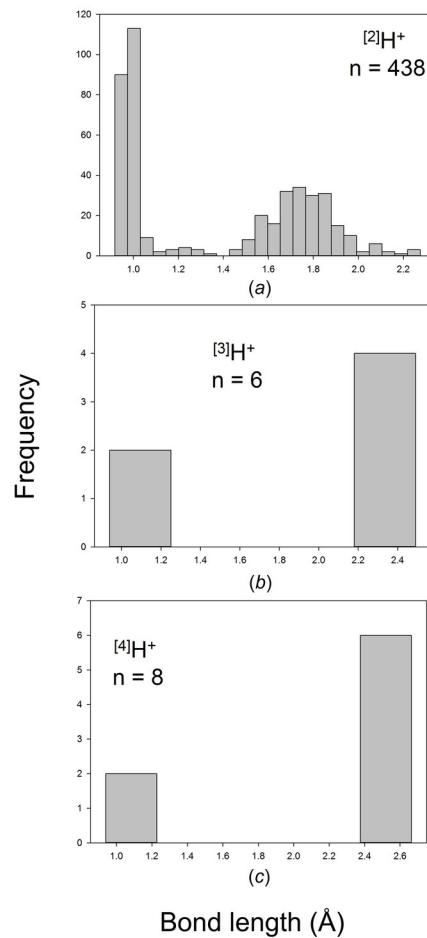
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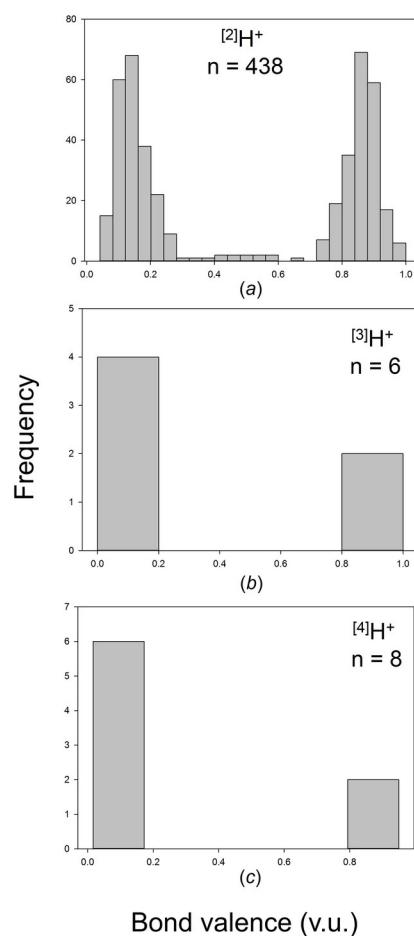
**Bond-length distributions for ions bonded to oxygen: results for the non-metals and discussion of lone-pair stereoactivity and the polymerization of PO<sub>4</sub>**

**Olivier Charles Gagné and Frank Christopher Hawthorne**

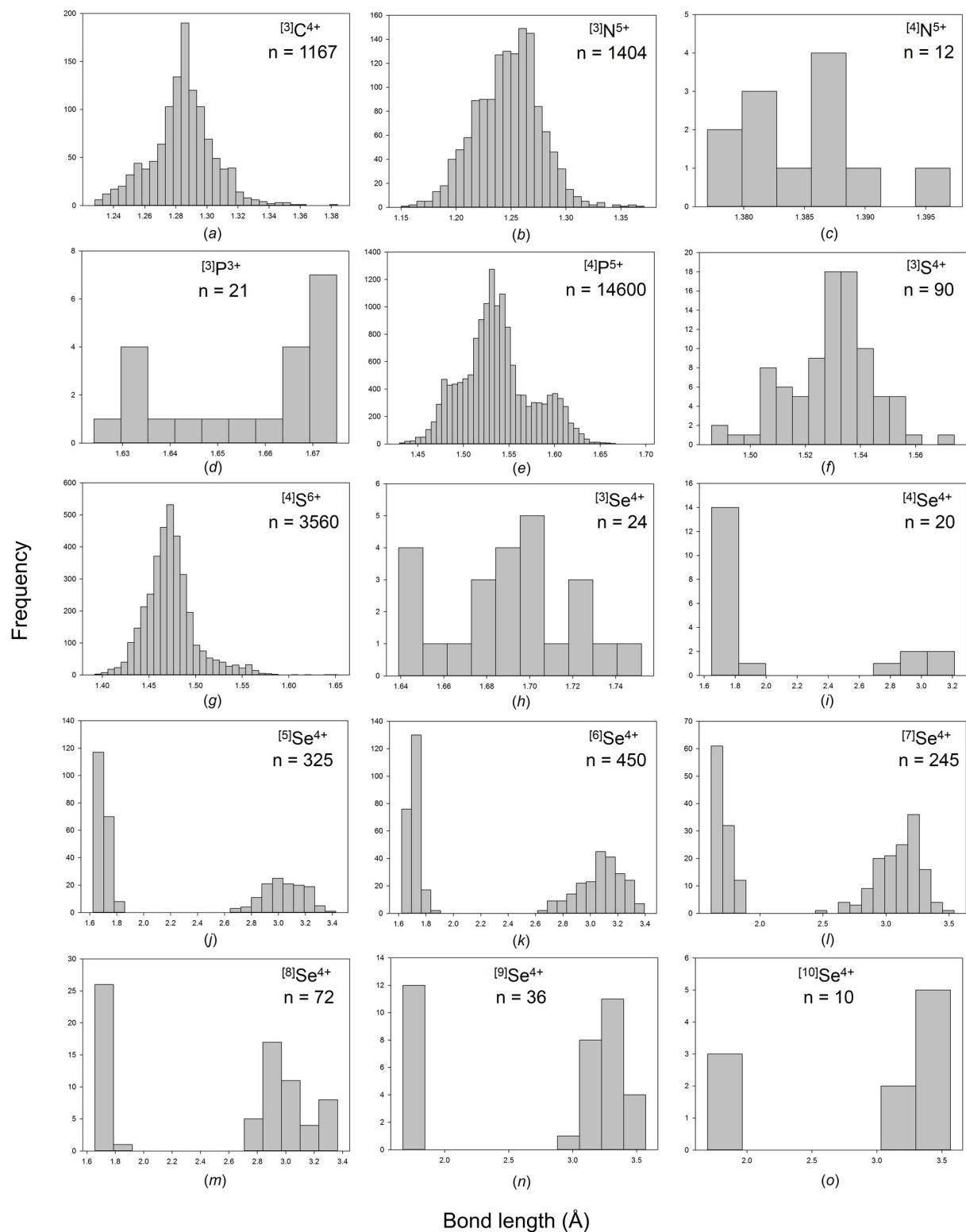
**Figure S1** Bond-length distributions for all configurations of the hydrogen ion bonded to O<sup>2-</sup>: (a) <sup>[2]</sup>H<sup>+</sup>, (b) <sup>[3]</sup>H<sup>+</sup>, (c) <sup>[4]</sup>H<sup>+</sup>.

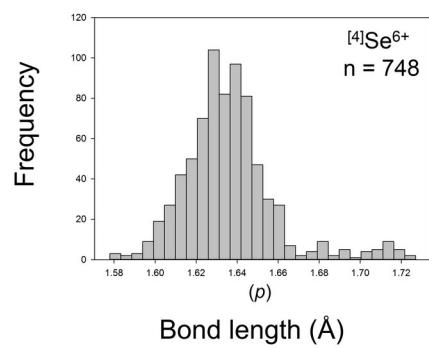


**Figure S2** Bond-valence distributions for all configurations of the hydrogen ion bonded to O<sup>2-</sup>: (a) <sup>[2]</sup>H<sup>+</sup>, (b) <sup>[3]</sup>H<sup>+</sup>, (c) <sup>[4]</sup>H<sup>+</sup>.

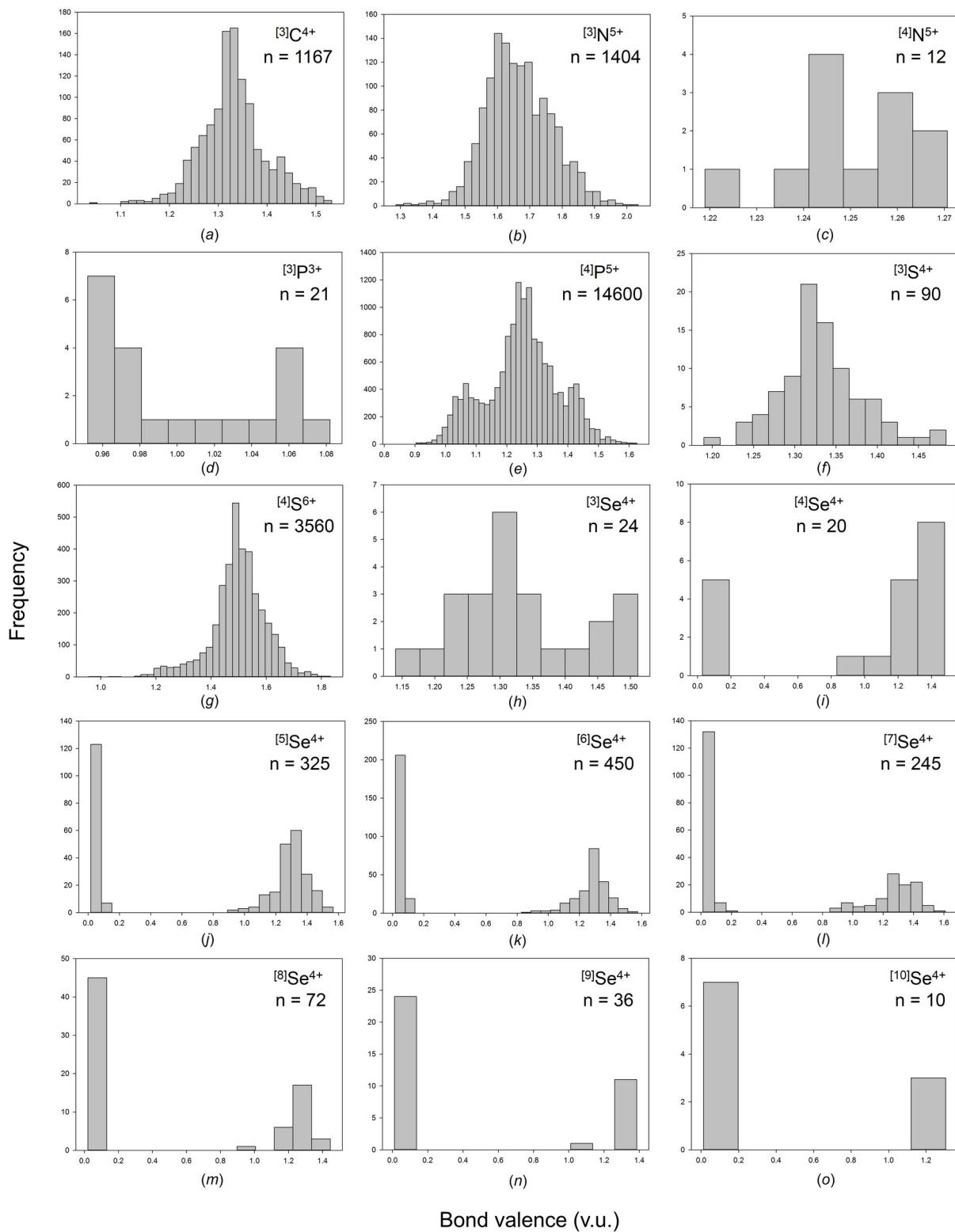


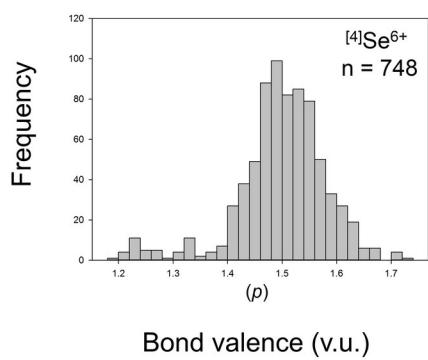
**Figure S3** Bond-length distributions for all configurations of the group 14-16 non-metal ions bonded to O<sup>2-</sup>: (a) <sup>[3]</sup>C<sup>4+</sup>, (b) <sup>[3]</sup>N<sup>5+</sup>, (c) <sup>[4]</sup>N<sup>5+</sup>, (d) <sup>[3]</sup>P<sup>3+</sup>, (e) <sup>[4]</sup>P<sup>5+</sup>, (f) <sup>[3]</sup>S<sup>4+</sup>, (g) <sup>[4]</sup>S<sup>6+</sup>, (h) <sup>[3]</sup>Se<sup>4+</sup>, (i) <sup>[4]</sup>Se<sup>4+</sup>, (j) <sup>[5]</sup>Se<sup>4+</sup>, (k) <sup>[6]</sup>Se<sup>4+</sup>, (l) <sup>[7]</sup>Se<sup>4+</sup>, (m) <sup>[8]</sup>Se<sup>4+</sup>, (n) <sup>[9]</sup>Se<sup>4+</sup>, (o) <sup>[10]</sup>Se<sup>4+</sup>, (p) <sup>[4]</sup>Se<sup>6+</sup>.



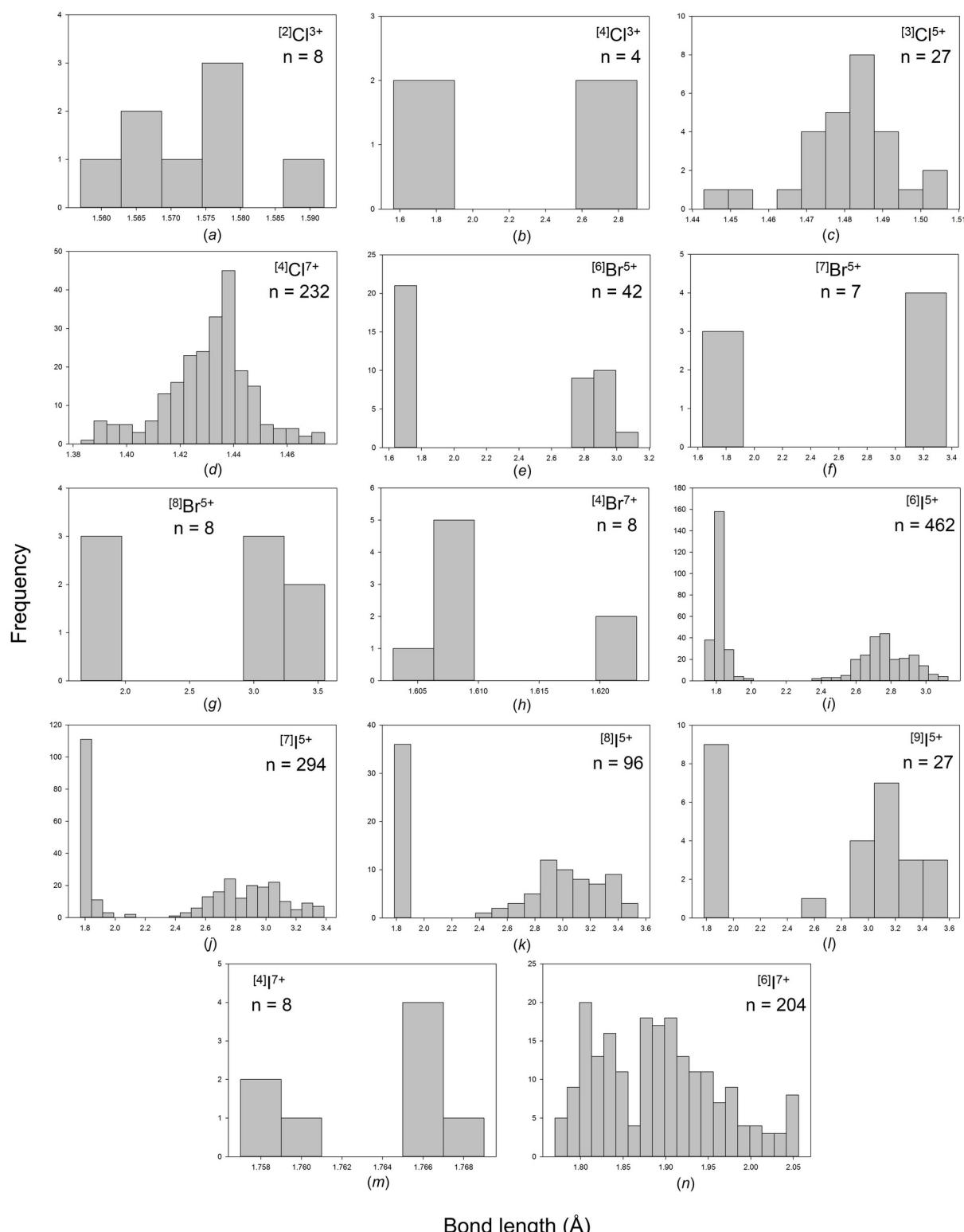


**Figure S4** Bond-valence distributions for all configurations of the group 14-16 non-metal ions bonded to O<sup>2-</sup>: (a) <sup>[3]</sup>C<sup>4+</sup>, (b) <sup>[3]</sup>N<sup>5+</sup>, (c) <sup>[4]</sup>N<sup>5+</sup>, (d) <sup>[3]</sup>P<sup>3+</sup>, (e) <sup>[4]</sup>P<sup>5+</sup>, (f) <sup>[3]</sup>S<sup>4+</sup>, (g) <sup>[4]</sup>S<sup>6+</sup>, (h) <sup>[3]</sup>Se<sup>4+</sup>, (i) <sup>[4]</sup>Se<sup>4+</sup>, (j) <sup>[5]</sup>Se<sup>4+</sup>, (k) <sup>[6]</sup>Se<sup>4+</sup>, (l) <sup>[7]</sup>Se<sup>4+</sup>, (m) <sup>[8]</sup>Se<sup>4+</sup>, (n) <sup>[9]</sup>Se<sup>4+</sup>, (o) <sup>[10]</sup>Se<sup>4+</sup>, (p) <sup>[4]</sup>Se<sup>6+</sup>.

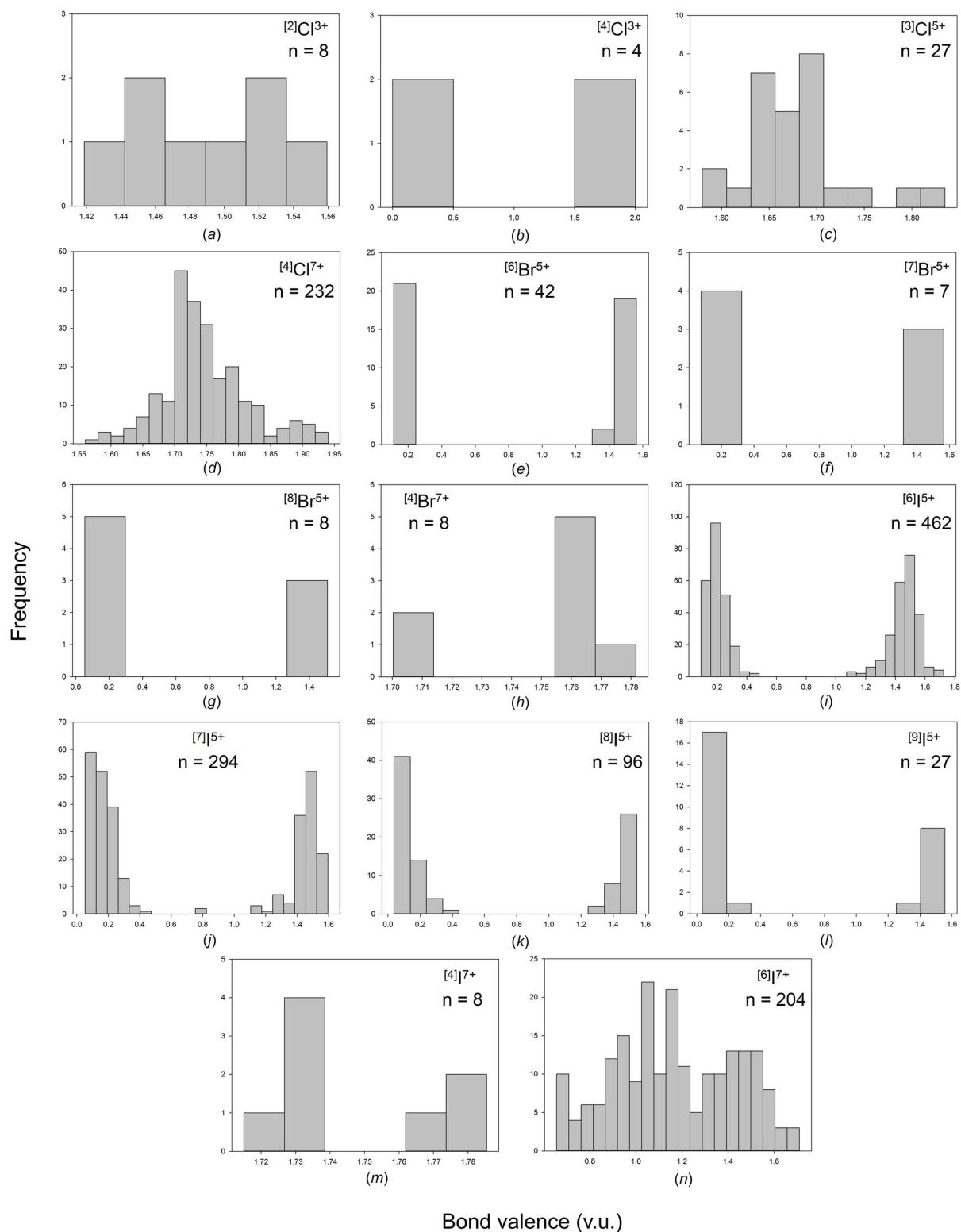




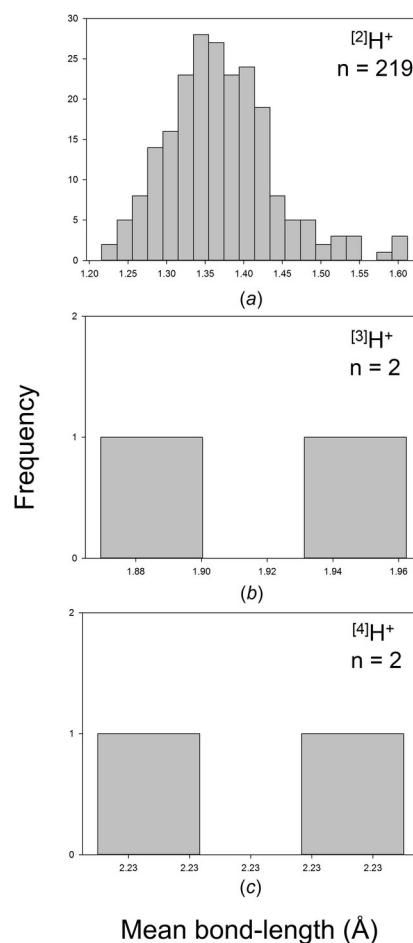
**Figure S5** Bond-length distributions for all configurations of the group 17 non-metal ions bonded to O<sup>2-</sup>: (a) <sup>[2]</sup>Cl<sup>3+</sup>, (b) <sup>[4]</sup>Cl<sup>3+</sup>, (c) <sup>[3]</sup>Cl<sup>5+</sup>, (d) <sup>[4]</sup>Cl<sup>7+</sup>, (e) <sup>[6]</sup>Br<sup>5+</sup>, (f) <sup>[7]</sup>Br<sup>5+</sup>, (g) <sup>[8]</sup>Br<sup>5+</sup>, (h) <sup>[4]</sup>Br<sup>7+</sup>, (i) <sup>[6]</sup>I<sup>5+</sup>, (j) <sup>[7]</sup>I<sup>5+</sup>, (k) <sup>[8]</sup>I<sup>5+</sup>, (l) <sup>[9]</sup>I<sup>5+</sup>, (m) <sup>[4]</sup>I<sup>7+</sup>, (n) <sup>[6]</sup>I<sup>7+</sup>.



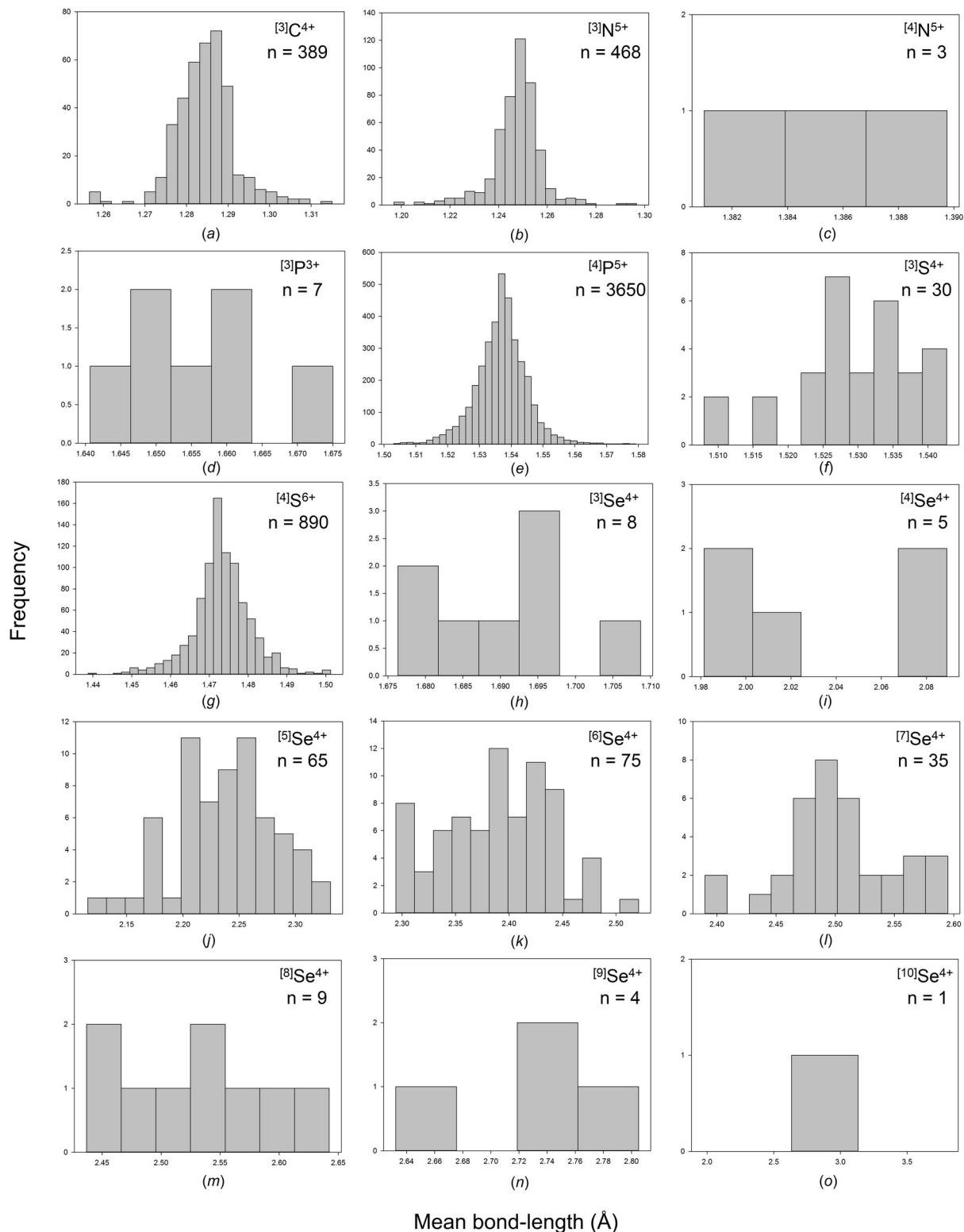
**Figure S6** Bond-valence distributions for all configurations of the group 17 non-metal ions bonded to O<sup>2-</sup>: (a) <sup>[2]</sup>Cl<sup>3+</sup>, (b) <sup>[4]</sup>Cl<sup>3+</sup>, (c) <sup>[3]</sup>Cl<sup>5+</sup>, (d) <sup>[4]</sup>Cl<sup>7+</sup>, (e) <sup>[6]</sup>Br<sup>5+</sup>, (f) <sup>[7]</sup>Br<sup>5+</sup>, (g) <sup>[8]</sup>Br<sup>5+</sup>, (h) <sup>[4]</sup>Br<sup>7+</sup>, (i) <sup>[6]</sup>I<sup>5+</sup>, (j) <sup>[7]</sup>I<sup>5+</sup>, (k) <sup>[8]</sup>I<sup>5+</sup>, (l) <sup>[9]</sup>I<sup>5+</sup>, (m) <sup>[4]</sup>I<sup>7+</sup>, (n) <sup>[6]</sup>I<sup>7+</sup>.

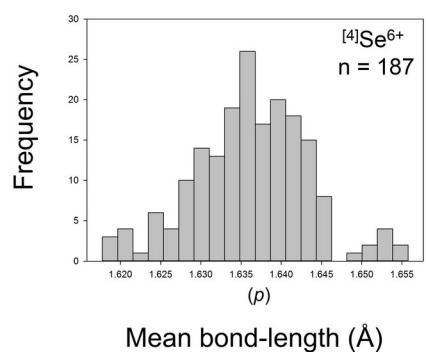


**Figure S7** Mean-bond-length distributions for all configurations of the hydrogen ion bonded to O<sup>2-</sup>:  
(a) <sup>[2]</sup>H<sup>+</sup>, (b) <sup>[3]</sup>H<sup>+</sup>, (c) <sup>[4]</sup>H<sup>+</sup>.

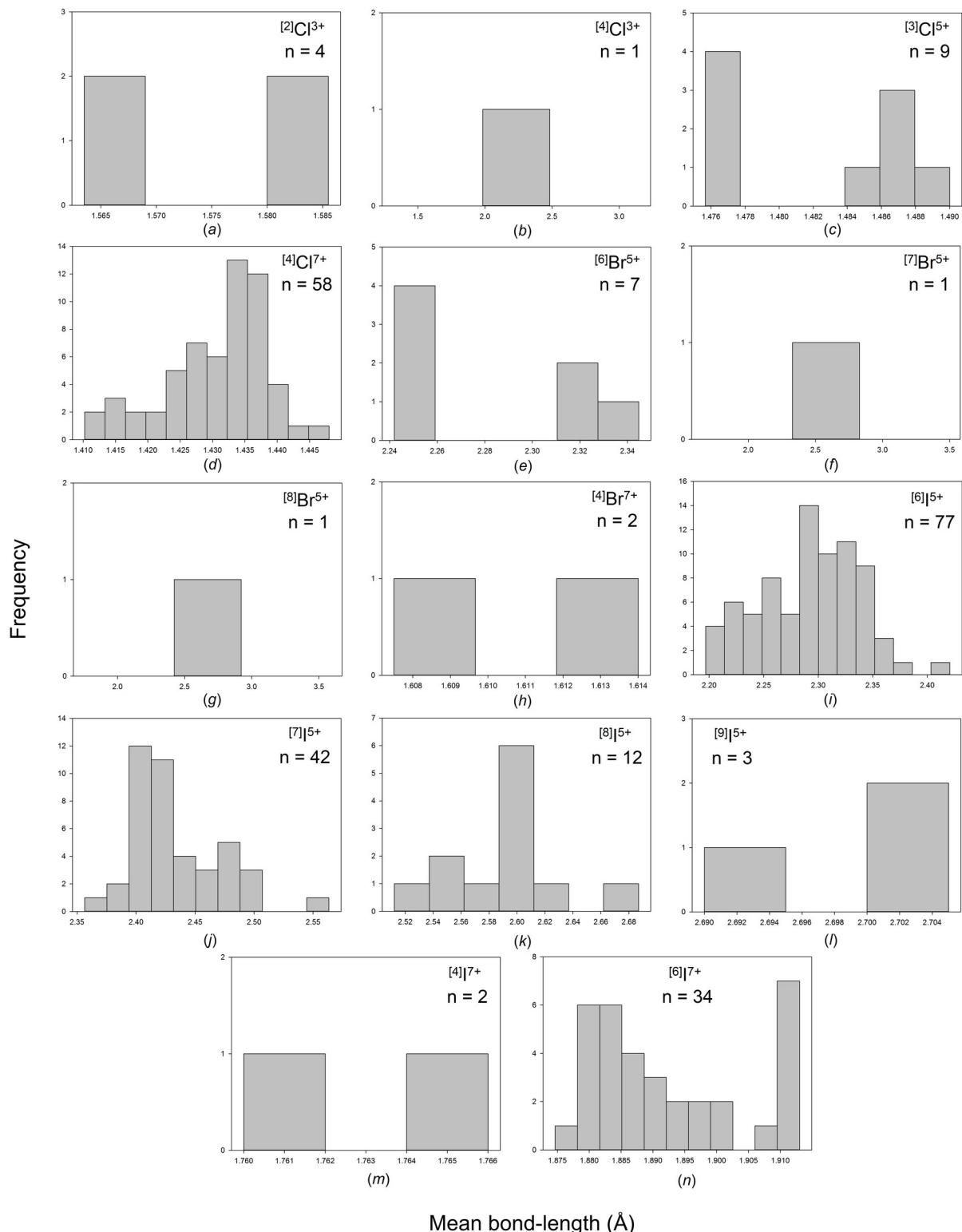


**Figure S8** Mean-bond-length distributions for all configurations of the group 14-16 non-metal ions bonded to O<sup>2-</sup>: (a) <sup>[3]</sup>C<sup>4+</sup>, (b) <sup>[3]</sup>N<sup>5+</sup>, (c) <sup>[4]</sup>N<sup>5+</sup>, (d) <sup>[3]</sup>P<sup>3+</sup>, (e) <sup>[4]</sup>P<sup>5+</sup>, (f) <sup>[3]</sup>S<sup>4+</sup>, (g) <sup>[4]</sup>S<sup>6+</sup>, (h) <sup>[3]</sup>Se<sup>4+</sup>, (i) <sup>[4]</sup>Se<sup>4+</sup>, (j) <sup>[5]</sup>Se<sup>4+</sup>, (k) <sup>[6]</sup>Se<sup>4+</sup>, (l) <sup>[7]</sup>Se<sup>4+</sup>, (m) <sup>[8]</sup>Se<sup>4+</sup>, (n) <sup>[9]</sup>Se<sup>4+</sup>, (o) <sup>[10]</sup>Se<sup>4+</sup>, (p) <sup>[4]</sup>Se<sup>6+</sup>.

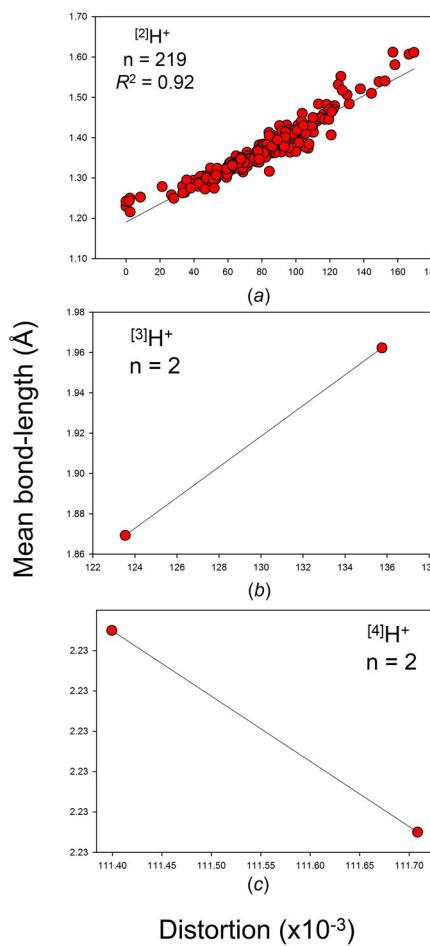




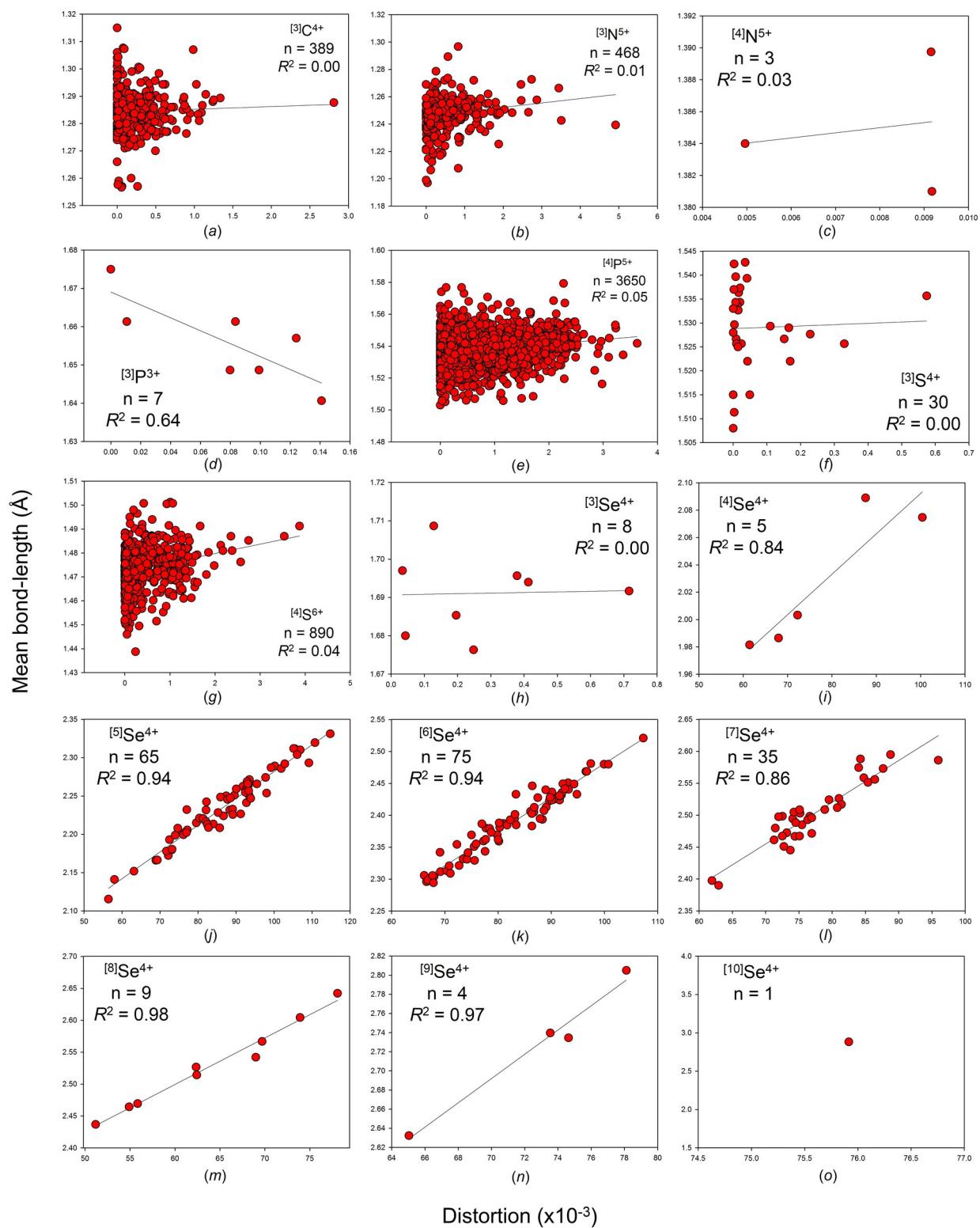
**Figure S9** Mean-bond-length distributions for all configurations of the group 17 non-metal ions bonded to O<sup>2-</sup>: (a) <sup>[2]</sup>Cl<sup>3+</sup>, (b) <sup>[4]</sup>Cl<sup>3+</sup>, (c) <sup>[3]</sup>Cl<sup>5+</sup>, (d) <sup>[4]</sup>Cl<sup>7+</sup>, (e) <sup>[6]</sup>Br<sup>5+</sup>, (f) <sup>[7]</sup>Br<sup>5+</sup>, (g) <sup>[8]</sup>Br<sup>5+</sup>, (h) <sup>[4]</sup>Br<sup>7+</sup>, (i) <sup>[6]</sup>I<sup>5+</sup>, (j) <sup>[7]</sup>I<sup>5+</sup>, (k) <sup>[8]</sup>I<sup>5+</sup>, (l) <sup>[9]</sup>I<sup>5+</sup>, (m) <sup>[4]</sup>I<sup>7+</sup>, (n) <sup>[6]</sup>I<sup>7+</sup>.

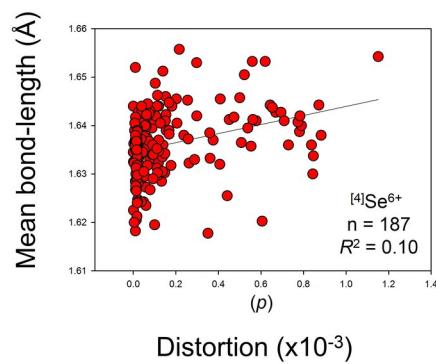


**Figure S10** The effect of bond-length distortion on mean bond-length for all configurations of the hydrogen ion bonded to O<sup>2-</sup>: (a) <sup>[2]</sup>H<sup>+</sup>, (b) <sup>[3]</sup>H<sup>+</sup>, (c) <sup>[4]</sup>H<sup>+</sup>.



**Figure S11** The effect of bond-length distortion on mean bond-length for all configurations of the group 14-16 non-metal ions bonded to O<sup>2-</sup>: (a) <sup>[3]</sup>C<sup>4+</sup>, (b) <sup>[3]</sup>N<sup>5+</sup>, (c) <sup>[4]</sup>N<sup>5+</sup>, (d) <sup>[3]</sup>P<sup>3+</sup>, (e) <sup>[4]</sup>P<sup>5+</sup>, (f) <sup>[3]</sup>S<sup>4+</sup>, (g) <sup>[4]</sup>S<sup>6+</sup>, (h) <sup>[3]</sup>Se<sup>4+</sup>, (i) <sup>[4]</sup>Se<sup>4+</sup>, (j) <sup>[5]</sup>Se<sup>4+</sup>, (k) <sup>[6]</sup>Se<sup>4+</sup>, (l) <sup>[7]</sup>Se<sup>4+</sup>, (m) <sup>[8]</sup>Se<sup>4+</sup>, (n) <sup>[9]</sup>Se<sup>4+</sup>, (o) <sup>[10]</sup>Se<sup>4+</sup>, (p) <sup>[4]</sup>Se<sup>6+</sup>.





**Figure S12** The effect of bond-length distortion on mean bond-length for all configurations of the group 17 non-metal ions bonded to O<sup>2-</sup>: (a) <sup>[2]</sup>Cl<sup>3+</sup>, (b) <sup>[4]</sup>Cl<sup>3+</sup>, (c) <sup>[3]</sup>Cl<sup>5+</sup>, (d) <sup>[4]</sup>Cl<sup>7+</sup>, (e) <sup>[6]</sup>Br<sup>5+</sup>, (f) <sup>[7]</sup>Br<sup>5+</sup>, (g) <sup>[8]</sup>Br<sup>5+</sup>, (h) <sup>[4]</sup>Br<sup>7+</sup>, (i) <sup>[6]</sup>I<sup>5+</sup>, (j) <sup>[7]</sup>I<sup>5+</sup>, (k) <sup>[8]</sup>I<sup>5+</sup>, (l) <sup>[9]</sup>I<sup>5+</sup>, (m) <sup>[4]</sup>I<sup>7+</sup>, (n) <sup>[6]</sup>I<sup>7+</sup>.

