

## 9. BASIC STRUCTURAL FEATURES

Table 9.4.1.1. Atomic distances between halogens and main-group elements (cont.)

| Atom pair                         | <i>N</i> | Mean  | s.u. | <i>d</i> <sub>1</sub> | Smallest 5% | First quartile | Median | Third quartile | <i>d</i> <sub>2</sub> |
|-----------------------------------|----------|-------|------|-----------------------|-------------|----------------|--------|----------------|-----------------------|
| Ge <sup>4+</sup> —F <sup>-</sup>  | 20       | 176.7 | 3.9  | 150.0                 | 168.0       | 176.0          | 177.1  | 178.4          | 210.0                 |
| Sn <sup>4+</sup> —F <sup>-</sup>  | 24       | 195.8 | 6.4  | 0.0                   | 184.4       | 194.6          | 196.3  | 198.0          | 500.0                 |
| Pb <sup>4+</sup> —F <sup>-</sup>  | 9        | 209.7 | 7.2  | 0.0                   | 196.9       | 206.5          | 210.5  | 212.8          | 500.0                 |
| C <sup>4+</sup> —Cl <sup>-</sup>  | 6        | 163.0 | 21.8 | 120.0                 | 120.6       | 157.0          | 174.0  | 175.5          | 200.0                 |
| Sn <sup>4+</sup> —Cl <sup>-</sup> | 46       | 238.7 | 5.7  | 0.0                   | 230.1       | 235.0          | 240.4  | 242.7          | 500.0                 |
| Pb <sup>4+</sup> —Cl <sup>-</sup> | 9        | 249.0 | 2.0  | 0.0                   | 244.9       | 248.4          | 249.0  | 249.6          | 500.0                 |
| Sn <sup>4+</sup> —Br <sup>-</sup> | 5        | 251.0 | 9.7  | 0.0                   | 236.5       | 244.5          | 255.0  | 258.8          | 500.0                 |
| Ge <sup>4+</sup> —I <sup>-</sup>  | 3        | 254.3 | 4.6  | 0.0                   | 248.3       | 249.5          | 256.5  | 257.2          | 500.0                 |
| Sn <sup>4+</sup> —I <sup>-</sup>  | 10       | 263.4 | 20.9 | 0.0                   | 209.0       | 263.5          | 265.0  | 269.0          | 500.0                 |
| Pb <sup>4+</sup> —I <sup>-</sup>  | 2        | 310.0 | 1.4  | 0.0                   | 308.2       | 309.0          | 310.0  | 311.0          | 500.0                 |
| P <sup>5+</sup> —F <sup>-</sup>   | 40       | 155.6 | 6.4  | 130.0                 | 144.0       | 151.3          | 156.8  | 159.3          | 200.0                 |
| As <sup>5+</sup> —F <sup>-</sup>  | 89       | 164.6 | 6.7  | 130.0                 | 155.4       | 160.9          | 165.5  | 168.4          | 200.0                 |
| Sb <sup>5+</sup> —F <sup>-</sup>  | 81       | 182.6 | 6.5  | 150.0                 | 174.1       | 179.2          | 182.7  | 184.7          | 230.0                 |
| Bi <sup>5+</sup> —F <sup>-</sup>  | 9        | 192.1 | 11.3 | 0.0                   | 178.4       | 188.2          | 189.7  | 195.5          | 500.0                 |
| P <sup>5+</sup> —Cl <sup>-</sup>  | 52       | 193.2 | 3.6  | 170.0                 | 187.2       | 190.6          | 193.3  | 195.4          | 210.0                 |
| Sb <sup>5+</sup> —Cl <sup>-</sup> | 66       | 233.1 | 6.6  | 200.0                 | 220.6       | 229.8          | 233.8  | 236.4          | 270.0                 |
| P <sup>5+</sup> —Br <sup>-</sup>  | 12       | 211.2 | 5.1  | 0.0                   | 201.2       | 208.0          | 213.0  | 214.7          | 500.0                 |
| Sb <sup>5+</sup> —Br <sup>-</sup> | 6        | 254.0 | 2.1  | 250.0                 | 250.6       | 252.5          | 254.0  | 255.5          | 270.0                 |
| S <sup>6+</sup> —F <sup>-</sup>   | 25       | 151.1 | 4.2  | 140.0                 | 141.2       | 150.1          | 152.1  | 153.7          | 160.0                 |
| Te <sup>6+</sup> —F <sup>-</sup>  | 9        | 176.1 | 6.9  | 0.0                   | 160.9       | 174.5          | 179.0  | 180.5          | 500.0                 |
| S <sup>6+</sup> —Cl <sup>-</sup>  | 10       | 197.6 | 5.7  | 170.0                 | 185.0       | 195.5          | 197.3  | 201.0          | 220.0                 |
| I <sup>7+</sup> —F <sup>-</sup>   | 6        | 179.7 | 4.7  | 0.0                   | 170.6       | 179.0          | 180.7  | 181.7          | 500.0                 |

Table 9.4.1.2. Atomic distances between halogens and main-group elements in their special oxidation states

| Atom pair                         | <i>N</i> | Mean  | s.u. | <i>d</i> <sub>1</sub> | Smallest 5% | First quartile | Median | Third quartile | <i>d</i> <sub>2</sub> |
|-----------------------------------|----------|-------|------|-----------------------|-------------|----------------|--------|----------------|-----------------------|
| Tl <sup>1+</sup> —F <sup>-</sup>  | 36       | 282.6 | 19.0 | 250.0                 | 259.8       | 267.1          | 273.0  | 297.3          | 350.0                 |
| Tl <sup>1+</sup> —Cl <sup>-</sup> | 38       | 326.2 | 19.0 | 0.0                   | 291.8       | 316.3          | 326.0  | 339.0          | 500.0                 |
| Tl <sup>1+</sup> —Br <sup>-</sup> | 17       | 335.0 | 9.1  | 0.0                   | 309.7       | 332.5          | 336.5  | 341.8          | 500.0                 |
| Tl <sup>1+</sup> —I <sup>-</sup>  | 28       | 347.6 | 9.4  | 0.0                   | 333.4       | 340.0          | 346.7  | 356.0          | 500.0                 |
| C <sup>2+</sup> —F <sup>-</sup>   | 17       | 131.2 | 2.4  | 110.0                 | 126.8       | 130.1          | 131.3  | 132.7          | 160.0                 |
| Sn <sup>2+</sup> —F <sup>-</sup>  | 38       | 205.6 | 8.8  | 170.0                 | 189.8       | 200.2          | 205.7  | 209.4          | 250.0                 |
| Pb <sup>2+</sup> —F <sup>-</sup>  | 49       | 247.5 | 10.3 | 160.0                 | 227.4       | 239.5          | 250.5  | 256.5          | 290.0                 |
| Ge <sup>2+</sup> —Cl <sup>-</sup> | 7        | 227.3 | 10.4 | 0.0                   | 210.7       | 215.5          | 231.0  | 235.2          | 500.0                 |
| Sn <sup>2+</sup> —Cl <sup>-</sup> | 26       | 253.3 | 9.0  | 220.0                 | 236.6       | 250.2          | 253.0  | 257.8          | 290.0                 |
| Pb <sup>2+</sup> —Cl <sup>-</sup> | 69       | 297.9 | 19.2 | 0.0                   | 274.5       | 285.2          | 293.5  | 311.9          | 500.0                 |
| Sn <sup>2+</sup> —Br <sup>-</sup> | 12       | 287.8 | 28.4 | 0.0                   | 253.2       | 264.0          | 280.0  | 314.0          | 500.0                 |
| Pb <sup>2+</sup> —Br <sup>-</sup> | 31       | 296.0 | 14.0 | 250.0                 | 275.1       | 288.4          | 294.8  | 302.2          | 350.0                 |
| Ge <sup>2+</sup> —I <sup>-</sup>  | 3        | 283.0 | 8.0  | 260.0                 | 274.3       | 275.5          | 283.0  | 290.5          | 310.0                 |
| Sn <sup>2+</sup> —I <sup>-</sup>  | 17       | 316.4 | 17.6 | 0.0                   | 295.7       | 303.6          | 307.5  | 330.8          | 500.0                 |
| Pb <sup>2+</sup> —I <sup>-</sup>  | 32       | 322.7 | 18.4 | 270.0                 | 296.6       | 316.0          | 320.0  | 338.0          | 380.0                 |
| N <sup>3-</sup> —F <sup>-</sup>   | 218      | 275.1 | 23.6 | 170.0                 | 233.8       | 266.2          | 278.1  | 289.9          | 350.0                 |
| N <sup>2-</sup> —F <sup>-</sup>   | 26       | 270.2 | 29.6 | 0.0                   | 212.6       | 260.5          | 268.0  | 277.0          | 500.0                 |
| P <sup>3+</sup> —F <sup>-</sup>   | 7        | 153.6 | 3.8  | 140.0                 | 148.4       | 149.8          | 153.5  | 156.5          | 170.0                 |
| As <sup>3+</sup> —F <sup>-</sup>  | 6        | 165.0 | 5.1  | 150.0                 | 156.6       | 162.5          | 164.0  | 169.0          | 200.0                 |
| Sb <sup>3+</sup> —F <sup>-</sup>  | 73       | 193.4 | 5.5  | 170.0                 | 186.6       | 190.9          | 192.7  | 194.5          | 240.0                 |
| Bi <sup>3+</sup> —F <sup>-</sup>  | 21       | 235.7 | 18.8 | 0.0                   | 218.1       | 222.1          | 226.5  | 253.5          | 500.0                 |

## 9.4. TYPICAL INTERATOMIC DISTANCES: INORGANIC COMPOUNDS

Table 9.4.1.2. *Atomic distances between halogens and main-group elements (cont.)*

| Atom pair                         | <i>N</i> | Mean  | s.u. | <i>d</i> <sub>1</sub> | Smallest 5% | First quartile | Median | Third quartile | <i>d</i> <sub>2</sub> |
|-----------------------------------|----------|-------|------|-----------------------|-------------|----------------|--------|----------------|-----------------------|
| N <sup>3-</sup> —Cl <sup>-</sup>  | 349      | 323.0 | 24.4 | 250.0                 | 279.6       | 311.1          | 325.0  | 335.2          | 410.0                 |
| N <sup>2-</sup> —Cl <sup>-</sup>  | 28       | 305.9 | 18.4 | 250.0                 | 274.8       | 290.0          | 306.0  | 319.5          | 350.0                 |
| As <sup>3+</sup> —Cl <sup>-</sup> | 7        | 211.6 | 7.5  | 200.0                 | 202.7       | 205.5          | 209.5  | 216.5          | 250.0                 |
| Sb <sup>3+</sup> —Cl <sup>-</sup> | 36       | 272.1 | 43.6 | 0.0                   | 205.6       | 235.3          | 262.0  | 306.0          | 500.0                 |
| Bi <sup>3+</sup> —Cl <sup>-</sup> | 39       | 292.8 | 34.0 | 0.0                   | 246.9       | 265.5          | 304.2  | 318.5          | 500.0                 |
| N <sup>3-</sup> —Br <sup>-</sup>  | 113      | 342.8 | 24.4 | 280.0                 | 297.6       | 324.8          | 343.9  | 353.6          | 420.0                 |
| As <sup>3+</sup> —Br <sup>-</sup> | 4        | 232.0 | 4.8  | 200.0                 | 224.4       | 226.0          | 234.0  | 235.0          | 260.0                 |
| Sb <sup>3+</sup> —Br <sup>-</sup> | 14       | 283.3 | 23.3 | 0.0                   | 245.4       | 271.0          | 278.0  | 293.5          | 500.0                 |
| Bi <sup>3+</sup> —Br <sup>-</sup> | 26       | 307.7 | 28.3 | 250.0                 | 270.1       | 279.0          | 316.4  | 321.0          | 370.0                 |
| N <sup>3-</sup> —I <sup>-</sup>   | 61       | 366.8 | 25.2 | 290.0                 | 326.0       | 360.5          | 368.8  | 377.5          | 440.0                 |
| P <sup>2+</sup> —I <sup>-</sup>   | 4        | 244.5 | 3.8  | 0.0                   | 238.4       | 240.0          | 246.0  | 247.0          | 500.0                 |
| As <sup>3+</sup> —I <sup>-</sup>  | 6        | 268.3 | 9.6  | 250.0                 | 254.6       | 261.0          | 268.0  | 278.5          | 300.0                 |
| Sb <sup>3+</sup> —I <sup>-</sup>  | 28       | 307.2 | 27.4 | 0.0                   | 274.4       | 288.0          | 304.5  | 312.0          | 500.0                 |
| Bi <sup>3+</sup> —I <sup>-</sup>  | 18       | 322.6 | 25.3 | 0.0                   | 283.8       | 305.0          | 316.0  | 350.5          | 500.0                 |
| S <sup>4+</sup> —F <sup>-</sup>   | 8        | 152.2 | 7.6  | 130.0                 | 136.8       | 150.0          | 152.0  | 157.0          | 180.0                 |
| Te <sup>4+</sup> —F <sup>-</sup>  | 17       | 187.1 | 6.5  | 160.0                 | 178.9       | 182.2          | 186.5  | 191.5          | 230.0                 |
| S <sup>4+</sup> —Cl <sup>-</sup>  | 13       | 200.8 | 7.0  | 190.0                 | 194.3       | 195.6          | 197.2  | 207.5          | 240.0                 |
| Se <sup>4+</sup> —Cl <sup>-</sup> | 16       | 217.8 | 25.3 | 150.0                 | 153.6       | 210.0          | 215.0  | 239.5          | 300.0                 |
| Te <sup>4+</sup> —Cl <sup>-</sup> | 23       | 241.9 | 15.0 | 190.0                 | 224.1       | 229.8          | 247.5  | 252.2          | 290.0                 |
| Se <sup>4+</sup> —Br <sup>-</sup> | 6        | 245.3 | 13.7 | 0.0                   | 224.6       | 231.0          | 252.0  | 255.0          | 500.0                 |
| Te <sup>4+</sup> —Br <sup>-</sup> | 16       | 268.0 | 14.7 | 0.0                   | 243.6       | 267.0          | 268.7  | 269.6          | 500.0                 |
| Te <sup>4+</sup> —I <sup>-</sup>  | 13       | 282.4 | 12.5 | 0.0                   | 265.3       | 272.5          | 279.0  | 293.4          | 500.0                 |
| Br <sup>3+</sup> —F <sup>-</sup>  | 6        | 178.0 | 9.6  | 0.0                   | 168.3       | 169.5          | 172.0  | 188.5          | 500.0                 |
| I <sup>5+</sup> —F <sup>-</sup>   | 9        | 185.4 | 10.3 | 0.0                   | 168.9       | 180.2          | 183.0  | 195.5          | 500.0                 |
| I <sup>+</sup> —F <sup>-</sup>    | 5        | 326.6 | 31.5 | 0.0                   | 278.5       | 310.5          | 341.0  | 345.5          | 500.0                 |
| Br <sup>+</sup> —Cl <sup>-</sup>  | 9        | 290.1 | 4.6  | 0.0                   | 282.9       | 286.5          | 290.5  | 293.5          | 500.0                 |

Table 9.4.1.3. *Atomic distances between halogens and transition metals*

| Atom pair                        | <i>N</i> | Mean  | s.u. | <i>d</i> <sub>1</sub> | Smallest 5% | First quartile | Median | Third quartile | <i>d</i> <sub>2</sub> |
|----------------------------------|----------|-------|------|-----------------------|-------------|----------------|--------|----------------|-----------------------|
| Sc <sup>3+</sup> —F <sup>-</sup> | 17       | 206.8 | 13.5 | 0.0                   | 193.7       | 200.2          | 204.5  | 207.4          | 500.0                 |
| Ti <sup>3+</sup> —F <sup>-</sup> | 10       | 191.8 | 4.4  | 0.0                   | 186.5       | 188.5          | 191.0  | 193.5          | 500.0                 |
| Ti <sup>4+</sup> —F <sup>-</sup> | 37       | 190.1 | 11.2 | 0.0                   | 177.7       | 184.9          | 188.8  | 191.4          | 500.0                 |
| V <sup>4+</sup> —F <sup>-</sup>  | 14       | 183.3 | 11.1 | 0.0                   | 160.7       | 179.0          | 188.0  | 191.0          | 500.0                 |
| V <sup>5+</sup> —F <sup>-</sup>  | 13       | 183.6 | 9.1  | 0.0                   | 165.3       | 178.5          | 186.3  | 189.5          | 500.0                 |
| Cr <sup>2+</sup> —F <sup>-</sup> | 10       | 201.2 | 5.2  | 0.0                   | 195.0       | 197.5          | 199.3  | 207.0          | 500.0                 |
| Cr <sup>3+</sup> —F <sup>-</sup> | 68       | 192.6 | 12.1 | 0.0                   | 184.1       | 187.5          | 190.9  | 195.1          | 500.0                 |
| Cr <sup>4+</sup> —F <sup>-</sup> | 13       | 183.0 | 7.5  | 0.0                   | 167.3       | 180.5          | 185.5  | 188.5          | 500.0                 |
| Cr <sup>6+</sup> —F <sup>-</sup> | 3        | 163.0 | 5.3  | 140.0                 | 156.3       | 157.5          | 165.0  | 166.5          | 200.0                 |
| Fe <sup>2+</sup> —F <sup>-</sup> | 40       | 204.4 | 8.7  | 160.0                 | 188.0       | 199.2          | 204.3  | 208.0          | 250.0                 |
| Fe <sup>3+</sup> —F <sup>-</sup> | 103      | 189.7 | 6.5  | 150.0                 | 180.8       | 187.4          | 190.7  | 192.7          | 240.0                 |
| Co <sup>2+</sup> —F <sup>-</sup> | 28       | 200.9 | 8.0  | 180.0                 | 193.4       | 196.7          | 200.0  | 203.2          | 250.0                 |
| Co <sup>3+</sup> —F <sup>-</sup> | 12       | 189.2 | 2.6  | 160.0                 | 183.2       | 188.0          | 189.5  | 191.0          | 220.0                 |
| Ni <sup>2+</sup> —F <sup>-</sup> | 66       | 196.5 | 6.2  | 170.0                 | 188.9       | 193.0          | 195.9  | 199.4          | 250.0                 |
| Ni <sup>3+</sup> —F <sup>-</sup> | 8        | 186.0 | 3.2  | 0.0                   | 178.8       | 185.0          | 186.7  | 188.0          | 500.0                 |
| Ni <sup>4+</sup> —F <sup>-</sup> | 7        | 176.7 | 4.1  | 0.0                   | 170.4       | 171.8          | 178.3  | 179.5          | 500.0                 |
| Cu <sup>2+</sup> —F <sup>-</sup> | 82       | 195.6 | 12.8 | 160.0                 | 184.6       | 188.3          | 191.6  | 197.0          | 250.0                 |
| Cu <sup>3+</sup> —F <sup>-</sup> | 7        | 185.9 | 7.8  | 0.0                   | 172.7       | 182.5          | 183.7  | 194.2          | 500.0                 |
| Zn <sup>2+</sup> —F <sup>-</sup> | 48       | 197.2 | 11.2 | 150.0                 | 178.8       | 194.0          | 198.4  | 202.7          | 250.0                 |