9.4. Typical interatomic distances: inorganic compounds

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9.4.1. Introduction

In inorganic compounds, the intrinsic interatomic distances vary over a wide range, depending on atomic size, oxidation state, coordination number, bonding type, conditions of state, *etc*. The experimental values depend also on the conditions of measurement and possibly the defect structure of the sample in question.

To a first approximation, interatomic distances can be calculated from the sum of ionic radii taken from various tables. Mean values from experimental values from a limited number of structures determined up to 1960 are listed in *International Tables for X-ray Crystallography* (*IT* III, 1962). Today, databases allow all experimental results determined up to the present to be summarized and subjected to statistical analyses. For the Inorganic Crystal Structure Database (ICSD) (Bergerhoff & Brown, 1987), this analysis has been performed starting with 24 496 structure determinations in the 1990 version for all combinations of ions and atoms. For 8329 combinations, at least one distance inside the range 0 to 500 pm could be calculated. The statistical procedure is described in the following Section, and the results are given in Tables 9.4.1.1 to 9.4.1.12 for many pairs for which more than two distances had been determined. For more detailed discussions, and other ion pairs, the CD-ROM version of the ICSD is recommended. With the command 'check distances' in the *CVIS* program for the ICSD, the general distance distribution of a combination of elements can be compared with the distance distribution in a specific phase. Extreme values can be traced to their origin.

9.4.2. The retrieval system

By means of the retrieval system *CRYSTIN* (Sievers & Hundt, 1987), sets of structures were selected and combined; these contained:

(i) one ion in a specific oxidation state (if appropriate);
(ii) the other ion of the pair in a specific oxidation state (if appropriate);
(iii) structures determined at room temperature;
(iv) structures determined at normal pressure;
(v) no disordered structures;
(vi) no solid solutions;
(vii) no defect structures;
(viii) structures for which atomic coordinates were given;
(ix) only structures with $R < 6\%$ when there were many determinations.

For the M structures so defined, n interatomic distances were calculated for the atoms and ions in question. In so doing, all symmetrically equivalent and non-equivalent distances were taken into account. From these, a frequency distribution was calculated automatically. All distances d were collected into ranges of 2 pm. In (9.4.2.1)–(9.4.2.2), $n(d)$ is the number of distances in the range with midpoint d, d_1 is the midpoint of the lowest range, and d_2 is the midpoint of the highest range selected for the calculation of the mean. The choice of d_1 and d_2 is discussed in Section 9.4.3. The mean and the standard uncertainty (s.u.) of one set of distances were calculated by means of the equations

$$N = \sum_{d_1}^{d_2} n(d), \tag{9.4.2.1}$$

$$\text{mean} = \mu = N^{-1} \sum_{d_1}^{d_2} dn(d), \tag{9.4.2.2}$$

$$\text{s.u.} = \left(N^{-1} \sum_{d_1}^{d_2} (d - \mu)^2 n(d) \right)^{1/2}. \tag{9.4.2.3}$$

9.4.3. Interpretation of frequency distributions

It is obvious that the results have to be interpreted carefully when they are applied to crystal-structure discussions. In performing the analysis, the frequency distribution was inspected for each pair of ions. If all values were distributed around a single maximum, then d_1 and d_2 were set equal to zero and 500 pm, respectively. If there were two or more maxima, one was carefully selected and d_1 and d_2 were set to the left and right in such a way that the frequency was zero at both limits. In combinations with oxygen, so many distances were available for the most probable maximum that the program could select d_1 and d_2 automatically.

Maxima outside the selected range may come from errors in data or distances to ions in the second coordination sphere [*e.g.* Mg^{2+}—Cl^- in $Mg(H_2O)_6Cl_2$]. Generally, different oxidation states give rise to different maxima, which therefore have been tabulated separately (*e.g.* Cr^{2+}, Cr^{3+}, Cr^{4+}, Cr^{5+}, Cr^{6+} in combination with O^{2-}). In some typical cases, oxidation states cannot be clearly defined. Then the oxidation states have been omitted (*e.g.* Os—F, Rh—Br, N—S). Nevertheless, sometimes one oxidation state can be separated (*e.g.* W—Cl and W^{6+}—Cl^{1-}). Atomic distances between equally charged ions will be contact distances and vary over a wide range (*e.g.* O^{2-}—O^{2-} distances within SO_4^{2-} ions and between such ions).

Table 9.4.1.1. *Atomic distances between halogens and main-group elements in their preferred oxidation states*

Atom pair	N	Mean	s.u.	d_1	Smallest 5%	First quartile	Median	Third quartile	d_2
Li^+—F^-	108	193.0	14.2	150.0	166.4	184.6	195.0	202.7	250.0
Na^+—F^-	265	230.8	19.7	0.0	211.5	222.7	227.8	236.7	500.0
K^+—F^-	354	269.3	19.5	180.0	241.8	258.5	267.0	282.3	340.0
Rb^+—F^-	158	294.2	17.5	250.0	268.6	280.8	292.9	309.2	350.0
Cs^+—F^-	230	311.3	13.6	260.0	290.1	303.0	312.8	319.6	360.0
Li^+—Cl^-	30	246.1	11.1	210.0	223.0	240.3	247.0	255.0	300.0
Na^+—Cl^-	100	282.7	11.5	250.0	267.5	273.4	280.5	290.8	330.0
K^+—Cl^-	191	318.8	16.1	270.0	296.4	308.7	316.8	328.4	370.0
Rb^+—Cl^-	135	336.4	14.8	290.0	319.5	325.1	333.2	348.9	390.0
Cs^+—Cl^-	216	356.9	17.9	290.0	333.6	344.8	357.7	367.7	420.0
Li^+—Br^-	9	282.3	27.7	0.0	246.9	266.5	275.0	287.5	500.0
Na^+—Br^-	15	303.8	18.5	270.0	281.5	294.8	298.2	312.5	360.0
K^+—Br^-	72	331.8	26.4	0.0	289.2	314.0	332.0	342.7	500.0
Rb^+—Br^-	48	349.2	16.1	300.0	325.4	337.0	348.7	360.5	400.0
Cs^+—Br^-	64	372.2	15.3	350.0	352.4	360.0	368.3	385.0	430.0
Li^+—I^-	7	307.9	26.0	270.0	274.7	283.5	303.0	326.5	370.0
Na^+—I^-	7	342.1	24.5	0.0	320.7	322.8	325.0	372.2	500.0
K^+—I^-	24	363.6	29.2	0.0	334.4	344.0	364.0	374.0	500.0
Rb^+—I^-	29	372.0	16.3	320.0	340.9	362.8	373.0	381.2	430.0
Cs^+—I^-	63	393.4	13.8	350.0	374.8	381.9	391.7	404.8	450.0
Be^{2+}—F^-	78	150.6	6.3	120.0	140.6	148.2	152.2	153.9	200.0
Mg^{2+}—F^-	96	198.8	9.2	150.0	188.2	195.1	200.7	203.3	250.0
Ca^{2+}—F^-	127	230.9	16.9	0.0	216.2	223.8	228.7	236.2	500.0
Sr^{2+}—F^-	35	246.5	9.6	0.0	227.8	241.5	246.2	250.2	500.0
Ba^{2+}—F^-	94	266.6	9.3	0.0	256.7	259.9	264.6	269.3	500.0
Be^{2+}—Cl^-	2	200.0	1.4	0.0	198.2	199.0	200.0	201.0	500.0
Mg^{2+}—Cl^-	16	250.9	11.9	210.0	229.6	246.7	249.0	258.0	300.0
Ca^{2+}—Cl^-	55	286.2	15.1	260.0	271.8	275.1	280.8	293.2	350.0
Sr^{2+}—Cl^-	42	302.4	6.7	0.0	294.2	301.6	303.0	304.8	500.0
Ba^{2+}—Cl^-	64	316.3	12.2	270.0	298.8	308.7	314.8	324.0	370.0
Ca^{2+}—Br^-	10	300.6	18.9	250.0	259.0	290.5	308.0	311.0	350.0
Sr^{2+}—Br^-	30	305.4	15.5	0.0	279.0	291.0	311.0	315.0	500.0
Ba^{2+}—Br^-	17	331.9	13.2	0.0	307.7	320.5	337.0	340.8	500.0
Ca^{2+}—I^-	4	324.5	11.8	300.0	312.4	314.0	322.0	324.0	360.0
Sr^{2+}—I^-	20	305.7	20.6	250.0	278.0	284.7	312.7	322.0	350.0
Ba^{2+}—I^-	8	348.2	9.7	0.0	336.4	338.0	346.0	357.0	500.0
B^{3+}—F^-	39	136.6	7.1	110.0	125.9	133.8	136.8	139.1	180.0
Al^{3+}—F^-	121	180.6	7.5	150.0	170.1	176.6	179.3	184.6	230.0
Ga^{3+}—F^-	17	191.2	6.0	0.0	183.7	186.8	189.7	193.9	500.0
In^{3+}—F^-	24	204.0	9.1	0.0	192.4	202.0	204.6	206.7	500.0
Tl^{3+}—F–	14	203.0	6.7	0.0	189.4	199.0	203.3	208.5	500.0
B^{3+}—Cl^-	8	175.8	16.9	140.0	142.8	173.0	176.0	178.0	220.0
Al^{3+}—Cl^-	50	211.1	7.2	190.0	204.3	209.8	211.1	212.4	270.0
Ga^{3+}—Cl^-	12	212.8	4.4	0.0	204.6	211.0	213.3	216.0	500.0
In^{3+}—Cl^-	20	248.7	10.7	220.0	238.0	241.2	246.0	253.0	300.0
Tl^{3+}—Cl^-	19	248.2	6.9	200.0	233.9	243.5	249.0	253.2	300.0
B^{3+}—Br^-	3	197.7	13.6	150.0	186.3	187.5	193.0	212.5	250.0
Al^{3+}—Br^-	4	226.5	5.7	0.0	222.2	223.0	224.0	226.0	500.0
Ga^{3+}—Br^-	4	230.0	3.5	0.0	224.4	226.0	231.0	232.0	500.0
In^{3+}—Br^-	11	262.6	11.9	0.0	248.6	250.8	261.0	274.2	500.0
Tl^{3+}—Br^-	13	253.3	6.0	0.0	245.3	250.2	253.0	255.8	500.0
B^{3+}—I^-	2	240.0	41.0	200.0	210.2	211.0	212.0	269.0	300.0
Al^{3+}—I^-	3	248.3	2.3	220.0	246.1	246.8	247.5	250.5	280.0
Ga^{3+}—I^-	2	253.0	0.0	0.0	252.1	252.5	253.0	253.5	500.0
In^{3+}—I^-	7	275.9	10.3	250.0	264.4	265.8	275.0	280.5	320.0

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

Atom pair	N	Mean	s.u.	d_1	Smallest 5%	First quartile	Median	Third quartile	d_2
Ge^{4+}—F^-	20	176.7	3.9	150.0	168.0	176.0	177.1	178.4	210.0
Sn^{4+}—F^-	24	195.8	6.4	0.0	184.4	194.6	196.3	198.0	500.0
Pb^{4+}—F^-	9	209.7	7.2	0.0	196.9	206.5	210.5	212.8	500.0
C^{4+}—Cl^-	6	163.0	21.8	120.0	120.6	157.0	174.0	175.5	200.0
Sn^{4+}—Cl^-	46	238.7	5.7	0.0	230.1	235.0	240.4	242.7	500.0
Pb^{4+}—Cl^-	9	249.0	2.0	0.0	244.9	248.4	249.0	249.6	500.0
Sn^{4+}—Br^-	5	251.0	9.7	0.0	236.5	244.5	255.0	258.8	500.0
Ge^{4+}—I^-	3	254.3	4.6	0.0	248.3	249.5	256.5	257.2	500.0
Sn^{4+}—I^-	10	263.4	20.9	0.0	209.0	263.5	265.0	269.0	500.0
Pb^{4+}—I^-	2	310.0	1.4	0.0	308.2	309.0	310.0	311.0	500.0
P^{5+}—F^-	40	155.6	6.4	130.0	144.0	151.3	156.8	159.3	200.0
As^{5+}—F^-	89	164.6	6.7	130.0	155.4	160.9	165.5	168.4	200.0
Sb^{5+}—F^-	81	182.6	6.5	150.0	174.1	179.2	182.7	184.7	230.0
Bi^{5+}—F^-	9	192.1	11.3	0.0	178.4	188.2	189.7	195.5	500.0
P^{5+}—Cl^-	52	193.2	3.6	170.0	187.2	190.6	193.3	195.4	210.0
Sb^{5+}—Cl^-	66	233.1	6.6	200.0	220.6	229.8	233.8	236.4	270.0
P^{5+}—Br^-	12	211.2	5.1	0.0	201.2	208.0	213.0	214.7	500.0
Sb^{5+}—Br^-	6	254.0	2.1	250.0	250.6	252.5	254.0	255.5	270.0
S^{6+}—F^-	25	151.1	4.2	140.0	141.2	150.1	152.1	153.7	160.0
Te^{6+}—F^-	9	176.1	6.9	0.0	160.9	174.5	179.0	180.5	500.0
S^{6+}—Cl^-	10	197.6	5.7	170.0	185.0	195.5	197.3	201.0	220.0
I^{7+}—F^-	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	N	Mean	s.u.	d_1	Smallest 5%	First quartile	Median	Third quartile	d_2
Tl^+—F^-	36	282.6	19.0	250.0	259.8	267.1	273.0	297.3	350.0
Tl^+—Cl^-	38	326.2	19.0	0.0	291.8	316.3	326.0	339.0	500.0
Tl^+—Br^-	17	335.0	9.1	0.0	309.7	332.5	336.5	341.8	500.0
Tl^+—I^-	28	347.6	9.4	0.0	333.4	340.0	346.7	356.0	500.0
C^{2+}—F^-	17	131.2	2.4	110.0	126.8	130.1	131.3	132.7	160.0
Sn^{2+}—F^-	38	205.6	8.8	170.0	189.8	200.2	205.7	209.4	250.0
Pb^{2+}—F^-	49	247.5	10.3	160.0	227.4	239.5	250.5	256.5	290.0
Ge^{2+}—Cl^-	7	227.3	10.4	0.0	210.7	215.5	231.0	235.2	500.0
Sn^{2+}—Cl^-	26	253.3	9.0	220.0	236.6	250.2	253.0	257.8	290.0
Pb^{2+}—Cl^-	69	297.9	19.2	0.0	274.5	285.2	293.5	311.9	500.0
Sn^{2+}—Br^-	12	287.8	28.4	0.0	253.2	264.0	280.0	314.0	500.0
Pb^{2+}—Br^-	31	296.0	14.0	250.0	275.1	288.4	294.8	302.2	350.0
Ge^{2+}—I^-	3	283.0	8.0	260.0	274.3	275.5	283.0	290.5	310.0
Sn^{2+}—I^-	17	316.4	17.6	0.0	295.7	303.6	307.5	330.8	500.0
Pb^{2+}—I^-	32	322.7	18.4	270.0	296.6	316.0	320.0	338.0	380.0
N^{3-}—F^-	218	275.1	23.6	170.0	233.8	266.2	278.1	289.9	350.0
N^{2-}—F^-	26	270.2	29.6	0.0	212.6	260.5	268.0	277.0	500.0
P^{3+}—F^-	7	153.6	3.8	140.0	148.4	149.8	153.5	156.5	170.0
As^{3+}—F^-	6	165.0	5.1	150.0	156.6	162.5	164.0	169.0	200.0
Sb^{3+}—F^-	73	193.4	5.5	170.0	186.6	190.9	192.7	194.5	240.0
Bi^{3+}—F^-	21	235.7	18.8	0.0	218.1	222.1	226.5	253.5	500.0

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

Atom pair	N	Mean	s.u.	d_1	Smallest 5%	First quartile	Median	Third quartile	d_2
N^{3-}—Cl^-	349	323.0	24.4	250.0	279.6	311.1	325.0	335.2	410.0
N^{2-}—Cl^-	28	305.9	18.4	250.0	274.8	290.0	306.0	319.5	350.0
As^{3+}—Cl^-	7	211.6	7.5	200.0	202.7	205.5	209.5	216.5	250.0
Sb^{3+}—Cl^-	36	272.1	43.6	0.0	205.6	235.3	262.0	306.0	500.0
Bi^{3+}—Cl^-	39	292.8	34.0	0.0	246.9	265.5	304.2	318.5	500.0
N^{3-}—Br^-	113	342.8	24.4	280.0	297.6	324.8	343.9	353.6	420.0
As^{3+}—Br^-	4	232.0	4.8	200.0	224.4	226.0	234.0	235.0	260.0
Sb^{3+}—Br^-	14	283.3	23.3	0.0	245.4	271.0	278.0	293.5	500.0
Bi^{3+}—Br^-	26	307.7	28.3	250.0	270.1	279.0	316.4	321.0	370.0
N^{3-}—I^-	61	366.8	25.2	290.0	326.0	360.5	368.8	377.5	440.0
P^{2+}—I^-	4	244.5	3.8	0.0	238.4	240.0	246.0	247.0	500.0
As^{3+}—I^-	6	268.3	9.6	250.0	254.6	261.0	268.0	278.5	300.0
Sb^{3+}—I–	28	307.2	27.4	0.0	274.4	288.0	304.5	312.0	500.0
Bi^{3+}—I^-	18	322.6	25.3	0.0	283.8	305.0	316.0	350.5	500.0
S^{4+}—F^-	8	152.2	7.6	130.0	136.8	150.0	152.0	157.0	180.0
Te^{4+}—F^-	17	187.1	6.5	160.0	178.9	182.2	186.5	191.5	230.0
S^{4+}—Cl^-	13	200.8	7.0	190.0	194.3	195.6	197.2	207.5	240.0
Se^{4+}—Cl^-	16	217.8	25.3	150.0	153.6	210.0	215.0	239.5	300.0
Te^{4+}—Cl^-	23	241.9	15.0	190.0	224.1	229.8	247.5	252.2	290.0
Se^{4+}—Br^-	6	245.3	13.7	0.0	224.6	231.0	252.0	255.0	500.0
Te^{4+}—Br^-	16	268.0	14.7	0.0	243.6	267.0	268.7	269.6	500.0
Te^{4+}—I^-	13	282.4	12.5	0.0	265.3	272.5	279.0	293.4	500.0
Br^{3+}—F^-	6	178.0	9.6	0.0	168.3	169.5	172.0	188.5	500.0
I^{5+}—F^-	9	185.4	10.3	0.0	168.9	180.2	183.0	195.5	500.0
I^+—F^-	5	326.6	31.5	0.0	278.5	310.5	341.0	345.5	500.0
Br^+—Cl^-	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	N	Mean	s.u.	d_1	Smallest 5%	First quartile	Median	Third quartile	d_2
Sc^{3+}—F^-	17	206.8	13.5	0.0	193.7	200.2	204.5	207.4	500.0
Ti^{3+}—F^-	10	191.8	4.4	0.0	186.5	188.5	191.0	193.5	500.0
Ti^{4+}—F^-	37	190.1	11.2	0.0	177.7	184.9	188.8	191.4	500.0
V^{4+}—F^-	14	183.3	11.1	0.0	160.7	179.0	188.0	191.0	500.0
V^{5+}—F^-	13	183.6	9.1	0.0	165.3	178.5	186.3	189.5	500.0
Cr^{2+}—F^-	10	201.2	5.2	0.0	195.0	197.5	199.3	207.0	500.0
Cr^{3+}—F^-	68	192.6	12.1	0.0	184.1	187.5	190.9	195.1	500.0
Cr^{4+}—F^-	13	183.0	7.5	0.0	167.3	180.5	185.5	188.5	500.0
Cr^{6+}—F^-	3	163.0	5.3	140.0	156.3	157.5	165.0	166.5	200.0
Fe^{2+}—F^-	40	204.4	8.7	160.0	188.0	199.2	204.3	208.0	250.0
Fe^{3+}—F^-	103	189.7	6.5	150.0	180.8	187.4	190.7	192.7	240.0
Co^{2+}—F^-	28	200.9	8.0	180.0	193.4	196.7	200.0	203.2	250.0
Co^{3+}—F^-	12	189.2	2.6	160.0	183.2	188.0	189.5	191.0	220.0
Ni^{2+}—F^-	66	196.5	6.2	170.0	188.9	193.0	195.9	199.4	250.0
Ni^{3+}—F^-	8	186.0	3.2	0.0	178.8	185.0	186.7	188.0	500.0
Ni^{4+}—F^-	7	176.7	4.1	0.0	170.4	171.8	178.3	179.5	500.0
Cu^{2+}—F^-	82	195.6	12.8	160.0	184.6	188.3	191.6	197.0	250.0
Cu^{3+}—F^-	7	185.9	7.8	0.0	172.7	182.5	183.7	194.2	500.0
Zn^{2+}—F^-	48	197.2	11.2	150.0	178.8	194.0	198.4	202.7	250.0

Table 9.4.1.3. *Atomic distances between halogens and transition metals (cont.)*

Atom pair	N	Mean	s.u.	d_1	Smallest 5%	First quartile	Median	Third quartile	d_2
Sc^{3+}—Cl^-	9	255.7	6.9	0.0	240.9	254.2	255.7	257.8	500.0
Ti^{3+}—Cl^-	6	244.0	6.3	0.0	232.6	241.0	246.0	247.5	500.0
Ti^{4+}—Cl^-	16	225.0	17.0	170.0	181.6	219.0	224.0	234.7	270.0
V^{2+}—Cl^-	8	250.0	2.8	0.0	246.3	247.3	250.0	252.7	500.0
V^{3+}—Cl^-	10	235.6	4.6	0.0	227.0	233.0	236.0	237.7	500.0
V^{4+}—Cl^-	4	227.5	7.7	0.0	216.4	218.0	228.0	232.0	500.0
V^{5+}—Cl^-	5	221.0	5.8	200.0	212.5	218.5	221.0	223.5	250.0
Cr^{2+}—Cl^-	30	246.7	15.2	220.0	236.2	239.0	241.2	247.0	320.0
Cr^{3+}—Cl^-	17	231.6	4.8	200.0	217.7	229.5	232.5	233.9	270.0
Cr^{6+}—Cl^-	3	218.3	1.2	200.0	216.3	217.5	218.5	219.2	250.0
Fe^{2+}—Cl^-	29	244.9	10.2	200.0	222.4	243.2	247.8	251.2	280.0
Fe^{3+}—Cl^-	39	227.1	9.8	200.0	216.2	217.9	226.5	235.2	280.0
Co^{2+}—Cl^-	39	237.6	12.4	200.0	220.5	225.2	244.1	247.3	280.0
Co^{3+}—Cl^-	10	228.4	30.5	150.0	167.0	225.0	228.0	231.0	310.0
Ni^{2+}—Cl^-	12	238.3	6.1	200.0	221.2	237.0	240.0	242.0	280.0
Cu^{+}—Cl^-	38	245.5	25.5	210.0	217.3	229.0	235.2	270.5	320.0
Cu^{2+}—Cl^-	51	228.1	5.1	200.0	217.1	225.9	228.7	230.4	240.0
Zn^{2+}—Cl^-	54	227.5	9.1	200.0	218.4	222.7	225.0	230.1	280.0
Ti^{4+}—Br^-	3	249.0	18.0	0.0	230.3	231.5	249.0	266.5	500.0
V^{2+}—Br^-	5	259.8	6.3	0.0	248.5	260.2	261.5	263.5	500.0
V^{3+}—Br^-	5	250.6	2.6	0.0	246.5	248.5	251.0	252.8	500.0
Cr^{2+}—Br^-	7	247.3	8.0	0.0	238.7	240.8	243.0	255.2	500.0
Cr^{3+}—Br^-	7	244.1	4.7	210.0	238.7	240.8	243.0	246.5	290.0
Mn^{2+}—Br^-	12	261.2	11.2	220.0	235.2	259.0	265.0	268.0	320.0
Fe^{2+}—Br^-	7	247.9	10.9	220.0	232.7	235.5	249.0	258.5	290.0
Fe^{3+}—Br^-	4	239.0	13.4	220.0	230.4	232.0	233.0	234.0	290.0
Co^{2+}—Br^-	8	253.0	7.9	0.0	238.8	248.7	250.0	260.7	500.0
Ni^{2+}—Br^-	3	257.7	7.0	0.0	250.3	251.5	257.0	264.5	500.0
Cu^{+}—Br^-	22	260.8	20.1	210.0	236.2	246.5	253.0	277.5	310.0
Cu^{2+}—Br–	18	260.3	23.3	210.0	231.8	244.5	251.0	287.5	310.0
Zn^{2+}—Br^-	17	235.0	14.5	200.0	203.7	234.5	236.9	237.9	300.0
V^{2+}—I^-	4	287.0	7.3	0.0	278.4	280.0	284.0	292.0	500.0
Cr^{2+}—I^-	20	261.2	31.6	0.0	190.0	242.0	275.0	278.5	500.0
Mn^{2+}—I^-	10	287.2	6.4	0.0	275.0	281.0	290.0	291.7	500.0
Fe^{2+}—I^-	3	268.3	15.0	240.0	250.3	251.5	276.5	277.2	300.0
Ni^{2+}—I^-	4	295.5	11.0	250.0	278.4	280.0	300.7	301.3	310.0
Cu^{+}—I^-	36	268.7	16.9	0.0	248.8	258.0	264.4	272.0	500.0
Zn^{2+}—I^-	5	264.6	17.2	240.0	252.5	256.2	257.5	261.5	310.0
Y^{3+}—F^-	34	226.7	18.9	0.0	199.4	217.0	224.7	235.0	500.0
Zr^{4+}—F^-	66	203.1	10.1	0.0	191.5	199.0	201.5	205.4	500.0
Nb^{3+}—F^-	6	195.0	2.2	0.0	190.6	194.3	195.3	196.5	500.0
Nb^{4+}—F^-	5	201.8	3.6	0.0	196.5	198.5	203.0	204.8	500.0
Nb^{5+}—F^-	52	191.0	12.7	150.0	159.2	184.5	192.0	199.5	240.0
Mo^{3+}—F^-	11	204.1	6.3	0.0	195.1	202.3	203.4	204.8	500.0
Mo^{5+}—F^-	8	185.5	10.1	160.0	172.4	174.0	185.0	186.0	230.0
Mo^{6+}—F^-	17	190.1	12.5	150.0	169.7	180.5	190.5	193.8	250.0
Ru^{5+}—F^-	7	182.1	9.0	0.0	166.7	176.8	183.0	190.2	500.0
Rh^{3+}—F^-	14	196.3	4.8	170.0	181.4	195.5	198.0	199.0	220.0
Pd^{2+}—F^-	9	206.8	11.6	0.0	192.4	194.5	211.0	216.8	500.0
Pd^{4+}—F^-	10	186.6	1.0	0.0	167.0	184.5	187.0	189.5	500.0
Ag^{+}—F^-	9	250.3	24.8	200.0	220.9	226.5	247.0	275.5	300.0
Ag^{2+}—F^-	12	205.5	4.8	180.0	195.2	204.0	206.4	207.6	240.0
Cd^{2+}—F^-	23	222.1	14.4	180.0	200.3	215.5	221.7	232.2	270.0

Table 9.4.1.3. *Atomic distances between halogens and transition metals (cont.)*

Atom pair	N	Mean	s.u.	d_1	Smallest 5%	First quartile	Median	Third quartile	d_2
Y^{3+}—Cl^-	10	274.0	23.4	220.0	227.0	259.0	278.0	285.5	330.0
Zr^{3+}—Cl^-	9	250.6	6.8	0.0	232.9	250.8	252.3	253.8	500.0
Zr^{4+}—Cl^-	9	240.1	6.7	0.0	230.4	232.5	244.2	245.4	500.0
Nb—Cl^-	9	245.4	11.2	0.0	228.9	238.5	243.0	258.5	500.0
Nb^{5+}—Cl^-	13	232.8	18.1	200.0	215.3	224.2	227.0	231.5	300.0
Mo^{2+}—Cl^-	11	240.8	6.2	0.0	227.1	238.5	240.5	244.5	500.0
Mo^{3+}—Cl^-	11	240.1	2.1	0.0	236.6	238.5	240.2	241.6	500.0
Mo^{4+}—Cl^-	3	224.3	5.8	0.0	220.1	220.8	221.5	230.5	500.0
Mo^{5+}—Cl^-	7	230.7	5.8	0.0	222.7	226.8	229.0	236.5	500.0
Mo^{6+}—Cl^-	12	229.3	4.7	210.0	221.2	225.3	230.0	233.3	260.0
Ru^{2+}—Cl^-	11	233.9	6.1	200.0	219.1	231.2	235.0	238.2	260.0
Ru^{3+}—Cl^-	15	234.7	5.4	220.0	230.4	231.9	233.4	235.5	270.0
Ru^{4+}—Cl^-	8	234.0	3.0	220.0	230.3	231.3	234.0	236.0	260.0
Rh^{3+}—Cl^-	9	232.3	2.8	210.0	228.4	230.2	231.7	234.8	260.0
Pd^{2+}—Cl^-	15	230.7	2.9	210.0	227.5	228.9	230.2	231.4	260.0
Pd^{4+}—Cl^-	3	210.3	16.3	0.0	198.3	199.5	203.0	228.5	500.0
Ag^+—Cl^-	16	261.9	13.5	0.0	237.6	250.0	262.0	271.0	500.0
Cd^{2+}—Cl^-	58	258.0	8.5	220.0	241.9	252.1	258.5	263.0	300.0
Zr^{3+}—Br^-	4	266.5	1.0	0.0	264.4	266.0	266.7	267.3	500.0
Nb^{5+}—Br^-	7	253.3	7.8	230.0	240.7	250.8	252.5	256.5	290.0
Mo—Br^-	12	257.7	14.0	0.0	229.2	254.5	256.0	260.0	500.0
Rh—Br^-	3	245.7	4.2	0.0	240.3	241.5	247.0	248.5	500.0
Ag—Br^-	6	267.7	17.8	0.0	254.6	258.5	260.0	267.0	500.0
Cd^{2+}—Br^-	16	274.0	12.1	250.0	253.6	264.0	276.7	284.0	310.0
Zr—I^-	21	287.1	1.7	250.0	284.0	286.2	287.1	288.0	320.0
Zr^{4+}—I^-	5	284.6	14.2	0.0	268.2	269.2	294.3	295.2	500.0
Nb—I^-	13	277.3	16.3	0.0	241.3	265.2	281.5	283.8	500.0
Nb^{5+}—I^-	4	274.5	8.7	0.0	262.4	264.0	274.0	280.0	500.0
Mo—I^-	4	270.0	12.7	0.0	250.4	252.0	276.0	277.0	500.0
Ru—I^-	3	269.7	2.3	250.0	266.3	267.5	270.5	271.2	300.0
Ag^+—I^-	61	283.1	11.6	250.0	267.0	278.2	281.2	284.9	330.0
Cd^{2+}—I^-	30	293.5	11.0	260.0	273.0	291.0	297.6	299.1	340.0
La^{3+}—F^-	30	240.9	5.8	0.0	234.3	237.4	240.6	242.2	500.0
Hf^{4+}—F^-	9	209.9	10.4	0.0	198.4	202.2	205.0	217.2	500.0
Ta^{5+}—F^-	29	190.6	5.5	160.0	178.9	188.4	191.2	194.6	220.0
W^{6+}—F^-	13	183.5	11.8	150.0	163.3	177.2	179.2	192.8	230.0
Re—F^-	18	187.6	14.9	150.0	163.8	179.0	182.0	195.0	240.0
Os—F^-	10	182.8	14.9	0.0	157.0	171.0	184.0	194.5	500.0
Pt^{4+}—F^-	12	189.0	6.8	0.0	169.2	188.6	189.4	192.0	500.0
Au^{3+}—F^-	7	196.1	3.8	180.0	190.4	191.8	198.2	199.1	220.0
Hg—F^-	19	278.1	26.8	0.0	215.9	271.8	282.3	287.5	500.0
Hg^{2+}—F^-	25	242.7	23.8	0.0	204.5	223.5	243.0	261.9	500.0
La^{3+}—Cl^-	21	293.1	16.1	0.0	256.0	294.2	297.0	302.4	500.0
Ta^{5+}—Cl^-	4	227.5	2.5	210.0	224.4	226.0	227.0	228.0	260.0
W—Cl^-	9	234.1	6.5	210.0	224.9	228.5	233.0	240.5	260.0
W^{6+}—Cl^-	8	219.2	11.1	190.0	202.8	208.0	224.0	228.0	270.0
Re—Cl^-	46	231.6	8.7	200.0	218.3	227.0	231.1	235.4	280.0
Os—Cl^-	14	239.3	6.8	200.0	226.7	236.2	238.0	243.8	280.0
Ir—Cl^-	11	235.4	7.4	200.0	223.1	230.8	234.5	240.5	270.0
Pt^{2+}—Cl^-	26	231.5	3.4	200.0	226.6	229.5	231.0	232.8	270.0
Pt^{4+}—Cl^-	31	231.9	7.0	0.0	225.1	230.2	232.1	234.2	500.0
Au^+—Cl^-	14	241.1	16.6	0.0	225.4	229.7	233.0	249.0	500.0
Au^{3+}—Cl^-	35	232.1	12.8	200.0	219.5	226.1	227.7	234.5	300.0
Hg^+—Cl^-	7	255.0	9.5	230.0	242.7	250.5	251.7	258.5	300.0
Hg^{2+}—Cl^-	68	250.5	25.5	200.0	223.4	231.0	238.0	276.7	310.0

Table 9.4.1.3. *Atomic distances between halogens and transition metals (cont.)*

Atom pair	N	Mean	s.u.	d_1	Smallest 5%	First quartile	Median	Third quartile	d_2
La^{3+}—Br^-	3	310.3	34.1	0.0	270.3	271.5	329.0	330.5	500.0
W^{6+}—Br^-	5	245.0	10.7	0.0	230.5	242.5	244.5	245.8	500.0
Re^{3+}—Br^-	4	237.5	6.6	0.0	232.2	233.0	234.0	238.0	500.0
Os^{4+}—Br^-	3	246.3	6.4	0.0	238.3	239.5	249.0	250.5	500.0
Ir^{3+}—Br^-	4	244.0	3.8	0.0	240.2	241.0	242.0	246.0	500.0
Pt^{2+}—Br^-	9	246.3	6.6	0.0	240.9	242.8	244.5	246.8	500.0
Pt^{4+}—Br^-	8	242.5	10.6	200.0	216.8	243.0	246.0	248.0	270.0
Pt—Br	22	247.4	7.9	230.0	240.2	243.2	246.0	248.5	290.0
Au^{3+}—Br^-	10	243.0	2.7	0.0	239.0	241.0	242.7	245.0	500.0
Hg^{+}—Br^-	5	263.0	14.3	0.0	240.5	256.5	269.0	271.5	500.0
Hg^{2+}—Br^-	27	268.8	25.9	230.0	238.7	247.5	257.0	294.5	330.0
Os—I	8	275.8	4.8	0.0	272.2	273.0	274.0	276.0	500.0
Pt^{4+}—I^-	10	266.2	2.1	0.0	262.5	264.5	266.5	267.8	500.0
Pt—I	24	265.4	3.9	0.0	258.4	263.0	265.2	268.0	500.0
Au^{+}—I^-	4	258.5	3.0	0.0	254.4	256.0	258.0	261.0	500.0
Au^{3+}—I^-	3	265.0	3.5	0.0	262.1	262.8	263.5	268.5	500.0
Hg^{2+}—I^-	40	284.2	27.3	0.0	258.0	267.3	273.6	281.0	500.0

Table 9.4.1.4. *Atomic distances between halogens and lanthanoids*

Atom pair	N	Mean	s.u.	d_1	Smallest 5%	First quartile	Median	Third quartile	d_2
Ce^{3+}—F^-	16	239.0	7.4	0.0	225.6	236.0	237.6	240.0	500.0
Ce^{4+}—F^-	4	216.5	14.9	0.0	198.4	200.0	214.0	220.0	500.0
Nd^{3+}—F^-	8	242.8	21.3	0.0	222.8	232.0	237.0	242.0	500.0
Sm^{3+}—F^-	6	232.0	8.2	0.0	220.6	223.0	234.0	237.5	500.0
Gd^{3+}—F^-	5	226.6	3.3	0.0	220.5	226.2	227.5	228.8	500.0
Tb^{3+}—F^-	3	229.0	7.2	0.0	220.3	221.5	231.0	234.5	500.0
Ho^{3+}—F^-	7	222.4	13.0	0.0	196.7	215.5	227.0	229.2	500.0
Er^{3+}—F^-	10	216.0	1.0	0.0	197.0	212.5	216.0	217.7	500.0
Yb^{3+}—F^-	16	217.2	7.2	0.0	208.5	211.0	218.0	222.0	500.0
Lu^{3+}—F^-	5	210.2	15.3	0.0	186.5	204.5	213.0	219.5	500.0
Pr^{3+}—Cl^-	18	286.2	12.1	0.0	253.8	277.0	289.0	291.0	500.0
Nd^{3+}—Cl^-	12	294.5	25.2	0.0	253.2	274.0	289.0	310.0	500.0
Eu^{3+}—Cl^-	5	285.4	12.4	0.0	276.2	277.2	282.5	283.8	500.0
Gd^{3+}—Cl^-	13	278.8	10.2	0.0	266.4	272.5	277.2	283.2	500.0
Gd—Cl	24	274.4	1.0	0.0	261.2	267.0	273.0	280.0	500.0
Tb^{3+}—Cl^-	4	271.0	5.4	0.0	266.4	268.0	269.0	270.0	500.0
Yb^{2+}—Cl^-	8	277.2	9.0	0.0	270.3	271.3	274.0	278.0	500.0
Nd^{3+}—Br^-	6	307.0	13.1	0.0	294.3	295.5	300.0	322.5	500.0
Gd^{3+}—Br^-	4	290.5	15.9	0.0	268.4	270.0	292.0	296.0	500.0
Eu^{2+}—I^-	4	330.5	11.0	0.0	324.1	324.7	325.3	326.0	500.0

Table 9.4.1.5. *Atomic distances between halogens and actinoids*

Atom pair	N	Mean	s.u.	d_1	Smallest 5%	First quartile	Median	Third quartile	d_2
Th^{4+}—F^-	26	233.3	10.4	0.0	219.3	226.8	231.3	237.0	500.0
Pa^{5+}—F^-	4	216.5	3.4	0.0	212.4	214.0	216.0	218.0	500.0
U^{4+}—F^-	35	232.1	12.7	0.0	216.8	222.5	228.3	241.2	500.0
U^{5+}—F^-	16	204.4	10.4	0.0	192.5	196.0	203.0	208.0	500.0
U^{6+}—F^-	25	211.8	21.4	170.0	180.2	187.6	220.3	223.9	280.0
Np^{4+}—F^-	8	215.8	17.8	0.0	172.8	218.0	220.0	222.0	500.0
Pu^{3+}—F^-	4	241.5	6.4	0.0	234.4	236.0	238.0	247.0	500.0
Th^{4+}—Cl^-	15	292.9	19.4	0.0	245.5	279.5	302.4	303.3	500.0
U^{4+}—Cl^-	14	268.1	17.7	0.0	241.4	261.0	264.7	267.5	500.0
U^{5+}—Cl^-	5	250.6	11.7	0.0	242.2	243.2	247.0	249.5	500.0
U^{6+}—Cl^-	17	264.6	20.1	0.0	229.7	246.5	273.0	275.9	500.0
Pu^{3+}—Cl^-	6	281.0	19.9	0.0	252.6	270.5	272.0	293.0	500.0
Am^{3+}—Cl^-	4	281.5	24.0	0.0	250.4	252.0	280.0	288.0	500.0
Th^{4+}—Cl^-	15	292.9	19.4	0.0	245.5	279.5	302.4	303.3	500.0
Th^{4+}—Br^-	5	288.6	26.7	0.0	256.5	282.5	285.0	287.5	500.0
U^{4+}—Br^-	5	281.0	24.2	0.0	260.5	270.5	273.0	277.5	500.0
Pu^{3+}—Br^-	4	309.0	8.2	0.0	302.4	304.0	306.0	308.0	500.0
U^{3+}—I^-	4	320.5	7.2	0.0	314.4	316.0	318.0	320.0	500.0

Table 9.4.1.6. *Atomic distances between oxygen and main-group elements in their preferred oxidation states*

Atom pair	N	Mean	s.u.	d_1	Smallest 5%	First quartile	Median	Third quartile	d_2
Li^+—O^{2-}	745	194.9	10.2	164.0	178.4	188.4	193.9	203.0	218.0
Na^+—O^{2-}	1914	233.6	10.8	196.0	214.9	227.6	233.7	239.4	268.0
K^+—O^{2-}	1434	276.4	13.0	254.0	259.3	267.4	273.8	282.6	326.0
Rb^+—O^{2-}	330	288.7	12.1	258.0	269.5	280.7	288.4	295.2	322.0
Cs^+—O^{2-}	290	305.2	12.4	270.0	280.5	297.5	306.3	314.1	328.0
Be^{2+}—O^{2-}	195	161.1	5.1	146.0	152.8	157.6	161.1	164.1	178.0
Mg^{2+}—O^{2-}	1121	201.6	9.0	166.0	185.2	197.6	202.8	206.6	228.0
Ca^{2+}—O^{2-}	1624	233.0	12.4	184.0	209.8	228.1	233.2	238.6	286.0
Sr^{2+}—O^{2-}	372	248.7	11.4	212.0	226.8	242.9	250.5	256.9	270.0
Ba^{2+}—O^{2-}	1012	273.8	14.6	222.0	246.9	265.4	274.9	283.0	312.0
B^{3+}—O^{2-}	407	134.3	3.6	116.0	127.1	132.8	134.8	136.6	142.0
Al^{3+}—O^{2-}	914	161.8	4.5	138.0	154.1	160.0	162.4	164.4	170.0
Ga^{3+}—O^{2-}	111	180.3	3.5	170.0	175.0	177.7	180.3	183.0	188.0
In^{3+}—O^{2-}	153	208.2	8.8	184.0	189.6	203.9	209.1	213.2	230.0
Tl^{3+}—O^{2-}	23	214.2	4.4	206.0	187.6	210.8	214.2	217.5	224.0
C^{4+}—O^{2-}	413	125.3	4.9	104.0	115.9	123.5	126.0	128.3	142.0
Si^{4+}—O^{2-}	2679	159.6	5.3	126.0	150.6	157.8	160.0	162.4	180.0
Ge^{4+}—O^{2-}	329	172.1	7.7	144.0	160.3	169.3	172.1	175.0	194.0
Sn^{4+}—O^{2-}	170	202.8	6.4	188.0	191.7	198.1	204.0	206.2	222.0
Pb^{4+}—O^{2-}	56	211.9	5.0	200.0	201.2	207.5	213.7	215.4	222.0
N^{5+}—O^{2-}	301	120.7	4.0	106.0	112.3	118.9	121.5	123.4	132.0
P^{5+}—O^{2-}	1391	149.6	4.7	122.0	142.3	147.3	150.1	152.4	172.0
As^{5+}—O^{2-}	251	166.0	3.9	150.0	159.4	164.4	166.3	167.7	182.0
Sb^{5+}—O^{2-}	161	197.7	7.1	184.0	188.0	193.2	196.7	200.0	220.0
Bi^{5+}—O^{2-}	6	229.0	0.0	228.0	226.5	227.2	228.2	229.1	230.0
S^{6+}—O^{2-}	998	144.3	5.5	118.0	135.6	142.5	144.7	146.6	178.0
Se^{6+}—O^{2-}	86	160.8	3.2	152.0	154.3	159.6	161.3	162.9	168.0
Te^{6+}—O^{2-}	113	189.2	4.1	176.0	182.2	186.8	190.0	191.5	200.0
Cl^{7+}—O^{2-}	89	139.5	5.5	122.0	128.3	136.8	140.9	143.1	150.0
Br^{7+}—O^{2-}	3	160.3	1.2	158.0	158.3	159.5	160.5	161.2	162.0
I^{7+}—O^{2-}	39	180.3	4.7	170.0	171.6	177.4	180.4	183.6	190.0

Table 9.4.1.7. *Atomic distances between oxygen and main-group elements in their special oxidation states*

Atom pair	N	Mean	s.u.	d_1	Smallest 5%	First quartile	Median	Third quartile	d_2
Tl^{+}—O^{2-}	101	265.4	12.9	240.0	244.2	254.2	268.6	275.7	286.0
C^{2+}—O^{2-}	308	110.5	4.5	88.0	102.7	108.8	111.2	112.9	124.0
Sn^{2+}—O^{2-}	14	201.1	2.3	196.0	196.7	200.2	201.3	202.8	206.0
Pb^{2+}—O^{2-}	367	233.2	16.1	190.0	208.1	222.5	232.0	244.2	268.0
N^{2+}—O^{2-}	23	115.3	3.5	108.0	110.3	112.8	114.3	117.6	124.0
N^{3+}—O^{2-}	166	119.9	5.4	102.0	109.5	116.7	121.5	123.9	130.0
N^{4+}—O^{2-}	5	119.0	0.0	118.0	117.8	118.2	118.8	119.4	120.0
P^{+}—O^{2-}	12	149.7	2.3	146.0	145.9	148.0	149.2	152.0	154.0
P^{3+}—O^{2-}	43	149.9	2.1	142.0	146.1	148.7	149.8	151.3	154.0
P^{4+}—O^{2-}	10	151.6	1.0	150.0	149.6	150.3	151.2	152.3	154.0
As^{3+}—O^{2-}	61	175.1	4.6	164.0	166.1	172.2	175.6	178.4	186.0
Sb^{3+}—O^{2-}	101	195.7	5.4	184.0	186.4	192.5	195.3	199.6	208.0
Bi^{3+}—O^{2-}	122	227.0	5.4	216.0	218.0	222.7	227.7	231.1	238.0
S^{2+}—O^{2-}	9	145.7	2.2	140.0	140.9	144.5	146.5	147.2	148.0
S^{4+}—O^{2-}	110	146.3	5.5	130.0	136.2	142.6	147.1	151.0	154.0
S^{5+}—O^{2-}	38	145.4	2.7	142.0	141.5	143.8	144.9	145.8	156.0
Se^{4+}—O^{2-}	125	166.5	3.1	154.0	160.8	164.9	166.5	168.5	176.0
Te^{4+}—O^{2-}	124	186.4	4.0	174.0	179.3	184.2	185.9	189.1	198.0
Cl^{3+}—O^{2-}	8	156.2	1.5	154.0	154.2	155.0	156.0	157.3	160.0
Cl^{5+}—O^{2-}	23	145.5	3.9	136.0	139.1	143.2	146.8	148.6	150.0
Br^{5+}—O^{2-}	11	164.5	0.9	162.0	166.0	164.2	164.6	165.3	166.0
Xe^{6+}—O^{2-}	4	172.5	1.9	170.0	170.2	171.0	172.0	174.0	176.0

Table 9.4.1.8. *Atomic distances between oxygen and transition elements in their preferred and special oxidation states*

Atom pair	N	Mean	s.u.	d_1	Smallest 5%	First quartile	Median	Third quartile	d_2
Y^{3+}—O^{2-}	208	228.7	7.6	212.0	217.4	222.3	228.0	235.5	244.0
Ti^{2+}—O^{2-}	7	206.4	2.2	202.0	202.7	204.8	206.5	208.2	210.0
Ti^{3+}—O^{2-}	79	200.4	4.0	188.0	192.0	197.9	201.7	203.1	208.0
Ti^{4+}—O^{2-}	661	188.7	10.2	156.0	169.9	182.2	190.3	196.1	212.0
V^{2+}—O^{2-}	10	206.6	3.4	202.0	213.8	204.2	205.5	209.0	214.0
V^{3+}—O^{2-}	112	198.0	3.7	188.0	191.7	196.1	197.7	199.8	210.0
V^{4+}—O^{2-}	93	165.8	8.8	150.0	156.2	159.3	163.3	171.8	190.0
V^{5+}—O^{2-}	328	165.1	8.5	142.0	152.8	160.5	164.2	168.8	196.0
Cr^{2+}—O^{2-}	13	203.8	2.8	198.0	196.3	201.5	203.7	206.4	208.0
Cr^{3+}—O^{2-}	215	196.4	4.0	186.0	190.2	194.0	196.3	198.6	208.0
Cr^{4+}—O^{2-}	4	167.5	1.0	166.0	166.1	166.7	167.3	168.0	170.0
Cr^{5+}—O^{2-}	3	169.0	0.0	168.0	164.3	165.5	167.0	168.5	170.0
Cr^{6+}—O^{2-}	164	159.9	5.0	144.0	150.8	157.2	159.6	163.1	172.0
Mn^{2+}—O^{2-}	507	210.0	10.4	178.0	193.1	204.1	209.8	215.6	240.0
Mn^{3+}—O^{2-}	151	191.5	6.1	176.0	181.2	187.6	191.1	195.9	208.0
Mn^{4+}—O^{2-}	74	191.5	6.1	180.0	182.9	187.3	190.5	194.6	208.0
Mn^{7+}—O^{2-}	9	158.8	1.6	156.0	154.8	157.1	158.8	159.9	162.0
Fe^{2+}—O^{2-}	640	203.6	9.3	172.0	187.3	198.5	203.8	209.3	236.0
Fe^{3+}—O^{2-}	900	192.9	9.1	164.0	176.9	187.4	193.4	198.7	224.0
Co^{2+}—O^{2-}	263	202.1	7.1	188.0	190.5	196.6	202.6	206.9	222.0
Co^{3+}—O^{2-}	118	191.8	4.9	176.0	183.9	189.2	191.3	193.9	206.0
Ni^{2+}—O^{2-}	282	200.3	7.9	176.0	185.1	195.9	202.4	205.3	218.0
Cu^{2+}—O^{2-}	614	193.5	7.3	164.0	180.7	190.2	193.7	196.5	220.0
Zn^{2+}—O^{2-}	432	198.1	8.0	182.0	186.7	192.4	196.6	203.2	228.0

Table 9.4.1.8. *Atomic distances between oxygen and transition elements (cont.)*

Atom pair	N	Mean	s.u.	d_1	Smallest 5%	First quartile	Median	Third quartile	d_2
Sc^{3+}—O^{2-}	151	205.1	5.2	188.0	196.6	201.6	205.7	208.4	222.0
Zr^{4+}—O^{2-}	268	203.4	7.3	176.0	188.6	201.1	204.4	207.4	222.0
Nb^{4+}—O^{2-}	7	189.9	1.1	188.0	185.9	187.5	189.4	190.8	192.0
Nb^{5+}—O^{2-}	416	186.6	9.4	166.0	171.4	179.1	186.3	194.8	208.0
Mo^{3+}—O^{2-}	6	207.0	1.8	204.0	200.9	204.5	207.0	208.5	210.0
Mo^{4+}—O^{2-}	34	192.1	5.7	182.0	182.0	185.8	194.8	196.9	200.0
Mo^{5+}—O^{2-}	26	165.8	3.7	158.0	160.3	163.2	165.6	167.6	176.0
Mo^{6+}—O^{2-}	357	171.5	8.3	146.0	158.9	167.6	170.7	174.8	202.0
Tc^{7+}—O^{2-}	4	171.0	0.0	170.0	169.1	169.8	170.5	171.2	172.0
Ru^{2+}—O^{2-}	3	263.0	0.0	262.0	261.6	262.1	262.7	263.4	264.0
Pd^{2+}—O^{2-}	31	201.0	2.7	194.0	196.6	199.1	200.9	202.9	208.0
Ag^{2+}—O^{2-}	6	205.3	2.3	202.0	202.3	203.5	205.0	207.0	210.0
Cd^{2+}—O^{2-}	276	221.9	10.8	184.0	200.8	217.1	222.5	227.8	254.0
La^{3+}—O^{2-}	317	244.1	9.2	222.0	230.1	237.7	243.1	249.9	268.0
Hf^{4+}—O^{2-}	11	202.8	1.7	198.0	201.1	202.2	203.0	203.8	206.0
Ta^{4+}—O^{2-}	5	193.0	1.4	190.0	190.5	192.2	193.0	193.8	196.0
Ta^{5+}—O^{2-}	262	191.7	7.6	168.0	177.7	186.5	193.5	196.8	210.0
W^{5+}—O^{2-}	12	189.5	3.1	184.0	179.0	187.0	189.3	192.5	194.0
W^{6+}—O^{2-}	355	180.0	11.3	150.0	161.8	171.8	178.9	190.0	206.0
Re^{5+}—O^{2-}	21	207.5	3.2	202.0	204.0	204.9	206.5	209.5	216.0
Re^{6+}—O^{2-}	3	163.0	0.0	162.0	161.8	162.2	162.8	163.4	164.0
Re^{7+}—O^{2-}	34	175.1	5.3	166.0	168.3	171.2	173.8	178.5	188.0
Os^{6+}—O^{2-}	3	175.0	0.0	174.0	173.6	174.1	174.8	175.4	176.0
Os^{8+}—O^{2-}	12	173.2	2.2	168.0	170.6	172.0	173.2	174.7	178.0
Ir^{3+}—O^{2-}	5	196.6	1.7	194.0	194.2	195.2	196.5	197.8	200.0
Ir^{4+}—O^{2-}	7	193.9	3.2	190.0	188.3	190.3	193.0	196.5	200.0
Pt^{2+}—O^{2-}	20	199.3	3.5	192.0	194.0	196.0	200.0	202.0	206.0
Pt^{4+}—O^{2-}	56	201.6	4.5	194.0	193.1	198.9	201.2	203.8	214.0
Au^{3+}—O^{2-}	9	198.3	1.0	196.0	195.7	197.3	198.5	199.2	200.0
Hg^{2+}—O^{2-}	94	209.3	11.0	192.0	194.9	202.6	205.7	214.5	236.0

Table 9.4.1.9. *Atomic distances between oxygen and lanthanoids*

Atom pair	N	Mean	s.u.	d_1	Smallest 5%	First quartile	Median	Third quartile	d_2
La^{3+}—O^{2-}	317	244.1	9.2	222.0	230.1	237.7	243.1	249.9	268.0
Ce^{3+}—O^{2-}	75	239.2	7.5	220.0	225.5	234.5	238.2	246.1	254.0
Ce^{4+}—O^{2-}	49	234.1	4.9	222.0	224.5	234.0	235.1	236.7	242.0
Pr^{3+}—O^{2-}	57	239.1	4.8	230.0	232.2	235.7	238.8	241.8	252.0
Nd^{3+}—O^{2-}	185	235.4	6.4	218.0	224.1	232.0	235.5	239.3	250.0
Sm^{3+}—O^{2-}	45	228.8	4.2	218.0	221.2	225.5	229.3	232.6	236.0
Eu^{3+}—O^{2-}	47	231.4	5.4	220.0	222.7	227.2	231.8	235.6	242.0
Gd^{3+}—O^{2-}	78	228.2	5.7	216.0	219.4	223.9	227.6	231.9	240.0
Tb^{3+}—O^{2-}	36	229.4	5.7	216.0	218.8	225.0	230.9	233.3	238.0
Dy^{3+}—O^{2-}	39	226.9	5.6	214.0	216.9	222.5	228.1	231.1	236.0
Ho^{3+}—O^{2-}	48	227.6	5.4	218.0	220.2	223.3	226.7	231.3	242.0
Er^{3+}—O^{2-}	69	224.6	5.4	212.0	214.4	220.9	224.6	228.8	236.0
Tm^{3+}—O^{2-}	24	223.3	4.9	214.0	216.5	220.0	223.3	226.0	234.0
Yb^{3+}—O^{2-}	78	221.8	4.4	210.0	214.5	218.9	221.4	224.9	234.0
Lu^{3+}—O^{2-}	35	220.4	7.3	208.0	210.1	213.8	220.5	226.2	234.0

9.4.1.10. *Atomic distances between oxygen and actinoids*

Atom pair	N	Mean	s.u.	d_1	Smallest 5%	First quartile	Median	Third quartile	d_2
Th^{4+}—O^{2-}	90	237.7	5.8	220.0	225.0	235.5	238.8	241.4	248.0
Pa^{5+}—O^{2-}	21	233.7	3.0	226.0	228.1	231.6	233.8	235.9	240.0
U^{6+}—O^{2-}	290	181.3	9.6	156.0	168.3	175.4	178.8	188.8	206.0
Np^{6+}—O^{2-}	2	173.0	0.0	172.0	171.6	172.1	172.8	173.4	174.0
Pu^{3+}—O^{2-}	6	235.0	0.0	234.0	233.3	233.8	234.6	235.3	236.0
Am^{3+}—O^{2-}	4	236.5	1.9	234.0	234.2	235.0	236.0	238.0	240.0

Table 9.4.1.11. *Atomic distances in sulfides and thiometallates*

Atom pair	N	Mean	s.u.	d_1	Smallest 5%	First quartile	Median	Third quartile	d_2
Li^{+}—S^{2-}	19	251.0	20.7	200.0	209.9	242.5	249.0	262.2	350.0
Na^{+}—S^{2-}	93	295.2	33.6	0.0	269.6	280.1	287.2	299.1	500.0
K^{+}—S^{2-}	82	325.0	13.3	300.0	308.0	316.1	323.5	331.1	380.0
Rb^{+}—S^{2-}	26	338.2	12.8	300.0	318.6	329.5	338.0	345.0	400.0
Cs^{+}—S^{2-}	51	358.8	11.7	300.0	341.1	349.5	359.7	368.9	400.0
Mg^{2+}—S^{2-}	9	249.4	10.0	200.0	234.9	240.5	253.0	258.5	300.0
Ca^{2+}—S^{2-}	21	283.8	12.7	0.0	260.1	274.5	285.0	293.5	500.0
Sr^{2+}—S^{2-}	13	300.8	6.0	270.0	292.6	296.6	300.3	305.5	350.0
Ba^{2+}—S^{2-}	86	317.3	13.6	250.0	300.4	309.8	315.0	326.5	370.0
B—S	10	180.2	8.3	150.0	161.0	178.3	180.0	183.7	250.0
Al^{3+}—S^{2-}	20	225.7	8.9	180.0	210.0	221.3	223.6	230.0	300.0
Ga^{3+}—S^{2-}	61	223.3	5.6	0.0	212.1	220.8	223.7	226.2	500.0
In^{3+}—S^{2-}	66	247.0	12.1	0.0	220.6	241.2	247.4	255.3	500.0
Tl^{+}—S^{2-}	67	305.4	16.5	0.0	278.4	294.8	306.2	316.1	500.0
C—S	19	170.6	11.8	140.0	143.9	164.8	173.0	179.2	210.0
Si^{4+}—S^{2-}	25	210.9	8.2	180.0	202.5	208.8	211.0	213.5	250.0
Ge^{4+}—S^{2-}	44	215.9	9.2	0.0	208.4	214.2	218.3	219.9	500.0
Sn^{2+}—S^{2-}	38	263.1	20.7	0.0	231.8	251.0	261.3	271.5	500.0
Sn^{4+}—S^{2-}	63	248.4	18.9	0.0	231.4	235.9	243.5	256.8	500.0
Pb^{2+}—S^{2-}	111	274.4	28.5	0.0	231.1	269.9	279.7	289.1	500.0
N—S	65	154.1	9.9	100.0	138.2	149.6	154.8	157.9	210.0
P—S	67	201.8	6.6	150.0	189.6	197.6	201.9	207.4	250.0
As^{5+}—S^{2-}	16	214.6	6.9	150.0	193.6	214.0	215.0	216.0	250.0
As—S	97	221.5	16.1	150.0	191.9	217.2	222.4	225.6	310.0
Sb^{3+}—S^{2-}	114	244.1	12.6	200.0	227.4	239.3	242.7	247.2	310.0
Sb^{5+}—S^{2-}	9	233.4	4.1	200.0	226.9	232.1	233.2	235.5	280.0
Bi^{3+}—S^{2-}	77	263.1	12.7	240.0	248.4	255.7	260.1	267.1	320.0
Sc^{3+}—S^{2-}	18	254.9	5.9	0.0	244.9	251.5	255.3	257.8	500.0
Ti^{4+}—S^{2-}	22	242.5	9.4	0.0	224.2	239.5	242.6	245.0	500.0
V^{5+}—S^{2-}	9	218.3	7.6	0.0	208.9	212.5	218.5	220.8	500.0
Cr^{3+}—S^{2-}	32	240.1	5.5	200.0	233.2	236.0	240.3	243.2	300.0
Mn^{2+}—S^{2-}	35	246.1	11.8	0.0	227.5	237.9	243.0	256.2	500.0
Fe—S	117	230.4	13.6	180.0	212.4	220.1	229.1	239.2	280.0
Co^{3+}—S^{2-}	8	226.0	2.4	222.0	222.4	224.0	226.0	228.0	230.0
Co^{2+}—S^{2-}	6	234.7	2.0	232.0	230.4	232.0	234.0	236.5	238.0
Co^{0}—S^{0}	18	214.9	2.0	210.0	211.4	213.4	214.9	216.2	220.0
Ni—S	64	229.4	13.5	190.0	213.1	218.5	228.0	238.0	280.0
Cu—S	221	226.0	8.1	190.0	211.4	222.3	226.4	230.8	270.0
Zn^{2+}—S^{2-}	37	232.8	8.1	200.0	214.9	230.8	233.4	235.3	270.0

Table 9.4.1.11. *Atomic distances in sulfides and thiometallates (cont.)*

Atom pair	N	Mean	s.u.	d_1	Smallest 5%	First quartile	Median	Third quartile	d_2
Y^{3+}—S^{2-}	3	275.0	6.0	0.0	268.3	269.5	275.0	280.5	500.0
Zr^{4+}—S^{2-}	10	257.2	7.1	0.0	248.5	252.5	256.0	260.5	500.0
Nb—S	28	242.8	11.0	210.0	215.4	240.0	247.0	249.1	280.0
Mo—S	76	236.4	9.6	180.0	217.1	235.0	239.2	241.1	280.0
Ru—S	9	236.3	7.8	200.0	218.9	234.2	236.5	241.5	270.0
Rh—S	4	223.5	15.4	0.0	200.4	202.0	228.0	232.0	500.0
Pd—S	29	232.7	4.2	0.0	225.4	229.2	233.2	236.2	500.0
Ag^{+}—S^{2-}	102	252.7	15.2	220.0	227.4	244.1	250.0	259.0	320.0
Cd^{2+}—S^{2-}	37	254.4	10.6	200.0	241.7	245.6	252.6	263.5	300.0
La^{3+}—S^{2-}	43	292.8	15.7	250.0	264.1	285.8	290.3	301.7	350.0
Hf—S	5	259.4	7.7	0.0	250.5	252.5	259.0	265.5	500.0
Ta—S	40	242.6	7.8	200.0	224.0	239.1	242.4	247.0	300.0
W—S	6	250.3	13.6	200.0	238.6	240.5	242.0	253.5	300.0
Re—S	15	233.4	12.1	0.0	199.5	233.5	237.0	238.2	500.0
Os—S	29	237.7	3.4	0.0	229.4	235.8	237.9	240.2	500.0
Pt—S	14	224.7	19.6	0.0	189.4	223.0	232.0	237.0	500.0
Au—S	7	234.1	19.5	200.0	216.7	226.8	229.0	231.2	300.0
Hg^{2+}—S^{2-}	63	244.5	11.1	200.0	229.1	238.4	244.1	251.5	300.0
Ce—S	31	290.5	9.5	0.0	278.3	283.4	288.2	298.2	500.0
Pr—S	7	288.4	15.7	0.0	270.7	275.5	287.0	308.2	500.0
Nd—S	12	286.8	7.8	0.0	276.4	278.0	287.0	294.7	500.0
Sm—S	15	276.9	13.7	0.0	233.5	276.8	281.2	284.5	500.0
Eu—S	26	292.5	9.4	0.0	275.3	285.0	294.0	299.2	500.0
Gd—S	5	289.0	27.1	0.0	274.2	274.8	275.7	283.5	500.0
Ho—S	8	263.8	7.6	0.0	246.8	261.0	267.0	268.7	500.0
Er—S	15	261.7	28.3	0.0	193.5	258.8	266.2	272.5	500.0
Yb—S	22	271.3	9.5	0.0	258.2	265.5	270.5	273.7	500.0
Lu—S	11	267.4	4.8	0.0	260.5	264.5	266.5	270.5	500.0
Th—S	15	283.9	11.0	0.0	259.5	278.8	285.5	290.5	500.0
U—S	46	277.8	9.1	0.0	264.6	274.3	276.4	279.1	500.0
Np—S	2	277.0	19.8	0.0	262.2	263.0	264.0	291.0	500.0
Pu—S	6	293.3	10.3	0.0	276.6	289.0	293.0	301.0	500.0

Table 9.4.1.12. *Contact distances between some negatively charged elements*

Atom pair	N	Mean	s.u.	d_1	Smallest 5%	First quartile	Median	Third quartile	d_2
O^{2-}—O^{2-}	14849	254.5	37.9	0.0	205.4	240.0	255.4	271.0	500.0
S^{2-}—S^{2-}	1414	343.1	42.8	0.0	279.7	325.9	342.6	364.0	500.0
Se^{2-}—Se^{2-}	314	360.5	46.3	0.0	245.4	339.6	363.2	388.2	500.0
Te^{2-}—Te^{2-}	135	392.5	51.2	0.0	281.5	373.8	401.5	425.6	500.0
F^{-}—F^{-}	2096	256.8	37.2	0.0	211.0	243.2	257.5	270.3	500.0
Cl^{-}—Cl^{-}	1667	341.3	41.6	0.0	301.7	326.1	341.2	359.7	500.0
Br^{-}—Br^{-}	534	364.3	47.5	0.0	314.4	350.5	367.5	384.9	500.0
I^{-}—I^{-}	489	396.4	46.9	0.0	313.6	384.6	402.8	419.8	500.0
O^{2-}—F^{-}	723	269.1	28.4	0.0	233.0	255.5	268.2	280.4	500.0
O^{2-}—Cl^{-}	827	313.5	35.3	0.0	267.3	302.9	314.4	328.3	500.0
O^{2-}—Br^{-}	230	332.0	32.9	0.0	293.5	319.4	331.7	344.3	500.0
O^{2-}—I^{-}	109	353.6	44.4	0.0	288.9	345.6	359.4	374.5	500.0
S^{2-}—F^{-}	27	294.3	61.7	0.0	160.7	259.8	299.0	334.2	500.0
S^{2-}—Cl^{-}	53	349.3	38.8	0.0	279.3	330.6	347.7	373.5	500.0
S^{2-}—Br^{-}	26	353.0	35.2	0.0	310.6	344.5	351.0	373.5	500.0
S^{2-}—I^{-}	42	357.9	54.9	0.0	306.1	360.7	368.0	375.0	500.0

9.2.2 (*cont.*)

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