International Tables for Crystallography (2006). Vol. C, Table 9.4.1.1, pp. 779–780.

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

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