

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> ₁	Smallest 5%	First quartile	Median	Third quartile	<i>d</i> 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	<i>N</i>	Mean	s.u.	<i>d</i> ₁	Smallest 5%	First quartile	Median	Third quartile	<i>d</i> 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

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

Atom pair	<i>N</i>	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

9.4. TYPICAL INTERATOMIC DISTANCES: INORGANIC COMPOUNDS

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

Atom pair	<i>N</i>	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

9. BASIC STRUCTURAL FEATURES

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

Atom pair	<i>N</i>	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	<i>N</i>	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