

9. BASIC STRUCTURAL FEATURES

9.4.1.10. Atomic distances between oxygen and actinoids

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

9.4. TYPICAL INTERATOMIC DISTANCES: INORGANIC COMPOUNDS

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