

9.6. TYPICAL INTERATOMIC DISTANCES: ORGANOMETALLIC COMPOUNDS AND COMPLEXES

Table 9.6.3.1. *Ligand index (cont.)*

Contact atom	Ligand class	Ligand class identifier
Nitrogen (<i>cont.</i>)	amidinate [RNC(R)NR]	4.11
	Schiff bases	4.12
	phthalocyanines, porphyrins, pyrroles	4.13
	pyrazolate, imidazolate and derivatives	4.14
	pyridine, polypryidyls (bpy, <i>o</i> -phen)	4.15
	pyrazines, pyridazines, pyrimidines	4.16
	other N ₂ ligands (NRNR ₂ , NNR ₂ , NRNR)	4.17
	triazenido (RNNNR)	4.18
	hydrazones and related species (NR ₂ N=CR)	4.19
	oximes	4.20
	<i>N</i> -nitrite (NO ₂)	4.21
	amine (NR ₃)	4.22
	borazines	4.23
	Oxygen	oxo (O)
hydroxy (OH)		5.2
alkoxy, aryloxy, <i>etc.</i> (OR)		5.3
<i>O</i> -ketones (OCR ₂), urea		5.4
carboxylates (O ₂ CR)		5.5
oxalate (O ₂ CCO ₂)		5.6
acetylacetonates [RC(O)CRC(O)CR]		5.7
α , β -diones (<i>e.g.</i> <i>o</i> -quinones)		5.8
carbonate (CO ₃ ²⁻)		5.9
<i>N</i> -oxides (<i>e.g.</i> pyridine <i>N</i> -oxide)		5.10
nitrate (NO ₃ ⁻)		5.11
<i>O</i> -nitrite (NO ₂ ⁻)		5.12
dioxygen, peroxides		5.13
phosphine oxides (OPR ₃)		5.14
phosphate (PO ₄ ³⁻)		5.15
other P—O anions		5.16
<i>O</i> -dialkyl sulfoxides (OSR ₂)		5.17
sulfate (SO ₄ ²⁻)		5.18
other S—O anions (sulfonates, <i>etc.</i>)		5.19
<i>O</i> -SO ₂		5.20
other oxyanions (<i>e.g.</i> ClO ₄ ⁻)		5.21
aqua		5.22
alcohols (ROH)		5.23
ethers (ROR')		5.24
miscellaneous (η^2 -acyl, η^2 -CO ₂ , μ -NCO)	5.25	
Fluorine	fluoride (F)	6.1
	fluoroanions (BF ₄ ⁻ , PF ₆ ⁻)	6.2
Silicon	miscellaneous	7.1
Phosphorus	phosphorus (P)	8.1
	phosphinidenes (PR)	8.2
	phosphides (PR ₂)	8.3
	oligo-phosphorus ligands (P ₃ , PR ₂ PR ₂ , PRPR, <i>etc.</i>)	8.4
	phosphines (PR ₃)	8.5
	diphosphines (<i>e.g.</i> diphos)	8.6
	phosphites [P(OR) ₃]	8.7
	aminophosphines, cyclotriphosphazanyl, misc. P—N ligands	8.8
Sulfur	sulfides (S)	9.1
	thiolates (SR)	9.2

Table 9.6.3.1. *Ligand index (cont.)*

Contact atom	Ligand class	Ligand class identifier	
Sulfur (<i>cont.</i>)	<i>S</i> -thiocyanate (SCN)	9.3	
	thioketones, thiourea (S=CR ₂)	9.4	
	thiocarboxylates (S ₂ CR ⁻)	9.5	
	thiocarbamates (S ₂ CNR ₂ ⁻)	9.6	
	xanthates (S ₂ COR ⁻), dithio-carbonates	9.7	
	trithiocarbonate (CS ₃ ²⁻), thioxanthates	9.8	
	α , β -dithiones	9.9	
	phosphine sulfides	9.10	
	dithiophosphinates (S ₂ PR ₂ ⁻)	9.11	
	polysulfur ligands (S ₂ , SSR, <i>etc.</i>)	9.12	
	thioethers (SR ₂)	9.13	
	<i>S</i> -SO ₂ , <i>S</i> -SO ₃ , <i>etc.</i>	9.14	
	disulfides (RSSR)	9.15	
	<i>S</i> -dialkyl sulfoxides (R ₂ SO)	9.16	
	miscellaneous (η^2 -CS ₂)	9.17	
	Chlorine	chloride (Cl)	10.1
	Arsenic	arsines (AsR ₃)	11.1
miscellaneous		11.2	
Selenium	miscellaneous	12.1	
Bromine	bromide (Br)	13.1	
Tellurium	miscellaneous	14.1	
Iodine	iodide (I)	15.1	

number of the metal. For a given metal, the first line of an entry in Table 9.6.3.3 gives statistics covering all appropriate occurrences of metal–ligand distances. Further lines give statistics for metal–ligand distances for subdivision based largely on chemical criteria (*e.g.* metal oxidation state or coordination number). Cases where one atom of a ligand bridges two or more metal atoms were included only when the metal atoms were all of the same type and, unless specified, only when the metal–ligand distances were symmetrical (range for distances ≤ 0.1 Å).

In many instances, the number of structures having interatomic distances involving a given metal for a particular ligand is too small (< 4) for statistics to be quoted. In these cases, individual structures, and the distances in them, are given. These structures are identified by their CSD reference code (*e.g.* BOZMIN); short-form literature references, ordered alphabetically by reference code, are in Appendix 2.

Each line of Table 9.6.3.3 contains nine columns of which six record the statistics of the bond-length distribution described above. The content of the remaining three columns: Bond, Substructure, and Note, are described below.

9.6.3.1. *The 'Bond' column*

This specifies the atom pair to which the line refers. Therefore, in the case of triethylphosphine complexes (section 8.5.2), there are 18 lines, in which the bond column contains P—C, followed by 17 entries for Ti—P through to Au—P, indicating statistics for both intraligand and metal–ligand atom pairs.

9.6.3.2. *Definition of 'Substructure'*

This column provides details of any subdivision of particular metal–ligand bonds that has been applied. Thus, for terminal