Supplement

Tables of Bond Lengths determined by *X*-Ray and Neutron Diffraction. Part 2.† Organometallic Compounds and Co-ordination Complexes of the *d*- and *f*-Block Metals

A. Guy Orpen * and Lee Brammer
Department of Inorganic Chemistry, The University, Bristol BS8 1TS
Frank H. Allen, Olga Kennard, and David G. Watson
Cambridge Crystallographic Data Centre, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW
Robin Taylor
I.C.I. Plant Protection Division, Jealott's Hill Research Station, Bracknell, Berkshire RG12 6EY

Average lengths for metal–ligand bonds are reported, together with some intraligand distances, for complexes of the *d*- and *f*-block metals. Mean values are presented for 325 different bond types involving metal atoms bonded to H, B, C, N, O, F, Si, P, S, Cl, As, Se, Br, Te, or I atoms of the ligands.

The determination of molecular geometry is of vital importance to our understanding of chemical structure and bonding. The majority of experimental data have come from *X*-ray and neutron diffraction, microwave spectroscopy, and electron diffraction. Over the years compilations of results from these techniques have appeared sporadically. The first major compilation was Chemical Society Special Publication no. 11: 'Tables of Interatomic Distances and Configuration in Molecules and Ions.'[1] This volume summarized results obtained by diffraction and spectroscopic methods prior to 1956; a supplementary volume[2] extended this coverage to 1959. Summary tables of bond lengths between carbon and other elements were also published in volume 3 of 'International Tables for *X*-Ray Crystallography.'[3] Some years later the Cambridge Crystallographic Data Centre[4] produced an atlas-style compendium of all organic, organometallic, and metal complex crystal structures published in the period 1960—1965.[5] More recently a survey of geometries determined by spectroscopic methods[6] has extended coverage in this area to mid-1977. A notable compendium of structural data, without geometric information, was given in 'Comprehensive Organometallic Chemistry,'[7] covering all complexes with metal–carbon bonds. The BIDICS series,[8] which finished in 1981, provided for some years a full coverage of metal complexes giving both bibliographic and geometric information. There have also been valuable annual summaries, without geometric information, on the structures of organometallic compounds determined by diffraction methods.[9]

The production of further comprehensive compendia of *X*-ray and neutron diffraction results has been precluded by the steep rise in the number of published crystal structures, as illustrated by Figure 1. Printed compilations have been effectively susperseded by computerized databases. In particular the Cambridge Structural Database (CSD) now contains bibliographic, chemical, and numerical results for some 70 000 organocarbon crystal structures. This machine-readable file fulfils the function of a comprehensive structure-by-structure compendium of molecular geometries. However the amount of data now held in CSD is so large that there is also a need for concise, printed tabulations of average molecular dimensions.

The only tables of average geometry in general use are those contained in the Chemical Society Special Publications[1,2] of 1958 and 1965, which list mean bond lengths for a variety of atom pairs and functional groups. Since these early tables were based on data obtained before 1960, we have used CSD to prepare a new table of average bond lengths in organic compounds[10] and in metal complexes. The table given here (Table 3) specifically lists average lengths for metal–ligand distances, together with intraligand distances, involving bonds between the *d*- and *f*-block metals (Sc–Zn, Y–Cd, La–Hg, Ce–Lu, and Th–U) and atoms H, B, C, N, O, F, Si, P, S, Cl, As, Se, Br, Te, and I of ligands. Mean values are presented for 325 different bond types involving such metal–ligand bonds.

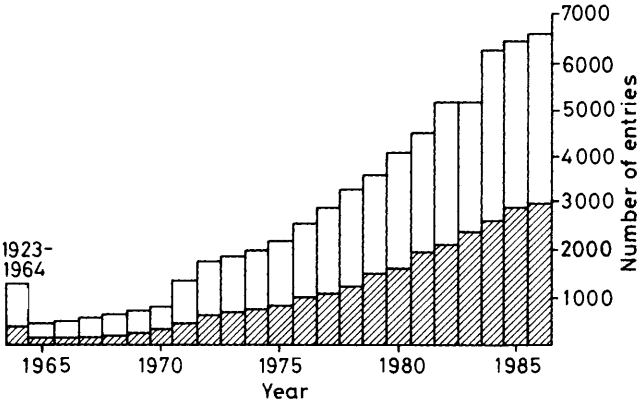


Figure 1. Growth of the Cambridge Structural Database as number of entries increases annually. The structures containing *d*- or *f*-block metals are indicated by shading

Methodology

Selection of Crystallographic Data.—All results given in Table 3 are based on *X*-ray and neutron diffraction results retrieved from the September 1985 version of CSD. Neutron diffraction data only were used to derive mean bond lengths involving hydrogen atoms. This version of CSD contained results for 49 854 single-crystal diffraction studies of organocarbon compounds; 9 802 of these satisfied the acceptance criteria listed below and were used in the averaging procedures.

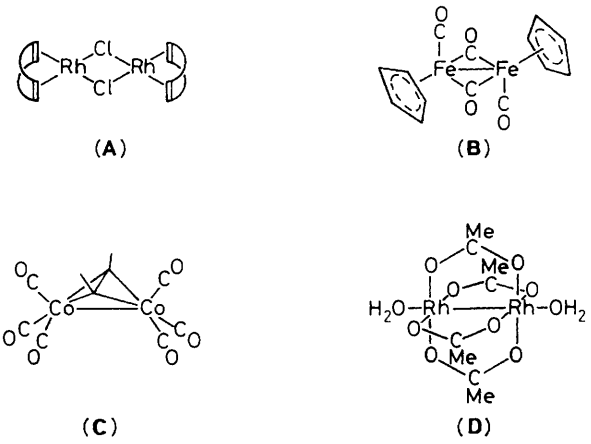
† Part 1 is ref. 10.

(*i*) The structure contains a *d*- or *f*-block metal; (*ii*) atomic co-ordinates for the structure have been published and are available in CSD; (*iii*) the structure was determined from diffractometer data; (*iv*) the structure does not contain unresolved numeric data errors from the original publication (such errors are usually typographical and are normally resolved by consultation with the authors); (*v*) only structures of higher precision were included on the basis that *either* (*a*) the crystallographic *R* factor was $\leqslant 0.07$ and the reported mean estimated standard deviation (e.s.d.) of the C–C bond lengths was $\leqslant 0.030$ Å (corresponds to AS flag = 1, 2, or 3 in CSD[4]), *or* (*b*) the crystallographic *R* factor $\leqslant 0.05$ and the mean e.s.d. for C–C bonds was not available in the database (AS = 0 in CSD); (*vi*) where the structure of a given compound has been determined more than once within the limits of (*i*)—(*v*), then only the most precise determination was used.

The structures used in Table 3 do not include compounds whose structure precludes them from CSD (*i.e.* not containing 'organic' carbon). In practice structures including at least one C–H bond are taken to contain 'organic' carbon. Thus the entry for Cr–CO distances has a contribution from $[NEt_4][Cr(\mu\text{-}H)(CO)_{10}]$ but not from $K[Cr(\mu\text{-}H)(CO)_{10}]$ or $[Cr(CO)_6]$.

Program System.—All calculations were performed on a University of Bristol VAX 11/750 computer. Programs BIBSER, CONNSER, RETRIEVE,[4] and GEOSTAT,[11,12] as locally modified, were used. A stand-alone program was written to implement the selection criteria, whilst a new program (STATS) was used for statistical calculations described below. It was also necessary to modify CONNSER to improve the precision with which it locates chemical substructures. In particular the program was altered to permit the location of atoms with specified co-ordination numbers. This was essential in the case of carbon so that atoms with co-ordination numbers two, three, and four (equivalent to formal hybridization states sp^1, sp^2, and sp^3) could be distinguished easily and reliably. Considerable care was taken to ensure that the correct molecular fragment was located by GEOSTAT in the generation of geometrical tabulations. Searches were conducted for all metals together, and statistics for individual metal elements and subdivision of the entry for a given metal carried out subsequently. An important modification of GEOSTAT allowed for calculation of metal atom co-ordination number with due allowance for multi-hapto ligands and μ ligands. Thus η^5-C_5H_5, η^6-C_6H_6, and other η^5 and η^6 ligands were assigned to occupy three co-ordination sites, η^3 and η^4 ligands such as allyls and dienes to occupy two co-ordination sites, and η^2 ligands such as alkenes to one site, and so on. The approach taken in dealing with (μ) bridging ligands was that when a metal–metal bond is bridged by one atom of a ligand [*e.g.* as in Cl, CO, OMe, *etc.* as in (**A**) and (**B**)] then only the non-metal atom is counted as occupying a co-ordination site. For the relatively rare case of bridging polyhapto ligands (in which the bridging atoms are linked by direct bonds) the assignment follows logically, thus μ-η^2,η^2-alkyne (see **C**) occupies one site on each metal. Bridging ligands which do not have one atom bonded to both metals [*e.g.* acetate in (**D**)] contribute to metal co-ordination numbers as do terminal ligands. In examples (**A**)—(**D**) below the metal atoms therefore have co-ordination numbers as follows: (**A**), Rh 4; (**B**), Fe 6; (**C**), Co 4; (**D**), Rh 6. For cases where co-ordination number is very difficult to assign, notably where a metal atom is bonded to more than one other metal atom as in metal cluster complexes, no assignment was attempted.

The non-location of hydrogen atoms presents major difficulties both in the determination of co-ordination numbers for metal atoms, and for correct identification of ligands (*e.g.* to distinguish methoxide from methanol). Care was therefore taken to exclude cases where any ambiguity existed [*e.g.* no data taken for $M\text{–}OCH_3$ and $M\text{–}O(H)CH_3$ distances when both are present in a structure in which hydrogen atom positions were not reported].



Classification of Bonds.—The classification of metal–ligand bonds in Table 3 is based on the ligating contact atom. Thus all metal–boron distances appear in sections 2.1—2.3 of Table 3, all metal–carbon distances in sections 3.1—3.22, and so on. Where intraligand interatomic distances (*e.g.* P–C distances in tertiary phosphines) are given in Table 3, they are averaged over all metals and precede the individual metal–ligand interatomic distances for that ligand.

Table 3 is designed to: (*i*) appear logical, useful, and reasonably self-explanatory to chemists, crystallographers, and others who may use it; (*ii*) permit a meaningful average value to be cited for each bond length. With reference to (*ii*), it was considered that a sample of bond lengths could be averaged meaningfully if: (*a*) the sample was unimodally distributed; (*b*) the sample standard deviation (σ) was reasonably small, ideally less than *ca.* 0.04 Å; (*c*) there were no conspicuous outlying observations (those which occurred at $>4\sigma$ from the mean were automatically eliminated from the sample by STATS, other outliers were inspected carefully); (*d*) there was no compelling chemical reason for further subdivision of the sample. It should be noted that Table 3 is not intended to be complete in covering all possible ligands. Its purpose is to provide information on the interatomic distances for ligands of the greatest *chemical* importance, notably for those which are simple and/or common.

Statistics.—Where there are less than four independent observations of a given bond length, then each individual observation is given explicitly in Table 3. In all other cases the following statistics were generated by the program STATS.

(*i*) The unweighted sample mean, *d*, where equation (1) holds

$$d = \sum_{i=1}^{n} d_i/n \qquad (1)$$

and d_i is the *i*th observation of the bond length in a total sample of *n* observations. Recent work [13–15] has shown that the unweighted mean is an acceptable (even preferable) alternative to the weighted mean, where the *i*th observation is assigned a weight equal to $1/\mathrm{var}(d_i)$. This is especially true where structures have been pre-screened on the basis of precision.

(*ii*) The sample median, *m*. This has the property that half of the observations in the sample exceed *m*, and half fall short of it.

(*iii*) The sample standard deviation, σ, where equation (2) holds.

$$\sigma = \left[\sum_{i=1}^{n} (d_i - d)^2/(n-1)\right]^{\frac{1}{2}} \qquad (2)$$

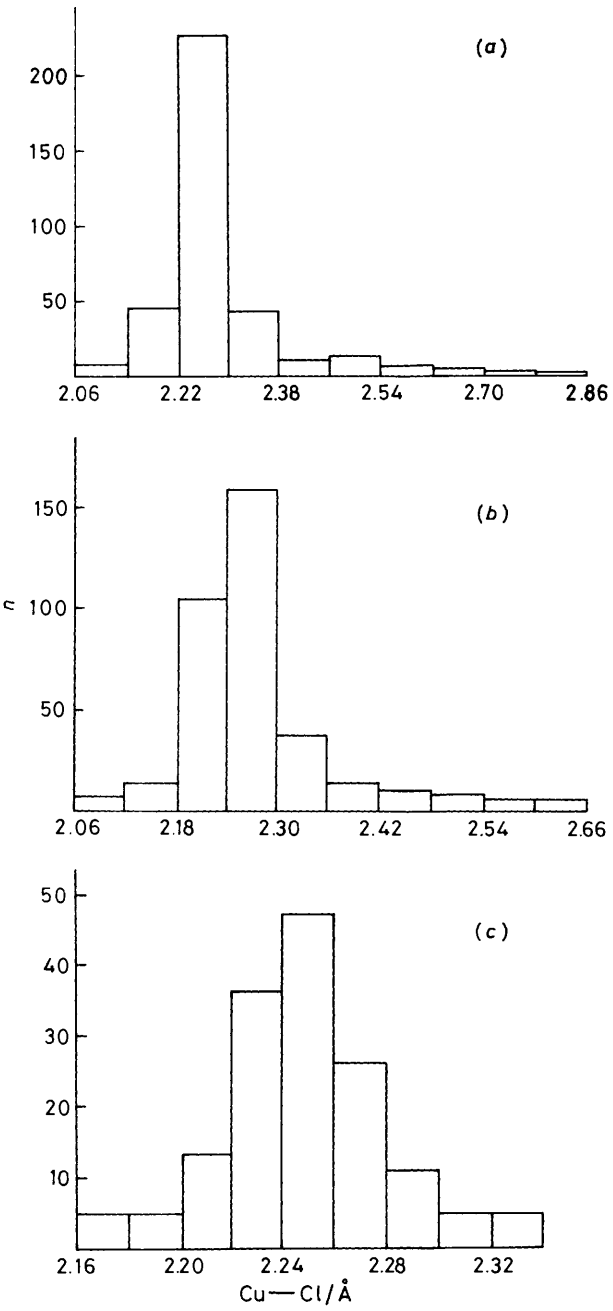


Figure 2. Effects of outlier removal and subdivision based on co-ordination number and oxidation state for the Cu–Cl bond. (*a*) All data; (*b*) all data without outliers [$>4\sigma$ (sample) from mean]; (*c*) all data for which Cu is four co-ordinate, Cu^{II}. Relevant statistics (see text) are:

	d	*m*	σ	q_l	q_u	*n*
(*a*)	2.282	2.255	0.105	2.233	2.296	366
(*b*)	2.276	2.254	0.092	2.232	2.292	362
(*c*)	2.248	2.246	0.032	2.233	2.263	153

(*iv*) The lower quartile for the sample, q_l. This has the property that 25% of the observations are less than q_l and 75% exceed it.

(*v*) The upper quartile for the sample, q_u. This has the property that 25% of the observations exceed q_u and 75% fall short of it.

(*vi*) The number, *n*, of observations in the sample.

The statistics given in Table 3 correspond to distributions for which the automatic 4σ cut-off (see above) had been applied and any manual removal of additional outliers (an infrequent operation) had been performed. In practice a very small percentage of observations was excluded by these methods. The major effect of removing outliers is to improve the sample standard deviation, as shown in Figure 2(*b*), in which four (out of 366) observations are deleted.

The statistics chosen for tabulation effectively describe the distribution of bond lengths in each case. For a symmetrical, normal distribution, the mean (*d*) will be approximately equal to the median (*m*), the lower and upper quartiles (q_l, q_u) will be approximately symmetric about the median ($m - q_l \approx q_u - m$), and 95% of the observations may be expected to lie within $\pm 2\sigma$ of the mean value. For a skewed distribution *d* and *m* may differ appreciably and q_l and q_u will be asymmetric with respect to *m*. When a bond length distribution is negatively skewed, *i.e.* very short values are more common than very long values, then it may be due to thermal motion effects; the distances used to prepare Table 3 were not corrected for thermal libration.

In a number of cases the initial bond length distribution was clearly not unimodal as in Figure 2(*a*). Where possible such distributions were resolved into their unimodal components [as in Figure 2(*c*)] on chemical or structural critieria. The case illustrated in Figure 2, for Cu–Cl bonds, is one of the most spectacular examples, due to the dramatic consequences of oxidation state and co-ordination number (and Jahn–Teller effects) on the structures of copper complexes.

Content and Arrangement of Table of Interatomic Distances

Table 1 indicates how the interatomic distances covered in Table 3 are subdivided. Metal–ligand distances are grouped according to the ligand contact atom, which leads to ordering by atomic number of that contact atom. For a given contact atom (H, B, C, *etc.*) the ligands are grouped by type as listed in Table 1. The class of ligand is identified numerically (*e.g.* alkoxides are class 5.3, alcohols class 5.23, ethers 5.24. *etc.*). Particular ligands are identified by a third number (*e.g.* methoxide is ligand 5.3.1). Finally, alternative bonding modes for a particular ligand are denoted by a fourth number [*e.g.* terminal alkoxides 5.3.1.1, bridging (μ) alkoxides 5.3.1.2]. In general the bonding modes are arranged in the sequence σ, η^2, ... η^n; μ, μ_3, *etc.*, where σ and η^n imply bonding of one or more atoms of the ligand to metal atoms, and μ, μ_3 *etc.* that two or more metal atoms are bonded to the ligand. Thus acetates are represented by entries headed 5.5.2.1 (σ), 5.5.2.2 (chelating), and 5.5.2.3 (bridging, μ). For each ligand the metal–ligand bonds then follow a sequence of ascending atomic number of the metal. For a given metal the first line of an entry in Table 3 gives statistics covering all appropriate occurrences of metal–ligand distances. Further lines give statistics for metal–ligand distances for subdivisions based largely on chemical criteria (*e.g.* metal oxidation state or co-ordination 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).

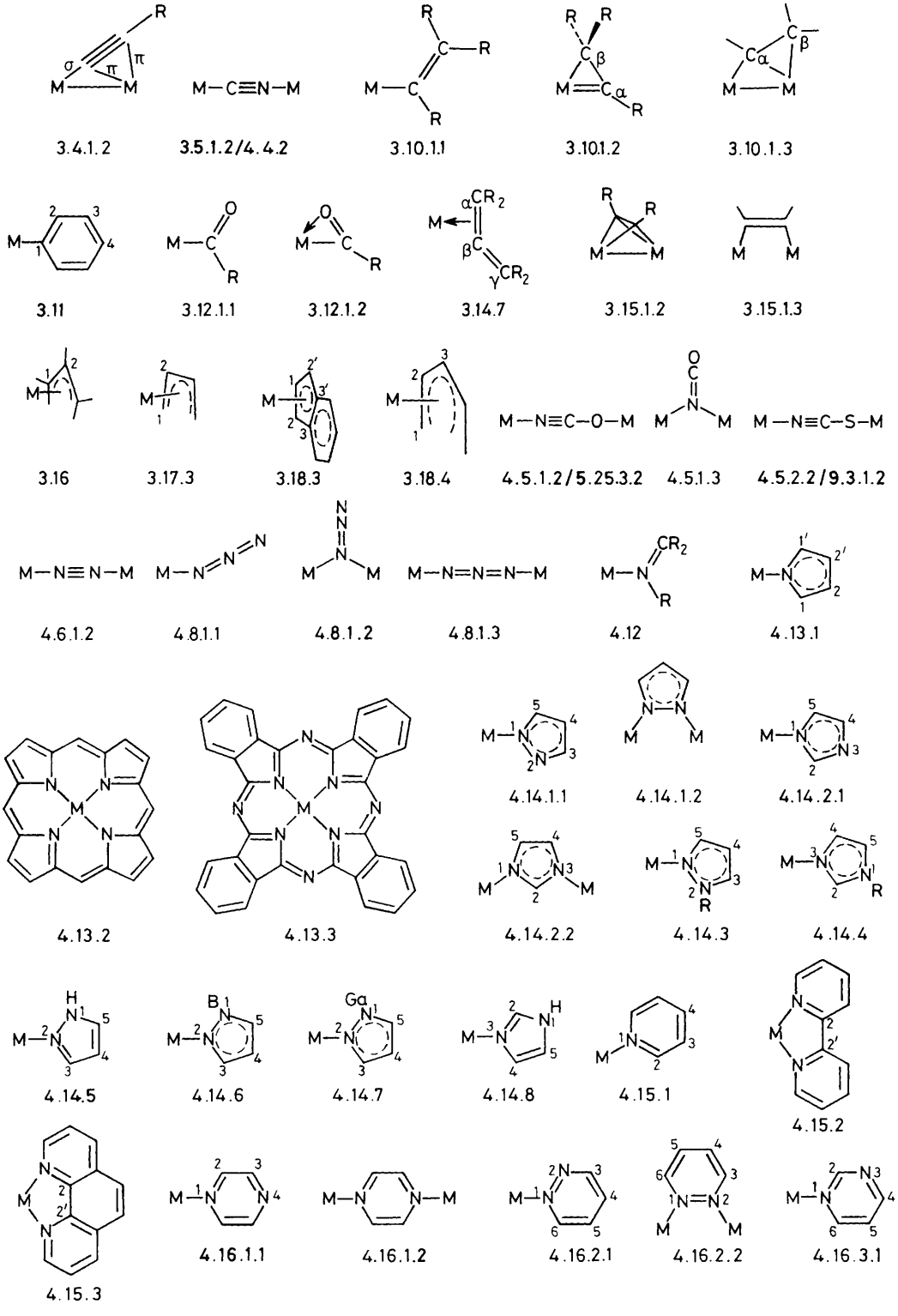
In many instances the number of structures having interatomic distances involving a given metal for a particular ligand is too small (<4) for statistics to be quoted. In these cases individual structures, and the distances in them, are given. These structures are identified by their CSD reference code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

Each line of Table 3 contains nine columns of which six record the statistics of the bond length distribution described

above. The contents of the remaining three columns, Bond, Substructure, and Note, are described below.

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.

Definition of 'Substructure'.—This column provides details of any subdivision of particular metal–ligand bonds which has been applied. Thus for terminal iron–chlorine bonds (in section 10.1.1.1) the second and third lines of the Fe–Cl entry refer to complexes in which the iron atom is four co-ordinate and in oxidation states (II) and (III) respectively. In some cases subdivision has been carried out on the basis of ligand substituents in those cases where a well defined sub-distribution was observed. For clarity in a number of cases the ligand structure and numbering scheme is illustrated in Figure 3. The reader will be aware that formal oxidation state is not always well defined; where no assignment was possible then this is indicated by (–) rather than the roman numeral used else-



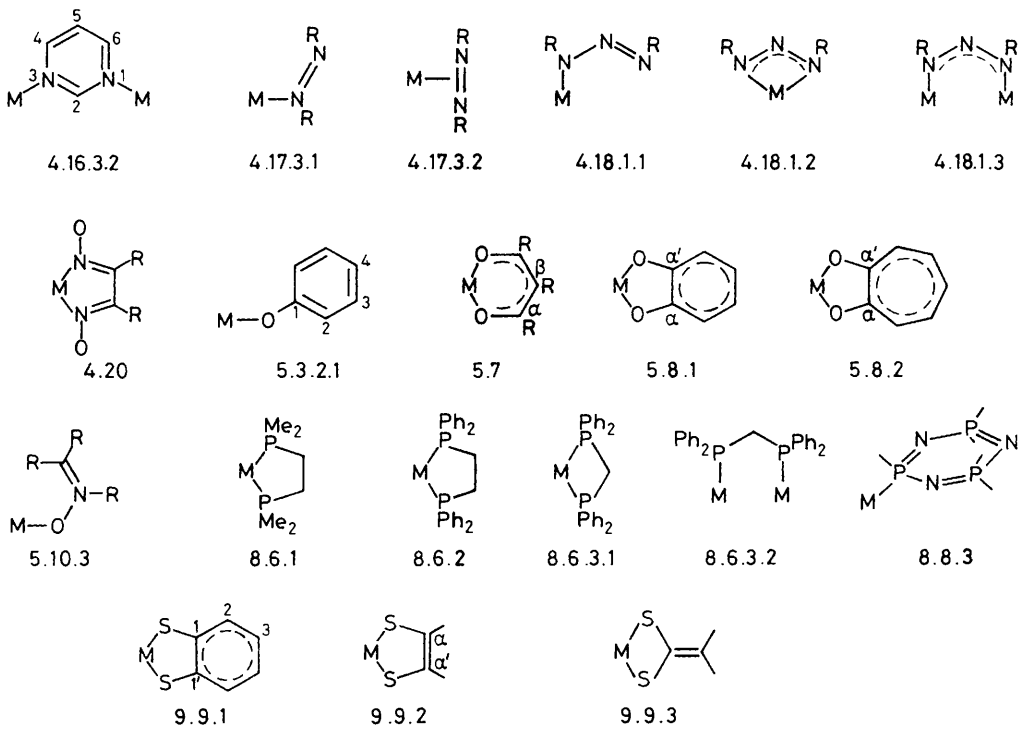


Figure 3. Diagrams of ligands in Table 3, showing table entry number and ligand atom labelling

where. Finally cases where the ligand oxidation state is variable are identified (*e.g.* for O_2, *ortho*-quinones, *etc.*) by references to the footnotes at the end of Table 3.

Use of the 'Note' Column.—The 'Note' column refers to the footnotes collected in Appendix 1. These record additional information as follows: (*a*) notable features of the distribution of distances, *e.g.* likely bias due to dominance by one structure or substructure, skewness, bimodality (subdivisions of the entry usually follow, which remove these features whenever possible); (*b*) further details of the chemical substructure, such as the exclusion of structures with particular *trans* ligands; (*c*) details of exclusion criteria used for a given entry or group of entries, such as the constraint that the two M–Cl distances, in bridging (μ) chloride complexes, differ by <0.1 Å (section 10.1.1.2); (*d*) references to previously published surveys of crystallographic results relevant to the entry in question. We do not claim that these entries are in any way comprehensive and we would be grateful to authors for notification (to A.G.O.) of any omissions. This will serve to improve the content of any future version of Table 3.

Locating an Entry in Table 3.—Table 2 provides a 'guide' to the contents of Table 3. The number of entries for which individual examples of metal–ligand distances are quoted, and the number of entries for which statistics are given in Table 3, are listed for each metal. Inspection of Table 2 shows which element pairs have no bond lengths recorded in Table 3. Thus while there are no cobalt–fluorine distances in Table 3, there are six classes of cobalt–phosphorus distances for which there are examples quoted, and ten for which statistics are given.

Let us say one wished to find typical lengths for cobalt–triethylphosphine (Co–PEt_3) bonds. Table 1 shows that PEt_3, a tertiary phosphine, falls under ligand class 8.5. In Table 3 the section dealing with such ligands starts with 8.5.1 (trimethylphosphine) followed by 8.5.2 (triethylphosphine). Under this section we find that Co–PEt_3 bonds average 2.208 Å in length (with sample standard deviation $\sigma = 0.039$ Å), and in cobaltacarbaboranes the average is 2.224 Å and for $Co(\eta\text{-}C_5H_5)L_2$ species the average is 2.147 Å.

Polydentate ligands with different elements able to act as contact atoms present particular difficulty. The convention we have adopted is to place the individual M–L interatomic distances under separate entries according to the contact element. Thus thiocyanate (SCN) appears in ligand class 4.5 when *N*-bonded (*i.e.* isothiocyanate M–NCS) and in ligand class 9.3 when *S*-bonded (M–SCN). When bridging with both S and N bonded to metals (as M–NCS–M′) then the M–N distances (as well as all intraligand distances) will be under ligand class 4.5 and M′–S distances under ligand class 9.3. Thus in such cases the intraligand dimensions will accompany the metal–ligand distances in the first ligand class (*i.e.* the lower numbered class).

Discussion

Table 3 has been derived from CSD, and as a result does not contain every precisely determined metal–ligand interatomic distance. For example there are many ammine (M–NH_3), carbonyl (M–CO), halide (M–Cl *etc.*), and aquo (M–OH_2) complexes which do not fall within the scope of CSD. For such bond types, and other metal–non-metal bond-length information, the interested reader is referred to the Inorganic Crystal Structure Database.[16]

The tabulation given here is a first attempt to obtain average dimensions for (*d*- and *f*-block) metal–ligand and intraligand bonds. Inspection of Table 3 shows that, in general, the sample standard deviations of metal–contact atom interatomic distances are typically larger than those of the intraligand distances [*e.g.* for Fe–PPh_3 complexes (section 8.5.3), Fe–P mean 2.237, σ 0.038 Å, *cf.* P–C mean 1.828, σ 0.014 Å]. There are several factors which cause this phenomenon. First, in many (but not all) cases, no account has been taken of substituent effects at the metal, such as the *trans* influence of other ligands. In contrast the substituent pattern at the ligand is usually well defined, therefore the chemical causes for variation in the metal–ligand and intraligand distances are different. Secondly, it is likely that metal–ligand bonds are softer, *i.e.* have lower force

Table 1. Ligand index

Contact atom	Ligand class	Ligand class identifier	Contact atom	Ligand class	Ligand class identifier
Hydrogen	Hydrides	1.1	Oxygen	Oxalate (O_2CCO_2)	5.6
	Tetrahydroborate (BH_4^-)	1.2		Acetylacetonates [RC(O)CRC(O)CR]	5.7
Boron	Borohydrides	2.1		α,β-Diones (*e.g. o*-quinones)	5.8
	Boranes/carbaboranes	2.2		Carbonates (CO_3^{2-})	5.9
	Boroles, borylenes, other heteroboracycles	2.3		*N*-Oxides (*e.g.* pyridine *N*-oxide)	5.10
Carbon	Carbide (C)	3.1		Nitrate (NO_3^-)	5.11
	Carbynes/alkylidynes (CR)	3.2		*O*-Nitrite (NO_2^-)	5.12
	Vinylidenes/alkenylidenes (CCR_2)	3.3		Dioxygen, peroxides	5.13
	Acetylides/alkynyls (CCR)	3.4		Phosphine oxides (OPR_3)	5.14
	Cyano (CN)	3.5		Phosphate (PO_4^{3-})	5.15
	Isocyanides (CNR)	3.6		Other P–O anions	5.16
	Carbon monoxide (CO)	3.7		*O*-Dialkyl sulphoxides (OSR_2)	5.17
	Thiocarbonyl (CS)	3.8		Sulphate (SO_4^{2-})	5.18
	Carbenes/alkylidenes (CR_2)	3.9		Other S–O anions (sulphonates, *etc.*)	5.19
	Vinyls/alkenyls ($CRCR_2$)	3.10		*O*-SO_2	5.20
	Aryls (C_6R_5)	3.11		Other oxyanions (*e.g.* ClO_4^-)	5.21
	Acyls [C(O)R]	3.12		Aquo	5.22
	Alkyls (CR_3)	3.13		Alcohols (ROH)	5.23
	η-Alkenes (C_2R_4, allenes, *etc.*)	3.14		Ethers (ROR′)	5.24
	Alkynes (RCCR)	3.15		Miscellaneous (η^2-acyl, η^2-CO_2, μ-NCO)	5.25
	η^3 Ligands (allyls, *etc.*)	3.16	Fluorine	Fluoride (F)	6.1
	η^4 Ligands (conjugated dienes, *etc.*)	3.17		Fluoro-anions (BF_4^-, PF_6^-)	6.2
	η^5 Ligands (dienyls, *etc.*)	3.18	Silicon	Miscellaneous	7.1
	η^6 Ligands (arenes, *etc.*)	3.19	Phosphorus	Phosphorus (P)	8.1
	η^7, η^8 Ligands	3.20		Phosphinidenes (PR)	8.2
	Carbaboranes, boroles	3.21		Phosphides (PR_2)	8.3
	Miscellaneous (CO_2, CS_2, *etc.*)	3.22		Oligo-phosphorus ligands (P_3, PR_2PR_2, PRPR, *etc.*)	8.4
Nitrogen	Nitride (N)	4.1		Phosphines (PR_3)	8.5
	Nitrenes/imides (NR)	4.2		Diphosphines (*e.g.* dppe)	8.6
	Alkylideneamido ($N{=}CR_2$)	4.3		Phosphites[$P(OR)_3$]	8.7
	Nitriles (NCR)	4.4		Amino-/iminoamino-phosphines, cyclotriphosphazene and other P–N	8.8
	Isocyanate, isothiocyanate (NCO, NCS)	4.5			
	Dinitrogen (N_2)	4.6			
	Diazoniums (N_2R), diazoalkanes (N_2CR_2)	4.7	Sulphur	Sulphides (S)	9.1
	Azide (N_3^-)	4.8		Thiolates (SR)	9.2
	Nitrosyl, thionitrosyl (NO, NS)	4.9		*S*-Thiocyanate (SCN)	9.3
	Amides (NR_2)	4.10		Thioketones, thiourea ($S{=}CR_2$)	9.4
	Amidinates [RNC(R)NR]	4.11		Thiocarboxylates (S_2CR^-)	9.5
	Schiff bases	4.12		Thiocarbamates ($S_2CNR_2^-$)	9.6
	Phthalocyanines, porphyrins, pyrroles	4.13		Xanthates (S_2COR^-), dithiocarbonates	9.7
	Pyrazolates, imidazolates and derivatives	4.14		Trithiocarbonates (CS_3^{2-}), thioxanthates	9.8
	Pyridine, polypyridyls (bipy, phen)	4.15		α,β-Dithiones	9.9
	Pyrazines, pyridazines, pyrimidines	4.16		Phosphine sulphides	9.10
	Other N_2 ligands ($NRNR_2$, NNR_2, NRNR)	4.17		Dithiophosphinates ($S_2PR_2^-$)	9.11
				Polysulphur ligands (S_2, SSR, *etc.*)	9.12
	Triazenido (RNNNR)	4.18		Thioethers (SR_2)	9.13
	Hydrazones and related species ($NR_2N{=}CR_2$)	4.19		*S*-SO_2, *S*-SO_3, *etc.*	9.14
				Disulphides (RSSR)	9.15
	Oximes	4.20		*S*-Dialkyl sulphoxides (R_2SO)	9.16
	N-Nitrite (NO_2)	4.21		Miscellaneous (η^2-CS_2)	9.17
	Amines (NR_3)	4.22	Chlorine	Chloride (Cl)	10.1
	Borazines	4.23	Arsenic	Arsines (AsR_3)	11.1
Oxygen	Oxo (O)	5.1		Miscellaneous	11.2
	Hydroxy (OH)	5.2	Selenium	Miscellaneous	12.1
	Alkoxy, aryloxy, *etc.* (OR)	5.3	Bromine	Bromide (Br)	13.1
	O-Ketones (OCR_2), urea	5.4	Tellurium	Miscellaneous	14.1
	Carboxylates (O_2CR)	5.5	Iodine	Iodide (I)	15.1

constants, than the intraligand bonds leading to a broader distribution of distances whatever the cause of variation. Finally it should be noted that a substantial contribution to the standard deviation of both metal–ligand and intraligand distances comes from random errors arising most importantly from the rather poor location of light (B, C, N, O, and F) atoms in the presence of 5*d*, 4*f*, and 5*f* metals (La–U). For example C–O bond lengths in carbonyl complexes (section 3.7.1) of the individual 3*d* metals show sample standard deviations (σ) in the range 0.011—0.024, while the 5*d* metals have σ in the range 0.023—0.035 Å. This last effect is somewhat reduced by the screening on AS flag, as described above. While other contributions to the variance in interatomic distances undoubtedly play a part, readers should be aware of these various factors when making use of the averages and other statistics of Table 3. In the longer term, as more structures are determined it will become possible to derive more precise averages by further subdivision of the distributions represented in Table 3.

Table 2. Numbers of entries in Table 3 [a]

Ligand atoms	H	B	C	N	O	F	Si	P	S	Cl	As	Se	Br	Te	I
Ligand classes	5	4	66	71	79	4	1	32	50	3	2	1	3	1	3
Metal [b,c]															
Sc [1]		1,0	0,1		0,4										
Ti [2,3]		2,0	6,8	14,5	4,15	1,0		1,2	4,3	1,2	1,0		1.0		
V [4–6]		2,0	8,8	6,5	10,10	0,1		3,3	2,6	0,2	1,0				1,0
Cr [7]	1,0	1,2	9,15	12,13	5,19	0,1		9,5	1,7	1,1	0,2	1,0	2,0	1,0	1,0
Mn		0,3	15,12	14,13	14,10	1,0	1,0	5,6	7,4	0,2	0,2	1,0	1,1	0,1	1,1
Fe	0,2	1,2	10,33	13,19	14,12		0,1	6,13	7,16	0,2	0,2	0,1	2,0	0,1	1,1
Co [8]	2,0	0,4	11,27	5,28	18,22			6,10	7,11	1,2	0,2		0,1		0,1
Ni [9,10]	0,1	2,1	7,20	9,23	9,18	1,0		6,8	12,13	0,2	1,1	0,1	0,2		1,1
Cu [11,12]	1,0	3,0	1,11	7,35	18,31	3,0		3,3	7,12	0,3	0,1	1,0	0,3		0,3
Zn	1,0	2,0	3,2	7,16	14,10				7,3	0,2			0,1		0,1
Y [1]		1,0	0,1		2,6					0,1					
Zr [13]		1,0	6,8	10,1	5,7	0,1		1,1	4,0	0,2		1,0			1,0
Nb [14]			4,6	3,5	2,9	0,1		2,0	1,6	1,2	0,1				
Mo [15,16]	1,1	1,0	11,25	17,26	7,28	1,1	1,0	5,11	3,20	1,2	0.2	1,0	0,2	1,0	0,2
Tc [17,18]			0,1	5,5	3,5			1,2	1,2	1,1	0,1		2,0		
Ru	0,1	2,1	12,25	19,9	11,8		0,1	2,13	4,4	0,2	0,2		0,2		1,1
Rh	2,1	0,2	11,25	12,18	11,14		1,0	5,13	6,7	0,2	1,1	0,1	0,2		0,2
Pd		0,1	9,15	14,13	6,6			8,7	4,10	1,2	1,1		0,1		1,1
Ag		1,0	4,2	8,6	8,2	1,0		2,3	4,6	2,1		1,0	1,0		1,2
Cd [19]				3,14	12,10			2,0	6,4	0,3			1,2		0,1
La [d]				1,1	4,7				1,0	1,0					
Ce [d]			0,2	0,1	4,4				0,1	1,0					
Pr [d]			1,1	1,0	2,5					2,0					
Nd [d]				2,2	7,5					1,0					
Sm [d]			0,1	1,1	8,6										
Eu [d]			0,1	0,1	3,6										
Gd [d]			0,1	1,0	2,4										
Tb [d]					1,0										
Dy [d]				2,1	1,2				0,1						
Ho [d]					0,1										
Er [d]			0,1	1,1	4,4					1,0					
Tm [d]									0,1						
Yb [d]			0,2	2,2	3,2					2,0					1,0
Lu [d]			1,2	1,0	0,1				0,1						
Hf [13]			2,4	1,0	2,2			0,2		1,0					
Ta [23]	1,0		5,7	4,1	4,2			2,2	2,4	0,2			1,0		
W [24,159]	0,2	1,1	9,20	10,7	4,12	1,0	1,0	4,6	7,5	1,2	1,0	1,0	0,1		1,1
Re	0,2	0,1	10,13	9,9	11,12	1,0	0,1	4,5	4,3	0,2	0,1	1,0	0,2		0,2
Os	0,2	2,0	12,11	9,7	6,6		1,0	4,6	3,3	0,2	1,0	1,0	1,0		0,1
Ir	1,1	1,1	11,12	12,4	3,4	1,0	1,0	5,9	5,5	0,2		1,0	0,2		0,2
Pt	2,0	0,1	4,25	11,13	8,10	1,0	0,1	6,13	8,11	0,2	0,1	1,0	0,2	1,0	0,2
Au [25]		0,1	4,3	6,0	4,0			5,3	7,3	0,1			0,1		1,0
Hg [26]		1,0	8,3	10,5	11,2		0,1	3,2	2,6	1,2		1,0	0,2	0,1	0,2
Th [d]	1,0		1,2	0,3	5,8			1,0	0,1	0,1					
U [d]		0,1	1,5	7,5	16,18	1,2		1,0	1,1	0,2			0,1		

[a] Numbers of entries for which <4 examples are known are given first, followed by numbers of entries for which statistics are quoted (*i.e.* those with >4 examples). [b] No entries at all for Pm, Pa, and Ac. [c] Superscript numbers refer to entries in Appendix 1. [d] See references 1 and 20—23 in Appendix 1.

Table 3. Interatomic distances (Å)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
1.1.1.1 Hydrides (terminal)								27
Fe–H	All BASLIQ10	1.609	1.610	0.004	1.605	1.612	6	
Zn–H	See MAEMAZ11 (1.617)							
Mo–H	See HCYPMO02 (1.684)							
Rh–H	See CONFEQ01 (1.578, 1.583)							
Ta–H	See TACPTH (1.769, 1.774, 1.776)							
W–H	All IPPHWH01	1.732	1.734	0.010	1.725	1.740	6	
Re–H	(8), (–)	1.684	1.681	0.015	1.676	1.697	12	
Os–H	All THMPOS01	1.659	1.656	0.017	1.646	1.677	4	
Ir–H	All DETSOK	1.603	1.607	0.021	1.582	1.623	5	
Pt-H	See CAKNEH01 (1.610)							
1.1.1.2 Hydrides (μ-H)								27
Cr–H	See KCPTCR01 (1.725, 1.723)							
Fe–H	All HMYCFE01	1.670	1.670	0.001	1.669	1.672	4	
Mo–H	(6,7), (II,III)	1.842	1.843	0.023	1.819	1.864	4	
Ru–H	(*), (–)	1.782	1.776	0.019	1.773	1.791	22	
Rh–H	(4,*), (I)	1.775	1.768	0.040	1.738	1.811	8	
W–H	(6), (0)	1.900	1.897	0.028	1.876	1.926	5	
Re–H	(8,*), (I,IV)	1.832	1.832	0.039	1.793	1.870	16	
Os–H	(*), (–)	1.817	1.824	0.029	1.798	1.837	34	
Ir–H	See CUSGAY (1.821, 1.847)							
Pt–H	See CAKNEH01 (range 1.656—2.049)							
1.1.1.3 Hydrides (μ_3-H)								27
Co–H	See HMPCIC01 (1.728, 1.731, 1.742)							
Ni–H	All TCPNIH11	1.691	1.684	0.022	1.673	1.715	9	
Rh–H	See HPMCRH11 (1.847, 1.855, 1.873)							
1.2.1.1 BH_4 [M(μ-H)B]								28
Cu–H	See TMPCUB01 (1.698)							
1.2.1.2 BH_4 [$M(\mu\text{-H})_2BH_2$]								
Co–H	See BEGBIY01 (1.707, 1.740)							
Th–H	See MCHFHB10 (2.069, 2.120)							
2.1 Borohydrides [M(–H–)BH_2R]								28
Sc–B	See BOVCAQ (2.528)							
Ti–B	See CPCLBT (2.178)							
Cr–B	See BOSKUP (2.294)							
Co–B	(–), (I): η^2-BH_4, μ-σ:σ′-BH_4	2.218	2.224	0.030	2.199	2.241	6	
Ni–B	See YBAENI (3.088)							
Cu–B	See BOLJAN (2.441), CICFID (2.204, 2.232), PHRLCU (2.079), TMPCUB01 (2.517)							
Zn–B	See CAPFOO (2.219), NBCZNB10 (2.252, 2.253)							
Y–B	See BUWBAW (2.478, 2.836), HBTHFY (2.574, 2.680)							
Zr–B	See CANFAY (2.335)							
Mo–B	See HBMPMO (2.468)							
Ru–B	See CIZBOC (2.237)							
Os–B	See COCKOU (2.300)							
U–B	(–), (III,IV): all	2.569	2.510	0.136	2.494	2.644	16	
	(–), (IV): $(\mu\text{-H})_3$BR	2.493	2.498	0.040	2.459	2.515	11	
2.2.1 Boranes/carbaboranes (not H-bridged) (see also 3.21.1)								29
Ti–B	See CEXTII (2.355, 2.375, 2.383)							
V–B	See BUPLAZ10 (2.246, 2.322, 2.333)							
Cr–B		2.228	2.252	0.054	2.178	2.266	9	
Mn–B		2.225	2.231	0.058	2.213	2.306	9	
Fe–B		2.140	2.135	0.066	2.103	2.179	111	
Co–B		2.086	2.082	0.073	2.036	2.124	270	
Ni–B		2.106	2.108	0.049	2.071	2.142	41	
Cu–B	See BOTPCU (2.209, 2.237), TPCUBF (2.273)							
Ru–B	All	2.263	2.324	0.167	2.041	2.377	16	30
	Short < 2.10	2.035	2.033	0.012	2.026	2.046	5	
	Long > 2.25	2.367	2.355	0.067	2.318	2.399	11	
Rh–B		2.224	2.219	0.061	2.188	2.252	55	
Pd–B		2.237	2.244	0.041	2.197	2.260	10	
Ag–B	See TPACUB (2.352, 2.420, 2.522)							
W–B		2.403	2.393	0.036	2.381	2.416	7	
Re–B		2.292	2.287	0.056	2.239	2.349	6	
Os–B	See BUVROZ (2.147, 2.184, 2.283)							
Ir–B		2.236	2.205	0.083	2.183	2.287	29	
Pt–B		2.243	2.244	0.062	2.213	2.283	94	
Au–B		2.238	2.228	0.034	2.206	2.256	11	
Hg–B	See COBHGA (2.201, 2.286), TPMCDB10 (2.204, 2.498, 2.521)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
2.2.2 Boranes/carbaboranes [M(–H–)B] (hydrogen located)								29
Mn–B		2.228	2.222	0.025	2.208	2.254	4	
Fe–B	See TPCUBF (2.115)							
Co–B		2.100	2.086	0.032	2.079	2.125	15	
Cu–B	See TPUCUBF (2.164)							
Zn–B	See CEXSAZ (2.264, 2.274)							
Ru–B	See COKTIF (2.327, 2.462)							
Rh–B		2.342	2.330	0.040	2.311	2.384	4	
W–B	See COVROU (2.413)							
Ir–B	See BELJEH (2.290, 2.281), CTPIRB (2.250), TPICBO (2.452, 2.480)							
2.3 Boracycles (see also 3.21.2 and 4.23)								31—33
V–B	See BOKXEE (2.369)							
Cr–B	Excluding BRNOCR (2.566)	2.340	2.349	0.026	2.312	2.360	7	
Mn–B		2.291	2.282	0.047	2.252	2.299	7	
Fe–B		2.227	2.185	0.097	2.163	2.279	13	
Co–B		2.123	2.097	0.076	2.073	2.189	12	
Ni–B	See CIDBOG (2.411), CPBORN (2.175), FMBCNI (2.260), SIBONI (2.226), VIBONI (2.500, 2.550)							
3.1.1.1 Carbide (μ_4-C)								34,35
Pt–B		2.243	2.244	0.062	2.213	2.283	94	
Pt–B		2.243	2.244	0.062	2.213	2.283	94	
Pt–B		2.243	2.244	0.062	2.213	2.283	94	
Hg–C	See FAHGME (2.042)							
3.1.1.2 Carbide (μ_5-C)								34,35
Ru–C		2.049	2.043	0.057	2.004	2.084	40	
Os–C		2.060	2.056	0.059	2.004	2.108	35	
3.1.1.3 Carbide (μ_6-C)								34,35
Ru–C		2.060	2.063	0.023	2.040	2.076	60	
Rh–C	See CBACRC (2.122, 2.132, 2.125)							
3.2.1.1 Carbynes/alkylidynes (terminal, CR, R = any C)								36,37
C–C		1.468	1.475	0.031	1.436	1.495	18	
Cr–C	(6), (–)	1.702	1.710	0.029	1.679	1.720	5	38
Mo–C	See BENFEF (1.799)							
Ta–C	See BESPIY (1.850), TABYCP10 (1.849)							
W–C	(5,6), (IV, VI)	1.815	1.821	0.041	1.777	1.840	9	
Re–C	See CECROR (1.742)							
3.2.1.2 Carbynes/alkylidynes (μ-CR, R = any C, H)								39
C–C		1.480	1.478	0.030	1.452	1.510	4	
Ru–C	See VCPRUB10 (1.933, 1.941), CIFXOE (1.936)							
W–C		1.955	1.947	0.021	1.940	1.973	6	
3.2.1.3 Carbynes/alkylidynes (μ_3-CR, R = any C, H)								
C–C		1.510	1.505	0.025	1.494	1.526	21	
Fe–C		1.928	1.933	0.024	1.910	1.939	15	
Co–C		1.896	1.895	0.035	1.874	1.920	27	
Mo–C		2.059	2.056	0.019	2.042	2.075	11	
Ru–C		2.084	2.089	0.027	2.067	2.102	6	
Rh–C	All R=H	1.964	1.970	0.020	1.945	1.980	7	
Os–C	All COTPOQ01	2.101	2.102	0.004	2.097	2.105	6	
3.2.2 Amino carbynes (terminal, CNR_2)								
(M)C–N		1.322	1.334	0.053	1.271	1.368	5	
N–C		1.469	1.470	0.027	1.441	1.485	8	
Cr–C	See BAMCOH (1.750), SNCOCR (1.743)							
Mo–C	See BITKIY (1.797)							
W–C	See CAVREW (1.776, 1.747)							
3.2.3 Thiocarbynes (terminal, CSR)								
C–S	(1.712, 1.713)							
Mo–C	See CAWSAU (1.801)							
W–C	See TPCPTW (1.810)							
3.3.1.1 Vinylidenes/alkenylidenes (terminal, CCR_2)								40
C=C		1.318	1.312	0.032	1.295	1.329	7	
Fe–C	See COPMID (1.780, 1.799)							
Mo–C	See BUJFIV (1.918), CVMOMP10 (1.833)							
Ru–C	See BOJJUF (1.845)							
Rh–C	See CAYMAQ (1.820)							
W–C	See CEFVUE (1.983)							
3.3.1.2 Vinylidenes/alkenylidenes (μ-CCR_2)								
C=C		1.317	1.315	0.023	1.305	1.326	7	
Mn–C	See EYCCMN (1.971, 1.978)							
Fe–C	See CHPECI (1.969, 1.955)							
Co–C		1.885	1.885	0.021	1.864	1.904	4	
Ru–C	See VCPRUA10 (2.025, 2.034)							
Rh–C	See BECVOU (1.987, 1.989)							
Os–C	See BEXJUJ (2.096, 2.102)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
3.4.1.1 Acetylides/alkynyls (terminal, CCR)								
C≡C		1.188	1.188	0.017	1.178	1.202	16	
C–C		1.456	1.451	0.030	1.436	1.465	16	
V–C	See CIJLUC (2.074)							
Fe–C	See CPFPEY (1.920)							
Rh–C	See BIMTEW (1.939)							
Pd–C	See EYPIPD (1.953)							
W–C	See BONSUS (2.134)							
Ir–C	See CEFPEI (2.041)							
Pt–C	(4,6), (II, IV)	1.992	2.000	0.032	1.985	2.009	8	41
Hg–C	See PEYHGP (2.047, 2.031)							
3.4.1.2 Acetylides/alkynyls (μ-CCR)†								42
C–C		1.231	1.232	0.026	1.206	1.256	4	
Fe–C σ	See ACYPCI (1.890)							
Fe–C π	See ACYPCI (2.117, 2.283)							
Ru–C σ	See BAYCOS (2.047), BOBTOB (2.044)							
Ru–C π	See BAYCOS (2.323, 2.423); (2.285, 2.508)							
Pt–C σ	See MSIPEP (1.964)							
Pt–C π	See MSIPEP (2.141, 2.468)							
3.5.1.1 Cyano (terminal CN)								43
C–N		1.146	1.146	0.014	1.138	1.154	168	
V–C	See CIRSAX (2.067), CIRSEB (2.088)							
Cr–C	(6), (–): all	2.058	2.063	0.024	2.031	2.080	8	7
Mn–C	See CAZJAO10 (1.996, 1.989)							
Fe–C	(5,6), (0,II,III): all	1.937	1.935	0.023	1.923	1.950	33	
Co–C	(5,6), (–): all	1.896	1.900	0.019	1.883	1.907	50	8
Ni–C	(4,5), (–): all	1.883	1.868	0.076	1.852	1.873	30	
	Excluding two >2.1	1.864	1.868	0.021	1.851	1.872	28	
Cu–C	(3,5), (–): all	2.003	1.975	0.101	1.924	2.098	5	12
Zn–C	(4), (–): all	2.000	1.997	0.012	1.991	2.013	4	
Mo–C	(6—8), (–): all	2.167	2.166	0.021	2.155	1.184	21	15,44
Ru–C	See BEPJIP (2.025)							
Pd–C	See BEJHUT (1.997)							
Ag–C	See COLSEB (2.093)							
Pt–C	(4,5), (II): all	1.943	1.931	0.031	1.916	1.977	5	
Au–C	See CIGCOK (2.003)							
Hg–C	See BINRAR (2.187, 2.174), CAHRUY (2.100)							
3.5.1.2 Cyano (μ-CN)† (see also 4.4.2)								
C–N		1.143	1.147	0.016	1.132	1.153	21	
Cr–C	See CYCRTF (1.999, 1.972, 1.965)							
Mn–C	See CAZJAO10 (1.995)							
Fe–C	(6), (III)	1.948	1.942	0.025	1.928	1.972	6	
Ni–C	(4), (II)	1.859	1.853	0.017	1.847	1.877	4	
Cu–C	(4), (I)	1.951	1.965	0.030	1.914	1.974	6	12
Pd–C	See BUSRIQ (2.011)							
3.6.1.1 Isocyanides (terminal, CNR, R = any C)								45,46
C–N		1.149	1.147	0.016	1.139	1.157	220	
V–C	See CIRSAX (2.003), CLBCNV (2.189)							
Cr–C	(6,7), (0—III): R = Ph, Bu^t, CH_2Ph	1.996	2.003	0.038	1.969	2.014	21	7
Mn–C	(6), (–): R = Ph, Bu^t, Me	1.927	1.924	0.028	1.900	1.947	15	
Fe–C	(5,6,*), (0—II): all	1.862	1.867	0.048	1.819	1.901	12	
	(6), (II): all	1.874	1.874	0.043	1.832	1.901	7	
Co–C	See BISJOC (1.851, 1.846, 1.866)							
Ni–C	(3,4), (0): R = Bu^t	1.853	1.854	0.021	1.838	1.870	6	
Cu–C	(3,4), (I): R = Bu^t, C_6H_4Me-*p*, C_6H_{11}	1.896	1.895	0.009	1.890	1.905	7	
Nb–C	(7,8), (–): R = Bu^t	2.241	2.237	0.036	2.208	2.270	6	
Mo–C	(5—8), (0—IV)	2.107	2.115	0.040	2.089	2.135	61	15
	(5—8), (II)	2.111	2.115	0.032	2.094	2.131	56	
	(5—7), (II): R = Bu^t	2.108	2.115	0.030	2.089	2.125	36	
Ru–C	(6,*), (–)	1.986	1.997	0.040	1.941	2.014	7	
Rh–C	(4—6), (–)	1.968	1.969	0.036	1.955	1.983	21	
	(4), (–)	1.956	1.962	0.031	1.947	1.975	13	
Pd–C	(3—5), (–)	1.985	1.974	0.036	1.958	2.020	18	47
	(4), (–)	1.978	1.972	0.035	1.955	1.994	15	
Ag–C	See BUXGAC (2.162, 2.136)							
Pr–C	See CXINPR10 (2.654)							
W–C	(7), (II): R = Bu^t	2.102	2.105	0.035	2.070	2.125	11	
Re–C	(6,7), (I—II)	2.002	2.008	0.022	1.980	2.018	12	
Os–C	See CIRJAO (1.983, 2.004), HOSTBC10 (2.032)							
Ir–C	See MCPEIR (1.945), MICPIR10 (1.986)							
Pt–C	(4,5,*), (–)	1.936	1.924	0.059	1.896	1.968	13	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
3.6.1.1 Isocyanides (terminal, CNR, R = any C)—(*continued*)								45,46
Pt–C	(4,5), (–)	1.944	1.966	0.036	1.912	1.968	7	
3.6.1.2 Isocyanides (μ-CNR)								
C–N		1.221	1.227	0.038	1.196	1.241	15	
Fe–C		1.941	1.941	0.025	1.920	1.948	12	
Ni–C	All MINCNI	1.881	1.880	0.022	1.861	1.903	4	
Os–C	See HYBIOS (2.072, 2.039)							
Pt–C	All BIDCAS	2.100	2.086	0.070	2.038	2.170	12	
3.7.1.1 Carbon monoxide (terminal, CO)								48
C–O		1.145	1.143	0.020	1.132	1.156	10 022	
Ti–C		2.003	1.997	0.030	1.980	2.030	5	49
V–C		1.946	1.946	0.037	1.924	1.974	60	
Cr–C		1.866	1.867	0.037	1.835	1.895	925	38
Mn–C		1.808	1.805	0.034	1.784	1.833	789	
Fe–C		1.782	1.784	0.030	1.765	1.801	2 572	50
Co–C		1.780	1.781	0.034	1.758	1.801	662	
Ni–C		1.771	1.776	0.029	1.750	1.794	34	51
Cu–C		1.787	1.782	0.019	1.776	1.807	18	12
Zr–C	See CCPZRA (2.187)							49
Nb–C		2.073	2.073	0.028	2.056	2.092	26	
Mo–C		1.978	1.973	0.041	1.947	2.007	748	15
Tc–C		1.884	1.883	0.021	1.866	1.904	4	17
Ru–C		1.896	1.896	0.036	1.873	1.919	1 453	
Rh–C		1.847	1.846	0.040	1.821	1.869	238	
Ta–C	See BISZIM (2.036), BUVGII (2.083), CPMPTA (2.008)							
W–C		2.002	2.007	0.043	1.971	2.034	508	24
Re–C		1.936	1.933	0.050	1.898	1.978	370	
Os–C		1.902	1.903	0.036	1.880	1.927	1 443	
Ir–C		1.870	1.876	0.042	1.839	1.898	148	
Pt–C		1.853	1.854	0.056	1.821	1.878	29	
3.7.1.2 Carbon monoxide (μ-CO)								52
C–O		1.171	1.171	0.022	1.159	1.183	279	
Mn–C	All	1.940	1.930	0.021	1.926	1.955	8	
	M–C–M < 70°	1.929	1.928	0.005	1.924	1.933	6	
Fe–C	All	1.941	1.925	0.041	1.914	1.971	104	
	M–C–M < 80°	1.985	1.995	0.037	1.953	2.018	20	
	80 < M–C–M < 86°	1.930	1.921	0.034	1.908	1.946	80	
Co–C		1.914	1.919	0.046	1.883	1.947	114	
Ni–C		1.882	1.880	0.021	1.870	1.892	14	
Cu–C		1.861	1.862	0.015	1.854	1.872	6	
Mo–C	All	2.127	2.091	0.095	2.045	2.237	6	
	Mo=Mo only	2.068	2.064	0.027	2.045	2.095	4	
Ru–C	All	2.072	2.055	0.047	2.038	2.099	66	
	Non-clusters	2.040	2.039	0.021	2.026	2.055	20	
	Clusters	2.086	2.087	0.048	2.043	2.114	46	
Rh–C	All	2.040	2.037	0.055	1.994	2.076	180	
	M–C–M < 85°	2.057	2.058	0.059	2.000	2.111	106	
	85 < M–C–M < 95°	2.018	2.029	0.037	1.984	2.046	68	
	M–C–M > 115°	1.983	1.982	0.007	1.977	1.990	4	
Pd–C	All	2.004	1.997	0.039	1.979	2.015	14	
Re–C	All BAWTOI	2.073	2.072	0.009	2.063	2.080	6	
Os–C		2.081	2.063	0.057	2.042	2.122	6	
Ir–C		2.065	2.072	0.039	2.026	2.093	30	
Pt–C		2.044	2.039	0.032	2.018	2.063	6	
3.7.1.3 Carbon monoxide (μ_3-CO)								42
C–O		1.190	1.191	0.038	1.173	1.202	33	
Fe–C		2.002	1.990	0.037	1.980	1.997	15	
Co–C		1.950	1.949	0.032	1.937	1.962	15	
Ni–C	See TCPDNI01 (1.931, 1.932)							
Ru–C		2.171	2.169	0.020	2.153	2.193	8	
Rh–C	See POSHRH10 (2.205, 2.155, 2.238)							
Pd–C	See BUJYIO (2.190, 2.078, 2.157)							
3.8.1.1 CS (terminal)								
C–S		1.563	1.570	0.030	1.536	1.587	5	
Cr–C	See BUGRIE (1.778), MBZCRC (1.797), TLCSCR (1.751)							
Mn–C	See ICPNMN (1.803)							
Fe–C	See BEPDEF (1.662)							
3.8.1.2 CS (μ-CS)								
C–S	(1.597, 1.606, 1.618)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
3.8.1.2 CS (μ-CS)—(*continued*)								
Fe–C	All CPTCFF	1.886	1.889	0.007	1.878	1.891	4	
3.9.1.1 Carbenes/alkylidenes (terminal, CH_2)								36
Re–C	See CAHZUG (1.898)							
Os–C	See CAMTEP (1.924)							
3.9.1.2 Carbenes/alkylidenes (μ-CR_2, R = any C, H)								39,53
Mn–C	See BANGIG10 (2.026), MYCCMN10 (2.018, 2.019)							
Fe–C		2.006	1.990	0.045	1.974	2.052	6	
Co–C		1.934	1.925	0.025	1.909	1.961	7	
Ru–C		2.085	2.095	0.056	2.076	2.112	12	
Rh–C		2.048	2.059	0.033	2.017	2.075	15	
W–C	Excluding BIJJAF (2.127, 2.436)	2.298	2.296	0.035	2.266	2.331	4	
Re–C	All CEHFEA	2.141	2.132	0.030	2.119	2.171	4	
Os–C	Excluding CODCON (1.922, 1.909)	2.160	2.155	0.041	2.136	2.192	20	
Au–C		2.112	2.102	0.026	2.095	2.139	4	
3.9.2 Carbenes/alkylidenes (terminal, CHR)								
C–C		1.490	1.493	0.027	1.462	1.513	14	
Ta–C	(5,6,8), (V): all	1.963	1.938	0.065	1.932	2.030	7	54,55
W–C	(5—7), (IV,VI)	1.953	1.942	0.086	1.871	2.041	5	38,55
Re–C	See BOBYAS (1.949), CECROR (1.873)							
3.9.3 Carbenes/alkylidenes (terminal, CR_2)								
C–C	R = C (sp^3)	1.503	1.509	0.024	1.500	1.519	12	
Mn–C	See CERJIS (1.853), MCBCMN (1.864, 1.871)							
Fe–C	See CPCFEA10 (1.978)							
W–C	See DPCBWC (2.132, 2.154)							38,55
Ir–C	See PYBPIR (1.998)							
3.9.4 Alkoxy carbenes [terminal, CR(OR), R = any C]								
(M)C–O		1.318	1.314	0.023	1.300	1.338	18	
(M)C–C		1.501	1.503	0.032	1.479	1.524	18	
O–C		1.466	1.459	0.024	1.452	1.484	18	
Cr–C	(6), (–)	2.012	2.006	0.029	1.988	2.039	5	38,55
Mn–C	See BOCWAR (1.848), MNXCMN (1.890), NPMCMN (1.950)							55
Co–C	See PGECBC (1.912)							
Mo–C	See BEBTUX (2.087)							
W–C	(6), (–)	2.161	2.161	0.014	2.148	2.175	4	
Re–C	See CMNCBR (2.098)							
Os–C	See BODGUW10 (1.981)							
Pt–C	See CIPTMN (1.889), EOBCPT10 (1.920)							
3.10.1.1 Vinyls/alkenyls (σ-$CRCR_2$)†								41
C=C		1.345	1.344	0.024	1.333	1.357	98	
Ti–C	(8), (IV)	2.215	2.239	0.042	2.171	2.243	7	
Cr–C	All MPEYCR10	2.035	2.033	0.009	2.027	2.045	4	
Mn–C	See BIZJEZ (1.985), CECCIW (2.009), MASBCM (2.027)							
Fe–C	(5,6), (II)	1.991	1.997	0.039	1.954	2.030	10	
Co–C	(6), (–)	1.934	1.932	0.019	1.914	1.946	8	
Ni–C	(4,5), (–)	1.892	1.900	0.017	1.874	1.903	4	
Zr–C	See CPPHZR (2.249, 2.265)							
Mo–C	(7), (–)	2.204	2.223	0.049	2.151	2.247	5	
Ru–C	See CNBRUB (2.073), CXFMPR (2.082), PCFMRU10 (2.034)							
Rh–C		2.040	2.060	0.054	1.986	2.085	5	
Pd–C	(4), (II)	2.000	2.006	0.024	1.989	2.011	16	47
Hf–C	See CPTPHF (2.190, 2.219)							
W–C	See BEDGAS (2.202), COPMEZ (2.275), MCTCEW (2.194)							
Os–C	See CIRNOG (2.052)							
Ir–C	(5,6), (–)	2.071	2.073	0.044	2.036	2.103	6	
Pt–C	(4,5), (–)	2.024	2.022	0.037	1.991	2.058	17	41
Au–C	See BULPED (2.039, 2.045)							
3.10.1.2 Vinyls/alkenyls (η^2-$CRCR_2$)†								
C_α–C_β		1.408	1.407	0.013	1.418	1.442	8	
Mo–C_α		1.936	1.937	0.020	1.917	1.954	4	
Mo–C_β		2.292	2.293	0.027	2.265	2.316	4	
W–C_α		1.918	1.907	0.030	1.898	1.949	4	
W–C_β		2.251	2.249	0.078	2.181	2.324	4	
3.10.1.3 Vinyls/alkenyls (μ-σ:η^2-$CRCR_2$)†								39
C_α–C_β		1.408	1.407	0.022	1.395	1.421	43	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
3.10.1.3 Vinyls/alkenyls (μ-σ:η²-CRCR$_2$)†—(*continued*)								39
Mn^1–C_α	See BOWYOB (2.058, 2.053)							
Mn^2–C_α	See BOWYOB (2.086, 2.102)							
Mn^2–C_β	See BOWYOB (2.263, 2.263)							
Fe^1–C_α		1.996	2.004	0.036	2.000	2.009	8	
Fe^2–C_α		2.102	2.095	0.039	2.079	2.111	8	
Fe^2–C_β		2.219	2.197	0.046	2.183	2.260	8	
Co^1–C_α	See BOCCOC (1.973, 1.968), BULYOW (1.981)							
Co^2–C_α	See BOCCOC (2.009, 2.011), BULYOW (1.995)							
Co^2–C_β	See BOCCOC (2.132, 2.115), BULYOW (2.127)							
Mo^1–C_α	See BEDDAP (2.151, 2.140), CAMKIK (2.141)							
Mo^2–C_α	See BEDDAP (2.181, 2.181), CAMKIK (2.232)							
Mo^2–C_β	See BEDDAP (2.301, 2.301), CAMKIK (2.446)							
Ru^1–C_α		2.079	2.075	0.043	2.060	2.089	13	
Ru^2–C_α		2.221	2.227	0.057	2.191	2.260	13	
Ru^2–C_β		2.276	2.276	0.042	2.247	2.284	13	
Rh^1–C_α	See BATNIT (2.045), FMPENR (2.025, 2.028)							
Rh^2–C_α	See BATNIT (2.100), FMPENR (2.058, 2.102)							
Rh^2–C_β	See BATNIT (2.222), FMPENR (2.139, 2.205)							
W^1–C_α	(6,7), (0,II,IV): all	2.158	2.145	0.043	2.128	2.203	6	
W^2–C_α	(6), (IV): excluding 2.266, 2.124	2.412	2.412	0.034	2.380	2.445	4	
W^2–C_β	(6), (II,IV): excluding one at 2.220	2.458	2.470	0.047	2.410	2.500	5	
Re^1–C_α	See COTFAS (2.170, 2.098)							
Re^2–C_α	See COTFAS (2.359, 2.255)							
Re^2–C_β	See COTFAS (2.352, 2.307)							
Os^1–C_α	See CHVINO (2.108), HPETOS (2.154), UCHXOS (2.170)							
Os^2–C_α	See CHVINO (2.273), HPETOS (2.151), UCHXOS (2.188)							
Os^2–C_β	See CHVINO (2.362), HPETOS (2.300), UCHXOS (2.311)							
3.11 σ-Aryls†								
C^1–C^2		1.396	1.396	0.021	1.381	1.409	398	
C^2–C^3		1.393	1.392	0.022	1.379	1.406	398	
C^3–C^4		1.378	1.379	0.025	1.364	1.395	399	
Ti–C	See PFPBTI (2.135), PSIBTI (2.161)							
V–C	(4,6), (II,III)	2.114	2.115	0.012	2.102	2.124	4	
Cr–C	(5,6), (II,III)	2.075	2.072	0.019	2.061	2.089	10	38
Mn–C	(6), (I)	2.064	2.059	0.021	2.044	2.083	6	
Fe–C	(4,6), (I,II)	2.031	2.022	0.062	1.985	2.065	6	
	(6), (I,II)	2.008	2.021	0.021	1.974	2.030	5	
Co–C	See DMDECO01 (1.995), ETPSCO10 (1.997), TOPFCO10 (1.931)							
Ni–C	(4,5), (II,III)	1.917	1.929	0.038	1.893	1.942	18	
Cu–C	See CODJIO (2.020)							
Mo–C	(4,5,7), (0,II,IV): all	2.193	2.176	0.054	2.164	2.195	11	38
	(4,5), (II,IV)	2.172	2.169	0.016	2.160	2.187	9	
Ru–C	(5,6), (II)	2.092	2.121	0.057	2.013	2.136	7	
Rh–C	(5,6), (II,III)	2.011	2.000	0.026	1.990	2.037	9	
Pd–C	(4,*), (II): all	1.981	1.987	0.032	1.965	2.002	28	47
Lu–C	See CILCUV (2.425, 2.427, 2.455)							
Ta–C	(5), (V)	2.199	2.173	0.073	2.147	2.276	4	
Re–C	See PHTPRE (2.024, 2.029)							
Os–C	(6,*), (−)	2.090	2.092	0.032	2.058	2.120	4	
Ir–C	(4—6,*), (I,III): all	2.070	2.067	0.038	2.043	2.092	17	
	(6), (III)	2.053	2.049	0.024	2.037	2.071	10	
Pt–C	(4—6), (I,II,IV): all	2.049	2.061	0.046	2.033	2.079	35	41
	(4), (I,II)	2.055	2.062	0.039	2.043	2.079	28	
Au–C	(2—4,*), (I,III): all	2.059	2.062	0.024	2.052	2.073	22	
	(2,3), (I)	2.053	2.050	0.009	2.045	2.062	5	
	(4), (III)	2.062	2.068	0.031	2.055	2.081	13	
Hg–C	(2—4,*), (II): all	2.086	2.088	0.040	2.054	2.120	24	
	(2,3), (II)	2.053	2.057	0.027	2.040	2.075	12	
	(*), (−): all BIPHHG	2.120	2.119	0.014	2.115	2.126	12	
3.12.1.1 Acyls [σ-C(O)R]†								
C=O		1.210	1.209	0.023	1.195	1.218	60	
Mn–C	See PNMNCP (2.012), PYRMNC (2.076)							
Fe–C	(6), (II)	1.997	2.004	0.033	1.967	2.028	18	
Co–C	See BOBSUG (1.915), OXCOCP10 (2.055)							
Ni–C	(4,5), (II)	1.850	1.870	0.059	1.788	1.893	4	
Mo–C	See BOLCIO10 (2.049), MABUMO10 (2.168)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
3.12.1.1 Acyls [σ-C(O)R]†—(*continued*)								
Ru–C	See BEWMAR (2.091)							
Rh–C	(5,6), (III): all	1.995	1.996	0.031	1.969	2.006	10	
Pd–C	(4), (II): all	1.982	1.992	0.029	1.951	2.002	4	
Re–C	(6), (I):	2.190	2.183	0.027	2.175	2.214	7	
Os–C	See BUYMAJ (2.161)							
Ir–C	See NRBIRB (1.971), POIRID (2.067)							
Pt–C	(4), (II)	1.991	2.000	0.025	1.969	2.008	7	
3.12.1.2 Acyls [η^2-C(O)R]† (see also 5.25.1)								
C=O		1.240	1.238	0.014	1.227	1.248	10	
Zr–C	See BOPSII (2.181, 2.186)							
Mo–C		2.014	2.020	0.011	2.003	2.023	6	
W–C	See BUSYIX (2.030), COSSOS (2.000)							
3.13.1 Methyl (terminal, CH_3)								
Ti–C	See BASMOX (1.969), INDMTI (2.206)							
Cr–C	See CAMVER (2.168)							
Mn–C	(6), (IV): all CAJHOK	2.095	2.105	0.030	2.068	2.124	4	
Fe–C	See BNTLFE (2.080), CEDMON (2.065), CMZTFE (2.077)							50
Co–C	(6), (III)	2.014	2.014	0.023	1.993	2.032	16	
Ni–C	See BAPKEI (2.035), PEAMNI (2.023)							56
Zr–C	(4—6,8), (IV)	2.292	2.279	0.049	2.257	2.346	8	
Nb–C	See CPSNBA (2.346), CPSNBB (2.327)							54
Mo–C	(5—7), (II—IV,VI): all	2.254	2.282	0.065	2.189	2.296	15	
Ru–C	(5,6), (II)	2.179	2.156	0.045	2.143	2.226	5	
Rh–C	(5,6), (II,III)	2.092	2.101	0.027	2.064	2.113	4	
Hf–C	(8), (IV)	2.275	2.267	0.049	2.233	2.325	4	
Ta–C	(6,7), (III,V)	2.217	2.215	0.035	2.181	2.247	7	54
W–C	(4—6), (II,III,VI)	2.189	2.187	0.039	2.166	2.213	13	
Re–C	(5,6), (I,III)	2.173	2.188	0.051	2.123	2.201	8	
Ir–C	See BEJBEX (2.218), CODPIR10 (2.133)							
Pt–C	(4—6), (II,IV): all	2.083	2.077	0.045	2.047	2.117	58	41
	(4,5), (II)	2.107	2.115	0.044	2.069	2.136	30	
	(6), (IV)	2.057	2.056	0.028	2.038	2.077	28	
Au–C	(4), (III)	2.066	2.045	0.045	2.030	2.118	18	57
Hg–C	(2—4), (II)	2.072	2.071	0.026	2.056	2.092	29	
Th–C	See COSZOZ (2.567)							
3.13.2 Primary alkyls [CH_2, R = C (sp^3)]								
C–C		1.521	1.528	0.033	1.512	1.540	90	
Ti–C	See BILWIC (2.138, 2.152), BOYZOE (2.210)							
Mn–C	(4,6), (I,II)	2.176	2.173	0.024	2.154	2.199	5	
Fe–C	(6), (II)	2.091	2.082	0.030	2.071	2.102	8	
Co–C	(6), (II,III)	2.039	2.037	0.032	2.018	2.061	14	
Ni–C	See ACTPEN (1.970), BENIIB (1.973), DIPNIP (1.948)							56
Zn–C	See PMCZNE (1.964)							
Nb–C	See CPETNB (2.316), ONBCBU (2.322)							54
Mo–C	(4—8), (II—IV,VI): all	2.250	2.252	0.061	2.208	2.272	12	
	(4—8), (III,IV,VI)	2.230	2.234	0.042	2.195	2.269	10	
Ru–C	(4), (III): all CIBGEZ	2.036	2.033	0.010	2.029	2.045	6	
Rh–C	See CIDJEE (2.094), PBUDRI10 (2.098, 2.107)							
Pd–C	See BIHLOT01 (2.051), HIMPDA (2.009, 2.023)							
Ta–C	(5,7), (V)	2.225	2.208	0.056	2.183	2.289	6	54
W–C	See COPXIO (2.141, 2.126), DMPMPW10 (2.257)							
Re–C	See COMPRH (2.285), ETDYRE (2.296)							
Os–C	See BOTTAF (2.220, 2.219), BUYNEO (2.203)							
Pt–C	(4—6), (II,IV)	2.062	2.065	0.031	2.039	2.085	14	41
Hg–C	See CIRMAR (2.125)							
3.13.3 Primary alkyls [CH_2R, R = C (sp^2)]								
C–C		1.477	1.478	0.028	1.464	1.496	108	
Ti–C	See CEYCOY (2.203, 2.204)							
Cr–C	See BELTUH (2.101)							
Mn–C	See ACPMNA (2.209), BUFLET (2.199), CABYUZ (2.127)							
Fe–C	(5,6), (0,II)	2.131	2.133	0.038	2.098	2.155	9	
Co–C	(5,6), (−)	2.061	2.085	0.061	2.001	2.109	5	
Ni–C	See IPRNIP (1.977)							56
Zn–C	See CLPDZN (2.030)							
Zr–C	(8), (IV)	2.320	2.306	0.034	2.298	2.355	4	
Nb–C	(8), (IV,V)	2.289	2.291	0.024	2.271	2.306	14	54

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
3.13.3 Primary alkyls [CH_2R, R = C (sp^2)]—(*continued*)								
Mo–C	(4—6), (II,III,VI)	2.211	2.214	0.027	2.187	2.233	9	
Ru–C	See CALHIG (2.200)							
Rh–C	See CIHYOH (2.103)							
Pd–C	(4,5,*), (II, –)	2.050	2.044	0.042	2.019	2.071	20	
Hf–C	See CEYCUE (2.274, 2.284)							
Ta–C	See CBZYTA (2.304), CPBZTB (2.188, 2.233)							54
W–C	(5—8), (II,III,V): all	2.238	2.185	0.090	2.163	2.328	9	
Re–C	See BUVSOA (2.203), BZHREC (2.284)							
Os–C	See BUYMAJ (2.217)							
Ir–C	See BIYJIC (2.127), CIYKAW (2.167), POIRID (2.133)							
Pt–C	(4,5), (II)	2.067	2.081	0.033	2.032	2.089	4	41
Hg–C	See CHGACA (2.107), DBEZHG (2.064)							
Th–C	All CEKGEE	2.554	2.555	0.022	2.535	2.570	7	
U–C	(6,10), (IV)	2.509	2.521	0.039	2.468	2.539	4	
3.13.4 Secondary alkyls [terminal, CHR_2, R = C (sp^3)]								
C–C		1.532	1.534	0.033	1.510	1.554	72	
Fe–C	See BULLFE (2.168), CAGKEA (2.060), MEDOFE10 (2.079)							
Co–C	(6), (III)	2.086	2.090	0.028	2.058	2.111	4	
Ni–C	See CONBIQ (1.929)							56
Zr–C	See CALNUY (2.381)							
Ru–C	(5,6), (II)	2.145	2.153	0.032	2.112	2.171	4	
Rh–C	See HBUPRH (2.083)							
Pd–C	(4,5), (II)	2.035	2.041	0.036	2.003	2.051	9	
Ir–C	(5,6), (III)	2.107	2.107	0.035	2.074	2.141	7	
Pt–C	(4,5), (II)	2.078	2.073	0.038	2.046	2.116	4	41
Hg–C	See CHGALD (2.085)							
3.13.5 Secondary alkyls [CHR_2, $R_2 \neq C(sp^3)_2$]								
C–C	R = C (sp^2)	1.474	1.475	0.023	1.461	1.485	82	
	R = C (sp^3)	1.532	1.527	0.022	1.518	1.545	40	
Ti–C	See TCYPTI10 (2.332)							
Fe–C	(5,6), (–)	2.131	2.138	0.027	2.110	2.151	16	
Co–C	(6), (–)	2.075	2.086	0.029	2.052	2.093	5	
Zr–C	See PDPMZR10 (2.379, 2.396)							
Mo–C	See BIRLIX (2.405)							
Ru–C	See BDMFRU (2.180), CTERUC (2.138)							
Rh–C	See BIGHAA (2.192), CASDIJ (2.154)							
Pd–C	(4,5), (II)	2.083	2.092	0.040	2.052	2.106	11	
Re–C	(6), (I)	2.311	2.335	0.065	2.243	2.356	4	
Os–C	See BUYNEO (2.221), CINKAL (2.215), EYPCOS (2.185)							
Ir–C	See CAYGAK (2.420)							
Pt–C	(4,5), (II)	2.113	2.120	0.036	2.082	2.141	9	41
Au–C	See BAJZAN (2.146), CEPYIF (2.175)							57
Hg–C	See BAVMUG (2.122), TPHGDI10 (2.292)							
3.13.6 Tertiary alkyls (terminal, CR_3, R = any C)								
C–C		1.501	1.502	0.045	1.468	1.534	84	109
Fe–C	(5,6), (II)	2.127	2.128	0.027	2.098	2.153	6	
Co–C	See COJBOS (2.154)							
Zn–C	See COPLEY (2.050)							
Mo–C	See CYPRMO (2.414)							
Pd–C	(4), (II)	2.147	2.150	0.040	2.140	2.174	8	
Pt–C	(4), (II)	2.148	2.139	0.028	2.133	2.162	9	41
Au–C	See BENNOX (2.213), BUJXAF (2.197)							57
3.13.7 Trifluoromethyl (terminal, CF_3)								
C–F		1.347	1.343	0.030	1.329	1.355	22	
Pt–C	(4,5), (II)	2.098	2.087	0.057	2.056	2.146	5	
3.14.1 η-Ethene (C_2H_4)								
C=C		1.392	1.390	0.044	1.363	1.415	43	
Co–C	(5), (I)	2.035	2.033	0.012	2.025	2.048	4	
Ni–C	(3,4), (0)	1.985	1.978	0.025	1.970	1.989	18	
Cu–C	(3,4), (I)	2.010	2.011	0.011	2.001	2.019	6	12
Nb–C	See CPETNB (2.278, 2.320)							54
Ru–C	(6), (II)	2.198	2.204	0.022	2.174	2.215	4	
Rh–C	(4,5), (I)	2.129	2.135	0.033	2.091	2.160	12	
Ta–C	See NPNTAB (2.228, 2.285)							54
W–C	(5,6), (–)	2.205	2.185	0.043	2.176	2.246	8	
Ir–C	See CETPIR (2.124, 2.111)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
3.14.1 η-Ethene (C_2H_4)—(*continued*)								
Pt–C	(3,4,*), (0,II)	2.172	2.176	0.042	2.143	2.193	28	41,58
3.14.2 η-Alkenes (CH_2CHR, R = any C)								59
C=C		1.383	1.383	0.033	1.361	1.404	44	
Fe–C	(5), (0)	2.090	2.088	0.012	2.079	2.102	4	58,60
Co–C	(5), (I)	2.084	2.085	0.034	2.052	2.115	4	
Ni–C	(4,5), (II)	2.035	2.039	0.053	1.984	2.082	4	9,58,61
Cu–C	(3,*), (I)	2.060	2.061	0.025	2.046	2.080	6	12
Mo–C	(6), (0,II)	2.282	2.271	0.027	2.265	2.310	4	
Ru–C	(5,6), (−)	2.198	2.190	0.034	2.171	2.232	4	
Rh–C	(4,6), (I,−)	2.172	2.164	0.058	2.118	2.216	10	
	(4), (I)	2.150	2.141	0.040	2.117	2.194	8	
Pd–C	(4,5), (II)	2.189	2.179	0.040	2.151	2.233	12	
Ag–C	(3—5), (I)	2.535	2.542	0.050	2.486	2.582	6	
W–C	(6), (0): all	2.386	2.410	0.080	2.302	2.454	10	30
	: short < 2.35 (*trans* to C=C)	2.299	2.298	0.010	2.290	2.308	4	
	: long > 2.40 (*trans* to CO)	2.443	2.434	0.036	2.412	2.484	6	
Ir–C	See COPNIR (2.179, 2.162)							
Pt–C	(4), (II)	2.179	2.173	0.051	2.139	2.205	22	41
3.14.3 η-Alkenes (CH_2CR_2, R = any C)								
C=C		1.387	1.396	0.029	1.354	1.413	8	
Fe–C	(5), (0)	2.124	2.119	0.065	2.072	2.188	6	60
Ru–C	See BOVLUT (2.168, 2.203)							
Pd–C	See CARJOU (2.187, 2.107)							
Ag–C	All CIXYAJ	2.421	2.419	0.081	2.345	2.499	4	
3.14.4 η-Alkenes (CHRCHR, R = any C)								62
C=C		1.391	1.389	0.032	1.372	1.407	280	
V–C	See EFMCPV (2.213, 2.186)							
Cr–C	See MOBOCO10 (2.248, 2.300)							
Mn–C	See CPTOMN (2.193, 2.203)							
Fe–C	(5,6), (0,II): all	2.134	2.143	0.063	2.079	2.183	22	
	: R electron withdrawing	2.067	2.072	0.022	2.041	2.087	8	
	: R = alkyl	2.172	2.169	0.041	2.144	2.195	14	
Co–C	All NBPCCO	2.138	2.137	0.005	2.134	2.144	4	
Ni–C	(3—5), (0,II): all	2.057	2.054	0.050	2.000	2.095	17	9,58,61
	: R electron withdrawing	1.991	1.997	0.015	1.979	2.000	5	
	: 1,5-cod	2.084	2.089	0.028	2.052	2.107	12	
Cu–C	(3,4,*), (I): all	2.079	2.079	0.033	2.063	2.089	20	12
Mo–C	(6), (0,II): all	2.369	2.347	0.083	2.298	2.446	28	
	: *trans* to CO	2.468	2.463	0.039	2.428	2.499	10	
	: not *trans* to CO	2.314	2.310	0.034	2.284	2.346	18	
Ru–C	: all	2.223	2.196	0.076	2.172	2.251	64	63
	: nbd, 1,5-cod only	2.191	2.187	0.036	2.167	2.206	49	
Rh–C	(4—6,*), (I—III): all	2.157	2.143	0.049	2.123	2.188	206	
	: nbd, 1,5-cod only	2.156	2.143	0.047	2.122	2.189	184	
Pd–C	(4), (II)	2.214	2.208	0.037	2.194	2.221	30	
Ag–C	See BUZMUE (2.705, 2.611)							
W–C	(6), (−)	2.430	2.430	0.033	2.400	2.457	6	
Re–C	See BAXLER (2.275)							
Os–C	All R electron withdrawing	2.167	2.176	0.033	2.133	2.193	4	
Ir–C	(4—6,*), (I,III): all	2.170	2.160	0.061	2.124	2.200	94	
	: 1,5-cod only	2.163	2.160	0.051	2.124	2.186	76	
Pt–C	(4,5,*), (0,II): all	2.209	2.223	0.056	2.173	2.252	52	41,58
	: 1,5-cod only	2.230	2.236	0.039	2.193	2.254	40	
3.14.5 η-Alkenes ($CHRCR_2$, R = any C)								
C=C		1.411	1.403	0.025	1.392	1.427	12	
Mo–C	See OCTCMO10 (2.211, 2.227)							
Ru–C	See CXFMPR (2.171, 2.184)							
Rh–C	(4,5), (I)	2.130	2.121	0.023	2.111	2.155	14	
Ir–C	All COTFEW	2.148	2.150	0.020	2.130	2.165	4	
Pt–C	See COTFPT (2.059, 2.072)							41,58
3.14.6 η-Alkenes (CR_2CR_2, R = any C)								
C=C		1.436	1.438	0.044	1.415	1.454	15	
Fe–C	All	2.144	2.085	0.127	2.048	2.269	8	
	Excluding *trans* to CO	2.079	2.058	0.045	2.045	2.121	6	
Co–C	See EXPHCO (2.084, 2.134)							
Mo–C	See CPOMOA (2.231, 2.234)							
Rh–C	(4,5), (I)	2.175	2.173	0.025	2.153	2.199	4	
Pd–C	(4), (II)	2.248	2.258	0.055	2.191	2.296	4	
Ag–C	See BUGGAL (2.472, 2.632)							
Ir–C	See IRCNIR (2.098, 2.130)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
3.14.6 η-Alkenes (CR_2CR_2, R = any C)—(*continued*)								
Pt–C		2.130	2.128	0.026	2.106	2.156	4	41,58
Hg–C	See BODYEY (2.556, 2.577)							
3.14.7 η^2-Allenes (R_2CCCR_2)†								
C_α=C_β	Co-ordinated	1.403	1.403	0.028	1.375	1.431	5	
C_β=C_γ	Free	1.319	1.321	0.010	1.311	1.327	5	
Fe–C_α	See FPCYTP10 (1.982)							
Fe–C_β	See FPCYTP10 (1.897)							
Rh–C_α	See MARHAA10 (2.177, 2.178)							
Rh–C_β	See MARHAA10 (2.032, 2.027)							
Pd–C_α	See ALETPD (2.118)							
Pd–C_β	See ALETPD (2.068)							
Pt–C_α	See MALLPT (2.107)							41
Pt–C_β	See MALLPT (2.049)							
3.15.1.1 Alkynes (η^2-C_2R_2, R = any C)								64
C≡C	All	1.285	1.287	0.030	1.269	1.299	73	
	2e donor	1.269	1.271	0.034	1.242	1.284	23	
	3e donor	1.285	1.292	0.024	1.268	1.299	15	
	4e donor	1.304	1.309	0.027	1.280	1.321	15	
V–C	See CPFVLV (2.076)							
Cr–C	All PHACCS	1.960	1.960	0.009	1.952	1.969	6	
Mn–C	See HDYCMN (1.239)							
Co–C	See ACNCOB20 (1.977, 1.981), BETCUY10 (1.847, 1.856)							
Cu–C	(3), (I): R = $SiMe_3$, H	2.019	2.020	0.029	1.994	2.043	5	12
Nb–C	(6,8), (III): R = Ph	2.082	2.054	0.061	2.041	2.148	8	54
Mo–C	Varying electron donation (2—4e): all	2.078	2.072	0.050	2.043	2.143	40	65
	2e donor	2.129	2.131	0.031	2.099	2.148	12	
	3e donor	2.071	2.066	0.033	2.053	2.082	12	
	4e donor	2.027	2.035	0.028	1.997	2.049	12	
Rh–C	R = Ph, CF_3	2.041	2.045	0.015	2.030	2.051	6	
Pd–C	See FMEACA10 (2.040, 2.053)							
Ta–C		2.059	2.064	0.024	2.032	2.079	6	54
W–C	Varying electron donation (2—4e): all	2.060	2.059	0.036	2.034	2.083	36	65
	2e donor	2.080	2.076	0.041	2.059	2.104	14	
	3e donor	2.066	2.066	0.016	2.053	2.078	12	
	4e donor	2.025	2.022	0.014	2.013	2.036	10	
Re–C		2.043	2.042	0.022	2.029	2.063	6	
Ir–C		2.083	2.083	0.041	2.044	2.122	4	
Pt–C		2.025	2.029	0.016	2.020	2.037	18	41
3.15.1.2 Alkynes (μ-η^2: $\eta^{2\prime}$-C_2R_2)†								64
C≡C		1.353	1.355	0.031	1.337	1.365	29	
Co–C		1.954	1.940	0.033	1.930	1.966	47	
Ni–C	All FLCPNI	1.910	1.909	0.011	1.901	1.921	4	61
Mo–C		2.171	2.178	0.050	2.137	2.199	32	
Rh–C	All CFBYRH	2.054	2.056	0.029	2.026	2.081	4	
Ta–C	See ACTHTA (2.217, 2.418)							
W–C	All: show twisting from $C_{2v} \longrightarrow C_2$	2.122	2.099	0.102	2.050	2.214	12	
	Excluding CAMLAD	2.117	2.099	0.059	2.086	2.158	8	
3.15.1.3 Alkynes (μ-σ: σ′-C_2R_2)†								64
C≡C		1.315	1.316	0.024	1.301	1.340	14	
Co–C	See CAHHAU (2.066)							
Ru–C		2.084	2.091	0.016	2.068	2.094	4	
Rh–C		2.021	2.001	0.041	1.992	2.064	6	
Ir–C		2.112	2.109	0.041	2.082	2.156	8	
Pt–C		2.059	2.056	0.009	2.051	2.068	5	41
3.16 η^3-Allyls (R_2CCRCR_2)†								
C^1–C^2		1.404	1.404	0.035	1.388	1.421	375	
V–C^1	All ALCPPV	2.349	2.352	0.013	2.342	2.357	6	
V–C^2	(2.222, 2.228, 2.245)							
Cr–C^1	See CAMWOC (2.171, 2.247)							
Cr–C^2	(2.193)							
Mn–C^1	(6), (I)	2.223	2.227	0.018	2.205	2.233	8	
Mn–C^2		2.120	2.120	0.004	2.116	2.124	4	
Fe–C^1	(5,6), (0—II)	2.155	2.155	0.044	2.135	2.181	70	60
Fe–C^2		2.068	2.070	0.033	2.048	2.092	36	
Co–C^1		2.082	2.083	0.029	2.054	2.112	17	
Co–C^2		2.000	2.007	0.021	1.985	2.015	9	
Ni–C^1	(4,5), (−)	2.044	2.031	0.057	2.005	2.075	34	66
Ni–C^2		1.962	1.967	0.040	1.937	1.995	17	
Zr–C^1	(7), (II)	2.472	2.469	0.028	2.444	2.498	8	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
3.16 η^3-Allyls (R_2CCRCR_2)†—(*continued*)								
Zr–C^2		2.470	2.476	0.019	2.450	2.485	4	
Mo–C^1	(6,7), (−): most (7), (II)	2.353	2.352	0.057	2.321	2.375	73	
Mo–C^2		2.244	2.234	0.048	2.214	2.274	37	
Ru–C^1	(5,6), (−): most (6), (II)	2.254	2.247	0.058	2.209	2.293	27	
Ru–C^2		2.168	2.174	0.041	2.130	2.197	14	
Rh–C^1	(4—6), (I,III)	2.191	2.193	0.048	2.151	2.233	24	
Rh–C^2		2.148	2.138	0.041	2.122	2.159	12	
Pd–C^1	Most (4), (II)	2.142	2.133	0.041	2.115	2.172	62	
Pd–C^2		2.118	2.116	0.034	2.100	2.143	31	
W–C^1	(7), (II)	2.303	2.303	0.053	2.256	2.339	16	
W–C^2		2.240	2.229	0.061	2.182	2.293	8	
Ir–C^1	(5,6), (I,III): all	2.212	2.188	0.048	2.175	2.268	8	
Ir–C^2		2.168	2.165	0.059	2.113	2.225	4	
Ir–C^1	(5), (I)	2.174	2.176	0.006	2.167	2.179	4	
Ir–C^2	(2.100, 2.152)							
Ir–C^1	(6), (III)	2.249	2.260	0.039	2.208	2.279	4	
Ir–C^2	(2.241, 2.178)							
Pt–C^1	(4), (II)	2.194	2.191	0.044	2.159	2.242	10	41
Pt–C^2		2.170	2.184	0.034	2.138	2.194	5	
U–C^1	(7,9), (IV)	2.670	2.663	0.038	2.640	2.701	10	
U–C^2		2.748	2.781	0.070	2.674	2.806	5	
3.17.1 η^4-Cyclobutadiene (C_4H_4)								
C–C		1.423	1.434	0.035	1.409	1.441	16	
Fe–C		2.027	2.031	0.026	2.020	2.039	12	
Fe–centroid	(1.759, 1.757, 1.763)							
Co–C		1.990	1.974	0.034	1.965	2.024	6	
Co–centroid	(1.682, 1.748)							
3.17.2 η^4-Cyclobutadienes (C_4R_4, $R_4 \neq H_4$)								
C–C		1.462	1.464	0.019	1.455	1.472	136	
Mn–C	All BUKGET	2.107	2.109	0.019	2.088	2.124	4	
Mn–centroid	(1.837)							
Fe–C	(5), (0)	2.044	2.039	0.025	2.024	2.066	12	50
Fe–centroid	(1.760, 1.766, 1.779)							
Co–C	(5), (I)	1.989	1.987	0.026	1.975	2.003	51	
Co–centroid		1.704	1.694	0.037	1.689	1.706	13	
Ni–C	(4,5), most (II)	2.027	2.025	0.036	2.001	2.060	16	67
Ni–centroid		1.742	1.740	0.018	1.727	1.761	4	
Mo–C	(6), (0,I)	2.280	2.270	0.041	2.249	2.299	16	
Mo–centroid		2.032	2.033	0.036	1.998	2.065	4	
Mo–C	(6), (0)	2.308	2.298	0.040	2.276	2.338	8	
Mo–centroid	(2.060, 2.066)							
Mo–C	(6), (I)	2.253	2.252	0.018	2.240	2.269	8	
Mo–centroid	(1.995, 2.006)							
Ru–C	(5,6), (0,II)	2.224	2.184	0.086	2.168	2.312	8	
Ru–centroid	(2.006, 1.926)							
Ru–C	(5), (0): all COCLEL	2.261	2.256	0.116	2.159	2.368	4	
Ru–C	(6), (II): all CIMVID	2.188	2.184	0.015	2.176	2.204	4	
Rh–C	(5), (I)	2.114	2.105	0.025	2.102	2.120	8	
Rh–centroid	(1.850, 1.829)							
Pd–C	(4,5), (II)	2.148	2.135	0.065	2.106	2.160	16	
Pd–centroid		1.887	1.873	0.042	1.857	1.932	4	
Pd–C	(5), (II)	2.130	2.135	0.027	2.106	2.145	12	
Pt–C	All CBFPPT10	2.219	2.214	0.096	2.129	2.314	4	
Pt–centroid	(1.963)							
3.17.3 η^4-1,3-Butadienes ($R_2CCRCRCR_2$)†								68
C^1–C^2		1.420	1.420	0.021	1.409	1.433	213	
C^2–$C^{2'}$		1.405	1.404	0.023	1.392	1.416	108	
Cr–C^1		2.332	2.349	0.046	2.277	2.370	6	
Cr–C^2		2.147	2.134	0.043	2.110	2.200	6	
Mn–C^1	(5), (0)	2.134	2.135	0.007	2.128	2.141	8	
Mn–C^2		2.080	2.071	0.025	2.066	2.106	8	
Fe–C^1		2.130	2.128	0.029	2.111	2.148	113	60
Fe–C^2		2.059	2.058	0.018	2.050	2.068	113	
Co–C^1	(5,6), (0,I)	2.089	2.102	0.045	2.061	2.125	12	
Co–C^2		2.015	2.003	0.033	1.994	2.018	12	
Co–C^1	Excluding two < 2.015	2.105	2.106	0.025	2.095	2.132	10	
Co–C^2	Excluding two > 2.075	2.001	1.998	0.012	1.993	2.013	10	
Ni–C^1	See BUJFUH (2.360, 2.106)							
Ni–C^2	See BUJFUH (2.074, 2.018)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
3.17.3 η^4-1,3-Butadienes ($R_2CCRCRCR_2$)†—(*continued*)								68
$Zr-C^1$	(7,8), (−): all	2.402	2.323	0.162	2.305	2.526	14	69
$Zr-C^2$		2.522	2.549	0.120	2.397	2.582	14	
$Zr-C^1$	Structures with $Zr-C^1 < Zr-C^2$	2.314	2.311	0.021	2.298	2.326	10	
$Zr-C^2$		2.582	2.563	0.078	2.542	2.624	10	
$Mo-C^1$	(5—7), (−)	2.356	2.364	0.052	2.331	2.378	20	
$Mo-C^2$		2.280	2.280	0.038	2.251	2.309	20	
$Ru-C^1$	(5,6), (0,II)	2.254	2.246	0.060	2.223	2.267	17	
$Ru-C^2$		2.181	2.173	0.050	2.155	2.194	17	
$Ru-C^1$	Excluding two > 2.385	2.236	2.233	0.033	2.218	2.265	15	
$Ru-C^2$	Excluding two > 2.29	2.165	2.169	0.025	2.155	2.180	15	
$Rh-C^1$		2.214	2.224	0.047	2.165	2.252	4	
$Rh-C^2$		2.177	2.198	0.043	2.134	2.199	4	
$Hf-C^1$	(6), (0): all	2.369	2.368	0.019	2.350	2.387	8	69
$Hf-C^2$		2.400	2.400	0.006	2.395	2.407	8	
$W-C^1$	See HPMXCW10 (2.453, 2.460)							
$W-C^2$	See HPMXCW10 (2.335, 2.263)							
$Re-C^1$	See BIBJEB (2.310, 2.277)							
$Re-C^2$	See BIBJEB (2.276, 2.258)							
$Os-C^1$	See OXBUDC10 (2.243, 2.300)							
$Os-C^2$	See OXBUDC10 (2.198, 2.240)							
$Ir-C^1$	See BUHIPI (2.277, 2.162), CBUTIR (2.186)							
$Ir-C^2$	See BUHIPI (2.141, 2.202), CBUTIR (2.153)							
3.17.4 η^4-1,5-Cyclo-octadiene (1,5-cod) (see 3.14.4)								62
3.17.5 η^4-Norbornadiene (nbd) (see 3.14.4)								62
3.18.1 η^5-Cyclopentadienyl (cp)								
C–C		1.397	1.398	0.028	1.380	1.415	6 804	
Sc–C	All TCYPSC10	2.494	2.499	0.023	2.473	2.513	10	
Sc–centroid	(2.189, 2.194)							
Ti–C		2.374	2.375	0.031	2.354	2.396	832	
Ti–centroid		2.062	2.061	0.026	2.044	2.082	170	
V–C		2.281	2.281	0.026	2.260	2.301	226	
V–centroid		1.952	1.950	0.020	1.938	1.970	46	
Cr–C		2.225	2.226	0.033	2.197	2.250	295	
Cr–centroid		1.876	1.882	0.029	1.847	1.898	61	
Mn–C	All	2.166	2.149	0.094	2.127	2.164	321	30
Mn–centroid	All	1.824	1.786	0.132	1.775	1.798	67	30
Mn–C	(−), (−): low spin	2.143	2.146	0.026	2.125	2.161	300	
Mn–centroid	Low spin	1.783	1.784	0.018	1.774	1.794	61	
Mn–C	Mn(II), high spin	2.511	2.499	0.052	2.479	2.541	20	
Mn–centroid		2.237	2.229	0.051	2.196	2.262	6	
Fe–C		2.080	2.088	0.035	2.052	2.106	1 309	60
Fe–centroid		1.706	1.721	0.039	1.662	1.735	265	
Co–C		2.068	2.066	0.031	2.045	2.089	740	
Co–centroid		1.696	1.692	0.029	1.676	1.716	152	
Ni–C		2.116	2.113	0.033	2.093	2.138	315	70
Ni–centroid		1.748	1.750	0.025	1.734	1.762	65	
Cu–C	All TPCYCU	2.211	2.205	0.018	2.195	2.231	5	
Cu–centroid	(1.864)							
Zn–C		2.348	2.332	0.080	2.299	2.440	15	
Zn–centroid		2.044	2.038	0.027	2.021	2.072	4	
Y–C		2.649	2.646	0.040	2.626	2.668	75	
Y–centroid		2.382	2.379	0.041	2.356	2.386	15	
Zr–C		2.529	2.529	0.031	2.510	2.546	649	71
Zr–centroid		2.236	2.233	0.023	2.220	2.251	132	
Zr–C	Excluding BOYLUW	2.528	2.528	0.026	2.510	2.545	638	
Zr–centroid	Excluding BOYLUW	2.235	2.232	0.022	2.220	2.250	131	
Nb–C		2.408	2.406	0.037	2.385	2.435	353	54
Nb–centroid		2.093	2.093	0.029	2.075	2.110	71	
Mo–C		2.336	2.338	0.042	2.304	2.368	1 363	
Mo–centroid		2.011	2.010	0.033	1.992	2.026	278	
Ru–C		2.236	2.240	0.041	2.204	2.267	284	
Ru–centroid		1.892	1.898	0.042	1.857	1.929	58	
Rh–C		2.239	2.236	0.037	2.218	2.264	256	
Rh–centroid		1.895	1.898	0.032	1.879	1.914	53	
Pd–C	All BUPTEL	2.344	2.350	0.050	2.303	2.381	5	
Pd–centroid	(2.015)							
Pr–C	All CXINPR10	2.778	2.765	0.026	2.760	2.801	15	1,21
Pr–centroid	(2.526, 2.527, 2.526)							
Gd–C	All CPTHGD10	2.738	2.744	0.025	2.722	2.747	15	1,21
Gd–centroid	(2.472, 2.490, 2.494)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
3.18.1 η^5-Cyclopentadienyl (cp)—(*continued*)								
Er–C	All BOBWAQ	2.667	2.665	0.005	2.663	2.671	5	1,21
Er–centroid	(2.391)							
Yb–C	(8,10), (−)	2.657	2.642	0.047	2.621	2.693	25	1,21
Yb–centroid		2.383	2.383	0.043	2.340	2.426	5	
Lu–C	All OHCPLU	2.600	2.599	0.018	2.584	2.615	10	1,21
Lu–centroid	(2.309, 2.316)							
Hf–C		2.505	2.507	0.020	2.494	2.520	60	71
Hf–centroid		2.208	2.211	0.015	2.195	2.220	12	
Ta–C		2.392	2.395	0.036	2.373	2.411	60	54
Ta–centroid		2.072	2.068	0.031	2.040	2.101	12	
W–C		2.337	2.337	0.042	2.307	2.364	566	
W–centroid		2.005	2.007	0.035	1.985	2.026	114	
Re–C	(6—8), (−)	2.296	2.293	0.039	2.270	2.327	103	
Re–centroid		1.959	1.958	0.026	1.946	1.980	21	
Os–C	(6), (−)	2.235	2.233	0.032	2.220	2.262	10	
Os–centroid	(1.916, 1.856)							
Ir–C		2.263	2.273	0.030	2.244	2.281	35	
Ir–centroid		1.922	1.917	0.012	1.913	1.936	7	
U–C		2.759	2.765	0.031	2.740	2.776	63	
U–centroid		2.493	2.491	0.015	2.483	2.506	13	
3.18.2 η^5-Pentamethylcyclopentadienyl (C_5Me_5)								
C–C (ring)		1.417	1.418	0.024	1.404	1.433	1 164	
C–C (Me)		1.512	1.509	0.025	1.497	1.523	1 239	
Ti–C		2.403	2.394	0.028	2.384	2.418	61	
Ti–centroid		2.086	2.071	0.027	2.064	2.116	13	
V–C		2.334	2.339	0.054	2.283	2.357	30	
V–centroid		2.009	2.010	0.047	1.979	2.051	6	
Cr–C		2.209	2.204	0.017	2.197	2.232	10	
Cr–centroid	(1.847, 1.858)							
Mn–C		2.146	2.147	0.027	2.126	2.158	25	
Mn–centroid		1.777	1.777	0.027	1.755	1.800	5	
Fe–C		2.116	2.115	0.026	2.095	2.136	25	
Fe–centroid		1.739	1.730	0.026	1.715	1.766	5	
Co–C		2.098	2.099	0.035	2.078	2.118	155	
Co–centroid		1.717	1.722	0.035	1.705	1.735	31	
Ni–C	All BINFUZ	2.102	2.120	0.027	2.073	2.122	5	
Ni–centroid	(1.725)							
Cu–C	All BUPWOY10	2.271	2.271	0.051	2.223	2.319	5	
Cu–centroid	(1.920)							
Zr–C		2.545	2.545	0.031	2.522	2.562	55	
Zr–centroid		2.244	2.244	0.023	2.232	2.253	11	
Mo–C		2.365	2.364	0.047	2.328	2.407	78	
Mo–centroid		2.034	2.032	0.029	2.010	2.058	16	
Ru–C	All COPKEX	2.268	2.269	0.012	2.258	2.279	5	
Ru–centroid	(1.917)							
Rh–C		2.217	2.217	0.057	2.168	2.254	367	
Rh–centroid		1.856	1.870	0.060	1.795	1.908	75	
Pd–C	All BUSHEC	2.341	2.351	0.073	2.280	2.397	5	
Pd–centroid	(2.003)							
Sm–C	(8), (II,III): all	2.809	2.808	0.063	2.745	2.864	40	1,30,60
Sm–centroid		2.537	2.535	0.067	2.472	2.601	8	
Sm–C	(8), (II): all CALCEX	2.864	2.863	0.030	2.836	2.889	20	
Sm–centroid		2.599	2.601	0.006	2.593	2.604	4	
Sm–C	(8), (III): all BUFNOF	2.754	2.747	0.031	2.727	2.786	20	
Sm–centroid		2.475	2.475	0.005	2.470	2.479	4	
Eu–C	All CIFCAV	2.815	2.808	0.019	2.799	2.834	5	1,60
Eu–centroid	(2.550)							
Yb–C	All	2.608	2.597	0.052	2.576	2.631	127	1,60
Yb–centroid		2.320	2.324	0.053	2.283	2.340	27	
Yb–C	Excluding BIKTIY	2.597	2.592	0.035	2.574	2.619	117	
Yb–centroid		2.308	2.303	0.033	2.283	2.335	25	
Lu–C	All CIXTUY	2.710	2.731	0.090	2.623	2.780	10	1,60
Lu–centroid	(2.360, 2.493)							
Ta–C		2.439	2.435	0.039	2.404	2.469	53	54
Ta–centroid		2.122	2.118	0.029	2.095	2.137	11	
Re–C		2.297	2.289	0.041	2.266	2.336	30	
Re–centroid		1.956	1.976	0.034	1.913	1.979	6	
Os–C	All BIJKOU	2.244	2.218	0.043	2.211	2.291	5	
Os–centroid	See BIJKOU (1.887)							
Ir–C	(6,7), (III,V): all	2.158	2.157	0.043	2.139	2.185	56	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
3.18.2 η^5-Pentamethylcyclopentadienyl (C_5Me_5)—(*continued*)								
Ir–centroid	(6,7) (III,V): all	1.792	1.783	0.049	1.760	1.808	12	
Ir–C	(6), (III)	2.151	2.155	0.024	2.134	2.170	46	
Ir–centroid		1.773	1.778	0.025	1.753	1.791	10	
Ir–C	(7), (V): all CECKOK	2.245	2.249	0.018	2.227	2.258	10	
Ir–centroid	(1.875, 1.893)							
Th–C		2.817	2.822	0.026	2.793	2.838	15	
Th–centroid	(2.536, 2.547, 2.573)							
U–C		2.752	2.752	0.033	2.724	2.776	58	
U–centroid		2.479	2.484	0.022	2.460	2.493	12	
3.18.3 η^5-Indenyl (C_9H_7)†								
C^1–C^2		1.407	1.410	0.028	1.400	1.421	34	
C^2–C^3		1.444	1.449	0.020	1.428	1.458	34	
C^3–$C^{3'}$		1.432	1.427	0.017	1.420	1.441	17	
Cr–C^1	See BABFOZ (2.176)							
Cr–C^2	(2.184, 2.197)							
Cr–C^3	(2.288, 2.301)							
Cr–centroid	(1.869)							
Mo–C^1	(6), (−) (2.341, 2.346, 2.350)							
Mo–C^2		2.341	2.354	0.065	2.278	2.392	6	
Mo–C^3		2.409	2.430	0.041	2.370	2.439	6	
Mo–centroid	(2.051, 2.034, 2.025)							
Rh–C^1	(5,6), (−)	2.223	2.221	0.019	2.213	2.236	9	
Rh–C^2		2.226	2.224	0.034	2.200	2.243	18	
Rh–C^3		2.399	2.401	0.051	2.364	2.426	18	
Rh–centroid		1.948	1.954	0.037	1.921	1.961	9	
Ce–C^1	All INDCEP (2.748, 2.757, 2.782)							60
Ce–C^2		2.805	2.794	0.043	2.766	2.849	6	
Ce–C^3		2.961	2.964	0.036	2.933	2.988	6	
Ce–centroid	(2.587, 2.591, 2.606)							
U–C^1	See CAFNOM (2.709)							
U–C^2	(2.710, 2.720)							
U–C^3	(2.769, 2.813)							
U–centroid	(2.455)							
3.18.4 η^5-Dienyls (C_5H_7 and derivatives)†								72,73
C^1–C^3		1.408	1.403	0.026	1.391	1.422	24	
C^2–C^3		1.415	1.414	0.021	1.399	1.427	24	
V–C^1	All COGXOL	2.179	2.180	0.017	2.162	2.195	4	
V–C^2		2.231	2.233	0.011	2.219	2.240	4	
V–C^3	(2.236, 2.236)							
Cr–C^1	See COGXUR (2.159, 2.174)							
Cr–C^2	See COGXUR (2.147, 2.177)							
Cr–C^3	See COGXUR (2.166)							
Mn–C^1	See OAZPMN10 (2.209, 2.298)							
Mn–C^2	See OAZPMN10 (2.137, 2.143)							
Mn–C^3	See OAZPMN10 (2.146)							
Fe–C^1	All MEPEFE10	2.108	2.109	0.016	2.094	2.122	4	
Fe–C^2		2.073	2.072	0.015	2.060	2.088	4	
Fe–C^3	(2.081, 2.086)							
Co–C^1	(5), (I)	2.135	2.136	0.010	2.125	2.143	4	
Co–C^2		2.078	2.075	0.015	2.066	2.094	4	
Co–C^3	(2.060, 2.087)							
Zr–C^1	See HMPEZR (2.432, 2.446)							
Zr–C^2	See HMPEZR (2.428, 2.438)							
Zr–C^3	See HMPEZR (2.469)							
Ru–C^1	(6), (II)	2.169	2.171	0.016	2.154	2.181	6	
Ru–C^2		2.168	2.167	0.028	2.149	2.194	6	
Ru–C^3	(2.177, 2.257, 2.258)							
3.19.1 η^6-Benzene (C_6H_6)								74
C–C		1.399	1.398	0.023	1.385	1.413	105	
Ti–C	All BELGOO10	2.228	2.225	0.009	2.220	2.236	12	
Ti–centroid	(1.736, 1.742)							
Cr–C	(6), (0,I)	2.180	2.176	0.044	2.147	2.219	20	
Cr–centroid		1.676	1.691	0.056	1.618	1.725	5	
Fe–C	All BUVLEJ	2.059	2.063	0.025	2.035	2.077	12	
Fe–centroid	(1.542, 1.548)							
Co–C	See BNZCTC (2.123)							
Co–centroid	(1.603)							
Mo–C	(7), (II)	2.279	2.273	0.051	2.247	2.315	18	
Mo–centroid	(1.767, 1.805, 1.819)							
Ru–C	(6), (−): all	2.187	2.168	0.042	2.154	2.227	21	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
3.19.1 η^6-Benzene (C_6H_6)—(*continued*)								74
Ru–centroid	(6), (−): all	1.674	1.659	0.043	1.644	1.720	4	
Re–C	(5,6), (−)	2.217	2.214	0.034	2.186	2.249	30	
Re–centroid		1.725	1.725	0.026	1.703	1.747	5	
Os–C	(6), (−)	2.166	2.165	0.055	2.135	2.191	30	
Os–centroid		1.657	1.635	0.057	1.620	1.705	5	
3.19.2 η^6-Arenes (C_6R_6, R = any C, H)								74
C–C	Intra-ring	1.411	1.411	0.021	1.398	1.423	818	
Ti–C	(6,7), (0,II): all	2.330	2.247	0.125	2.240	2.479	18	30
Ti–C	(6), (0)	2.245	2.244	0.010	2.238	2.248	12	
Ti–centroid	(1.742, 1.744)							
Ti–C	(7), (II)	2.498	2.502	0.037	2.465	2.530	6	
Ti–centroid	(2.055)							
V–C	All DFBENV	2.192	2.192	0.010	2.181	2.203	6	
V–centroid	(1.692)							
Cr–C	(6), (0,I)	2.216	2.216	0.045	2.196	2.239	412	
Cr–centroid		1.710	1.718	0.046	1.699	1.733	73	
Fe–C	(5,6), (0,II)	2.101	2.097	0.036	2.078	2.114	82	
Fe–centroid		1.563	1.549	0.032	1.539	1.586	14	
Co–C	(5,6), (I,II)	2.167	2.131	0.060	2.122	2.228	13	
Co–centroid	(1.602, 1.766, 1.628)							
Ni–C	(5), (II)	2.209	2.216	0.041	2.170	2.238	10	75
Ni–centroid	(1.713, 1.699)							
Zr–C	All CLZRAL	2.590	2.592	0.030	2.558	2.619	9	
Zr–centroid	(2.164, 2.178)							
Nb–C		2.404	2.457	0.096	2.283	2.479	28	30
Nb–centroid		1.939	1.938	0.005	1.935	1.944	5	
Nb–C	Long > 2.425	2.473	2.474	0.016	2.459	2.484	18	
Nb–C	Short < 2.352	2.280	2.282	0.019	2.264	2.289	10	
Mo–C	(6,7), (0—III)	2.320	2.322	0.057	2.274	2.370	93	
Mo–centroid		1.841	1.838	0.061	1.794	1.904	16	
Ru–C	(5,6), (0,II)	2.247	2.235	0.051	2.212	2.264	78	
Ru–centroid		1.745	1.727	0.059	1.697	1.767	13	
Ru–C	(5,6), (0,II): excluding BENLOV	2.238	2.230	0.040	2.210	2.258	72	
Ru–centroid		1.733	1.727	0.042	1.695	1.757	12	
Rh–C	(5,6), (−)	2.327	2.315	0.052	2.291	2.363	22	
Rh–centroid		1.845	1.864	0.051	1.793	1.878	4	
Hf–C	All SNTLHF	2.481	2.493	0.041	2.433	2.519	6	
Hf–centroid	(2.041)							
W–C	(6,7), (0,II)	2.291	2.293	0.038	2.269	2.309	46	
W–centroid		1.803	1.805	0.043	1.768	1.821	8	
Re–C	All CIZNUU	2.327	2.328	0.005	2.323	2.331	6	
Re–centroid	(1.863)							
Os–C	(4,6), (−)	2.213	2.198	0.053	2.181	2.230	18	
Os–centroid	(1.638, 1.718, 1.719)							
3.20.1 η^7-Tropylium (C_7H_7) and derivatives								
C–C		1.408	1.409	0.022	1.393	1.418	126	
Ti–C	(7), (−)	2.228	2.236	0.020	2.204	2.242	21	
Ti–centroid	(1.484, 1.544, 1.569)							
Cr–C	(7), (−)	2.220	2.210	0.043	2.189	2.241	14	
Cr–centroid	(1.445, 1.571)							
Mo–C	(7), (−)	2.280	2.278	0.032	2.256	2.300	105	
Mo–centroid		1.607	1.596	0.035	1.577	1.649	15	
3.20.2 η^8-Cyclo-octatetraene (C_8H_8) and derivatives								
C–C		1.397	1.399	0.027	1.385	1.409	114	
Ti–C	(7), (III,IV)	2.349	2.373	0.043	2.319	2.384	32	
Ti–centroid		1.471	1.490	0.063	1.409	1.524	5	
Ti–C	(7), (III)	2.368	2.378	0.027	2.338	2.388	24	30
Ti–centroid		1.495	1.504	0.040	1.453	1.527	4	
Ti–C	Short < 2.35	2.329	2.328	0.009	2.321	2.336	7	
Ti–C	Long > 2.37	2.384	2.383	0.009	2.378	2.391	17	
Ti–C	(7), (IV): all CEXTII	2.291	2.293	0.023	2.270	2.311	8	
Ti–centroid	(1.377)							
V–C	All BUPLAZ10	2.282	2.281	0.039	2.257	2.293	8	
V–centroid	(1.376)							
Zr–C	(7), (II,IV)	2.461	2.459	0.017	2.449	2.474	16	
Zr–centroid	(1.685, 1.650)							
Ce–C	All COCTCE	2.710	2.709	0.015	2.700	2.720	8	1
Ce–centroid	(2.007)							
Th–C	(8), (IV)	2.712	2.710	0.016	2.701	2.724	16	
Th–centroid	(2.029, 2.003)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
3.20.2 η^8-Cyclo-octatetraene (C_8H_8) and derivatives—(*continued*)								
U–C	(8), (IV)	2.653	2.648	0.019	2.637	2.667	48	
U–centroid		1.917	1.919	0.005	1.913	1.921	5	
3.21.1 Carbaboranes (see also 2.2.1)								29
Ti–C	See CEXTII (2.265, 2.340)							
V–C	See BUPLAZ10 (2.191, 2.269)							
Cr–C		2.197	2.188	0.065	2.140	2.265	6	
Mn–C	See PMCMNB (2.043, 2.047)							
Fe–C		2.073	2.069	0.070	2.041	2.108	62	
Co–C		2.046	2.049	0.055	2.013	2.078	76	
Ni–C		2.087	2.071	0.071	2.045	2.145	15	
Ru–C	See RUCABO (2.097, 2.185)							
Rh–C		2.239	2.237	0.065	2.187	2.287	26	
Pd–C	See BICPDB (2.599), MPPDBN (2.414, 2.492)							
W–C		2.420	2.431	0.044	2.374	2.455	4	
Re–C	See CSCREC (2.310, 2.316)							
Pt–C	(Range 2.142—2.768)	2.441	2.447	0.199	2.277	2.591	12	
Hg–C		2.101	2.106	0.013	2.089	2.110	5	
3.21.2 Borylenes, *etc.* (see also 2.3)								31—33
V–C	See BOKXEE (2.297)							
Mn–C		2.197	2.188	0.037	2.167	2.234	10	
Fe–C		2.118	2.098	0.050	2.086	2.150	16	
Co–C		2.062	2.031	0.061	2.025	2.091	19	
Ni–C	All	2.120	2.091	0.085	2.053	2.193	9	
	Excluding FMBCNI	2.080	2.076	0.036	2.044	2.144	7	
3.22.1 η^2-CO_2 (see also 5.25.2)								
(None)								
3.22.2 η^2-CS_2 (see also 9.17)								
C=S	Co-ordinated	1.665	1.671	0.018	1.656	1.676	6	
C=S	Free	1.613	1.616	0.006	1.607	1.618	6	
V–C	See CPCDSV (2.075, 2.089)							
Fe–C	See SPHFEC10 (1.983)							
Co–C	See TPHCOA (1.882)							
Ni–C	See COGWOK (1.858)							
Nb–C	See CPSNBA (2.206)							
4.1.1.1 Nitride (terminal, N)								76
Cr–N	See BOZYIY (1.562)							
Mn–N	See ZEGGUN (1.512)							
Mo–N	(5,6), (VI)	1.636	1.636	0.006	1.630	1.641	4	77
Tc–N	See BAGWAH (1.604), CETKUH (1.629)							
Re–N	(5,6), (V): see BOCLOU (1.660), NEPPRE (1.788), NETPRE (1.602), NREDTC10 (1.656)							
4.1.1.2 Nitride (μ-N)								78
Mo–N (μ)	See BUPZIV (1.662, 2.150; 1.643, 2.167)							
Ru–N (μ)	See CEPBII (1.742)							
W–N (μ)	See CAWGAI (1.740, 2.661)							
Mo–N (μ_3)	See BAXFEL (range 1.900—1.979)							
Ru–N (μ_4)	See BITRAX (1.913, 1.943, 2.103, 2.114)							
Rh–N (μ_6)	See BOZBOH (range 2.124—2.137)							
4.2.1.1 Nitrenes/imides (terminal, NR, R = any C)								79
N–C		1.415	1.394	0.047	1.387	1.457	51	
V–N	See CIZTEK (1.730)							
Nb–N	See CAHJIE (1.783), COBLIO (1.733)							
Mo–N	(5—7), (V,VI)	1.729	1.728	0.019	1.719	1.733	20	
	(5—7), (V,VI): excluding one with Mo–N–C 139.4°	1.726	1.728	0.013	1.718	1.732	19	
Ta–N	See BEHHIF (1.765), COBDUS (1.762)							
W–N	(4—6), (V,VI)	1.738	1.739	0.026	1.725	1.754	13	
Re–N	(6), (V—VII)	1.701	1.694	0.019	1.688	1.709	9	
Os–N	See ADOOSA (1.697), ADOOSB (1.706, 1.720)							
U–N	See CESVUR (2.063)							
4.2.1.2 Nitrenes/imides (μ-NR)								
N–C	R = C (sp^2)	1.392	1.395	0.021	1.374	1.409	7	
	R = Bu^t	1.483	1.484	0.007	1.475	1.488	4	
Ti–N	See BIJJUZ10 (1.920), BUIMWB (1.921, 1.926)							
Zr–N	See TBIAZR (2.060, 2.071)							
Nb–N	All BENRAN	2.043	2.042	0.011	2.033	2.053	4	
Mo–N	(6), (−): excluding BUMEMO (1.819, 2.322)	1.970	1.973	0.010	1.958	1.978	6	
W–N	See BUIMWA (1.841, 2.288), CACRIH (1.891, 2.312)							
4.3 Alkylideneamido (N=CR_2, linear)								80
N–C	(1.258, 1.275, 1.259)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
4.3 Alkylideneamido (N=CR_2, linear)—(*continued*)								80
Zr–N	See CEFSIP (2.013)							
Mo–N	See BUDZEF (1.878), CPBUMO (1.892)							
4.4.1 Nitriles (NCR, R = any C)								
N–C		1.133	1.134	0.020	1.121	1.144	102	
Ti–N	See ECYFTI (2.245)							
V–N	See ACNCVO (2.097), BZTCOV (2.124), COPHAV (2.107)							
Fe–N	(5,6), (II,III): all	2.029	1.976	0.153	1.928	2.161	7	
	(5,6), (II): low spin	1.946	1.966	0.041	1.905	1.977	5	
Co–N	(4,5), (0,I): all	1.971	1.951	0.068	1.920	2.041	4	
Ni–N	See BCETPN (2.082), CARWAT (2.109), EFUMNI (1.873)							
Cu–N	(4—6,*), (I,II): all	2.121	2.005	0.249	1.968	2.321	11	
	(4,*), (I,II)	1.983	1.975	0.042	1.960	2.036	8	
Nb–N	(6), (IV,V): all	2.322	2.303	0.083	2.254	2.414	8	81
	(6), (IV,V)	2.282	2.292	0.042	2.238	2.315	6	44
Mo–N	(5—7), (II,VI)	2.147	2.144	0.041	2.125	2.177	9	44
Tc–N	See CETKUH (2.492)							
Ru–N	(5,6,*), (0,II,IV): all	2.090	2.108	0.037	2.052	2.118	5	
Rh–N	(4—6), (I,II)	2.139	2.152	0.091	2.052	2.232	11	30
	(4,5), (I)	2.050	2.052	0.006	2.045	2.056	5	
	(6), (II)	2.214	2.225	0.043	2.166	2.252	6	82
Pd–N	See CAKNIL10 (2.063)							
Cd–N	See CDCYAC (2.372)							
Re–N	(6), (I,II): all	2.107	2.125	0.040	2.065	2.137	13	
Os–N	(6,*), (−): all	2.098	2.096	0.028	2.084	2.124	10	
Ir–N	See BESSEX (2.054), CEYBEN (2.044), IRTCPP10 (2.024)							
Pt–N	(4,5), (I,II): all	2.003	1.982	0.048	1.978	2.036	8	
	(4), (II)	1.980	1.979	0.019	1.971	1.990	6	
U–N	See CIHLIO (2.604, 2.580)							
4.4.2 Cyano (μ-CN) (see also 3.5.1.2)†								
Cr–N	See CYCRTF (1.975, 1.975, 1.994)							
Mn–N	See CAZJAO10 (2.165), CAZJES10 (2.186)							
Cu–N	(4—6), (II): all	2.051	2.001	0.135	1.956	2.103	11	
	: excluding two > 2.3	1.994	1.995	0.052	1.955	2.022	9	
Pd–N	See BUSRIQ (2.067)							
Cd–N	(4,6), (II)	2.361	2.352	0.042	2.327	2.403	4	
4.5.1.1 Isocyanate (terminal, NCO) (see also 5.25.3.1)								83
N–C		1.141	1.148	0.020	1.125	1.156	16	
C–O		1.202	1.197	0.016	1.189	1.215	16	
Ti–N	See CPTICN10 (2.007, 2.018)							
Cr–N	See CPNOCC10 (1.980)							
Mn–N	See CENRES (1.919, 1.934), TRENCM (2.051)							
Co–N	See CNTPCP (1.949), CYZNIC10 (2.055)							
Cu–N	(4—6,*), (II): all	1.935	1.926	0.049	1.897	1.954	8	
4.5.1.2 Isocyanate (μ-NCO-*NO*) (see also 5.25.3.2)†								
N–C	(1.152, 1.154)							
C–O	(1.182, 1.216)							
Cu–N	See CNPRCV (1.946), ICNPCU10 (1.952)							
4.5.1.3 Isocyanate (μ-NCO-*N*)†								
N–C	(1.168)							
C–O	(1.173)							
Cu–N	See COVYIV (2.266, 2.023)							
4.5.2.1 *N*-Isothiocyanates (terminal, NCS) (see also 9.3.1.1)								84
N–C		1.149	1.150	0.017	1.141	1.159	230	
C–S		1.620	1.619	0.022	1.608	1.632	231	
Ti–N	See CPITTI (2.021)							
Cr–N	(6), (III): excluding CEFMAB (2.250)	1.999	1.998	0.016	1.984	2.012	12	85
Mn–N	(5—7), (II,III)	2.166	2.167	0.051	2.128	2.196	13	
	(6), (II): Mn–N–C > 152°	2.141	2.146	0.027	2.107	2.167	7	
Fe–N	(5—7), (II,III): all	2.063	2.095	0.084	1.982	2.133	12	
	(6,7), high spin (II)	2.108	2.106	0.031	2.088	2.139	7	
Co–N	(4—6), (II,III)	2.000	1.992	0.076	1.927	2.072	42	30
	(4), (II)	1.956	1.957	0.010	1.948	1.964	8	
	(5), (II)	2.034	2.028	0.050	2.004	2.064	6	
	(6), (II)	2.073	2.075	0.029	2.064	2.099	15	
	(6), (III): excluding ITDASC (2.117)	1.911	1.910	0.015	1.900	1.922	12	
Ni–N	(4—6), (II): all	2.035	2.064	0.079	2.026	2.077	44	30
	(4)	1.855	1.835	0.046	1.827	1.886	6	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
4.5.2.1 *N*-Isothiocyanates (terminal, NCS) (see also 9.3.1.1)—(*continued*)								84
Ni–N	(6)	2.064	2.068	0.027	2.054	2.079	36	
Cu–N	(4—6), (II): all	2.045	1.970	0.165	1.945	2.101	25	86
	(5), (II): Cu–N–C > 152°	2.013	1.968	0.102	1.946	2.073	21	86
Zn–N	(4—6), (II): all	1.988	1.945	0.081	1.923	2.083	8	30
	(4), (II)	1.931	1.929	0.013	1.919	1.945	5	
Zr–N	See TCBPZR (2.183)							
Nb–N	(6,8), (IV,V)	2.132	2.130	0.035	2.100	2.166	4	
Mo–N	(6,7), (V,VI)	2.148	2.166	0.077	2.065	2.183	11	81,87
Tc–N	(6), (II,III,V)	2.049	2.046	0.011	2.043	2.057	6	
Pd–N	(4), (II)	2.023	2.025	0.028	2.011	2.043	9	
Cd–N	(5,6), (II)	2.245	2.241	0.047	2.212	2.259	7	
Dy–N	See CIKTOF (2.433)							
Re–N	(6), (III,V)	2.024	2.018	0.023	2.009	2.038	7	
Pt–N	See PEYEPP (2.025)							
Th–N	(8), (IV)	2.496	2.496	0.024	2.474	2.513	9	
U–N	(8,9,11), (IV)	2.439	2.448	0.046	2.407	2.467	18	
4.5.2.2 Isothiocyanates (μ-NCS) (see also 9.3.1.2)†								
N–C		1.144	1.149	0.020	1.129	1.160	24	
C–S		1.642	1.643	0.017	1.632	1.650	24	
Mn–N	See TCMNET10 (2.143)							
Co–N	(6), (II)	2.111	2.118	0.020	2.091	2.128	5	
Ni–N	See TCYENI10 (2.031)							
Cu–N	(4,5), (II): excluding COHHIQ (2.205)	1.962	1.951	0.031	1.939	1.999	6	
Ag–N	See CENSUJ (2.281), CENTAQ (2.332)							
Cd–N	(5,6), (II)	2.287	2.294	0.019	2.267	2.300	4	
Pt–N	See TPPTCP01 (1.966)							
Hg–N	See TCHXPH10 (2.517), TCPPHG10 (2.405, 2.735)							
4.6.1.1 Dinitrogen (σ-N_2)								88
N–N		1.100	1.110	0.048	1.074	1.124	18	
Cr–N	See CAVMOB (1.957)							
Fe–N	See PHSNFE (1.866)							
Co–N	See CARKIP (1.814), PPHCHN10 (1.783, 1.832)							
Zr–N	See MCPNZR (2.187, 2.188)							
Mo–N	(6), (0,I)	2.013	1.996	0.056	1.971	2.072	4	89
Ru–N	See ENAZPU10 (1.893)							
Rh–N	See HNBPRH10 (1.970)							
W–N	See BUYBUS (2.038)							
Re–N	See BIBJAX (1.956), BUKMID (2.055), CNMPRE (1.966)							90
Os–N	See CAJCEV (1.909)							
4.6.1.2 Dinitrogen (μ-σ: σ′-N_2)†								
N–N	Excluding BEJGAY (1.282), IMNPTA10 (1.298)	1.155	1.155	0.020	1.137	1.174	5	
Ti–N	(7), (II): all NPMCTI	2.017	2.014	0.012	2.007	2.029	4	
Fe–N	See BALWUG (1.877)							
Zr–N	See MCPNZR (2.087, 2.075)							
Mo–N	See NMSPEM (2.042)							
Ta–N	See BEJGAY (1.796), IMNPTA10 (1.837)							
4.7.1 Diazoniums/diazenidos (σ-NNR)								80
N–N		1.219	1.224	0.032	1.210	1.236	14	
N–C		1.428	1.427	0.024	1.414	1.438	14	
Mn–N	See FTLAMN (1.696)							
Mo–N	(6,7), (0—VI): all Mo–N–N > 160°, N–N–C < 130°	1.806	1.816	0.028	1.778	1.832	8	
Ru–N	See CTZPRU (1.795)							
Rh–N	See CPZRHF10 (1.961)							
W–N	See CPCMZW (1.850)							
Os–N	See HPZPOS (1.867)							
Ir–N	See PAZMPI (1.834)							
4.7.2 Diazoalkanes (σ-$NNCR_2$)								
N–N	All bent N–N–C	1.319	1.312	0.027	1.300	1.346	8	
N–C		1.309	1.311	0.015	1.294	1.320	8	
Mn–N	See AZMLMN (1.796)							
Mo–N	See BAMTAK10 (1.759, 1.782), CIYBAN (1.797)							
W–N	See AZPPBW10 (1.723), BCAZWB (1.784), CIXJIC (1.776)							
Ir–N	See PCLPIR (1.825)							
4.8.1.1 Azido (σ-N_3)†								84
(M)N–N		1.180	1.183	0.020	1.175	1.193	37	
N–N		1.149	1.150	0.020	1.141	1.163	37	
Ti–N	See AZCPTI (2.025)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
4.8.1.1 Azido (σ-N_3)†—(*continued*)								84
Mn–N	See MNACAZ30 (2.244)							
Co–N	(5,6), (I,III)	1.991	1.967	0.047	1.952	2.030	7	
Cu–N	(4—6), (I,II): all	2.012	1.969	0.088	1.962	2.040	15	
	(4—6), (II): excluding three > 2.16	1.966	1.964	0.024	1.948	1.980	11	
Mo–N	(5,6), (II,VI): all	2.095	2.062	0.078	2.026	2.175	10	30
	(5,6), (VI)	2.037	2.036	0.025	2.019	2.054	6	
	(6), (II): all BUNZOZ	2.182	2.175	0.021	2.167	2.203	4	
Ru–N	See ENAZPU10 (2.122)							
Pd–N	See AZENPD10 (2.077), BEJJAB (2.044)							
U–N	See BOPTEF (2.382)							
4.8.1.2 Azido (μ-N_3-N^1)†								
N^1–N^2		1.210	1.202	0.025	1.195	1.220	11	
N^2–N^3	Excluding two > 1.25	1.135	1.136	0.015	1.127	1.146	9	
Cu–N	(4—6), (II): excluding one > 2.4	2.014	2.018	0.040	1.986	2.034	15	
Zr–N	See BAXFOV (2.202, 2.204)							
Rh–N	See AFMZRH (2.133, 2.105)							
4.8.1.3 Azido (μ-N_3-N^1N^3)†								
N–N		1.173	1.171	0.015	1.167	1.183	8	
Ni–N	See ZTANPB (2.196, 2.069)							
Cu–N	See BUVNIP (2.456, 1.979), MDNCAZ10 (2.252, 1.985), TTZZCU10 (2.013, 1.994)							
4.9.1.1 Nitrosyl (terminal, NO)								78,80
N–O	All	1.172	1.173	0.036	1.155	1.194	211	91
	M–N–O > 150°	1.176	1.175	0.030	1.156	1.194	197	
	M–N–O < 140°	1.114	1.125	0.057	1.064	1.164	10	
V–N	See BEYFEQ (1.809), BIVGAO (1.760)							
Cr–N	(4,6,7): Cr–N–O 166—180°	1.684	1.680	0.022	1.675	1.694	16	
Mn–N	(5,6): Mn–N–O 164—180°	1.651	1.648	0.013	1.641	1.659	14	
Fe–N	(4—6,*): Fe–N–O 144—180°	1.671	1.666	0.028	1.650	1.681	51	92
	: Fe–N–O > 155°	1.669	1.666	0.023	1.650	1.680	50	
Co–N	(4—6): Co–N–O 124—180°	1.697	1.667	0.084	1.640	1.805	22	8,30,92
	: Co–N–O > 158°	1.646	1.649	0.030	1.617	1.669	15	
	: Co–N–O < 133°, excluding BUBBAB (1.705)	1.822	1.815	0.020	1.806	1.842	6	
Ni–N	(3,4): Ni–N–O 161—180°	1.628	1.629	0.024	1.612	1.649	11	
Mo–N	(5—8): Mo–N–O 166—180°	1.787	1.779	0.041	1.760	1.804	44	
Ru–N	(4—6): Ru–N–O 143—180°	1.751	1.752	0.038	1.732	1.766	12	
	: Ru–N–O > 168°, excluding RUNCPP10 (1.839)	1.743	1.751	0.027	1.727	1.763	11	
Rh–N	See NSDPRH10 (1.801)							
W–N	(5—7): W–N–O 168—180°	1.792	1.800	0.034	1.770	1.822	7	
Re–N	(4—6): Re–N–O 170—180°	1.749	1.780	0.026	1.734	1.766	16	
Os–N	(4—6): Os–N–O 133—180°	1.751	1.748	0.067	1.732	1.776	7	92
	: Os–N–O > 174°, excluding NSOSPP10 (1.859)	1.733	1.743	0.051	1.708	1.771	6	
Ir–N	(4,5):Ir–N–O 124—180°	1.780	1.757	0.106	1.688	1.872	8	92
	: Ir–N–O > 163°, excluding CNOPIR (1.972), ICNPIR (1.900)	1.720	1.713	0.046	1.678	1.765	6	
4.9.1.2 Nitrosyl (μ-NO)								78
N–O		1.210	1.208	0.025	1.195	1.218	19	
Cr–N	See BRNOCR (1.892, 1.924)							
Mn–N		1.855	1.858	0.007	1.850	1.860	18	
Fe–N	See MENTFE (1.818)							
Co–N		1.817	1.821	0.012	1.804	1.826	4	
Ru–N	All BISKOD	1.918	1.919	0.005	1.913	1.922	4	
Rh–N	See COBGIJ (1.952)							
Os–N		2.042	2.040	0.029	2.014	2.073	6	
4.9.1.3 Nitrosyl (μ_3-NO)								78
N–O	(1.247)							
Mn–N	See TCPMNN10 (1.933, 1.917, 1.939)							
4.9.2 Thionitrosyl (terminal, NS)								80,93
N–S		1.518	1.509	0.022	1.504	1.541	4	
Cr–N	See CTNSCR10 (1.693)							
Ru–N	See COGHEL (1.729)							
Os–N	See CESNET (1.779), CIBKED (1.730)							
4.10.1 NH_2								
(None)								
4.10.2 Primary amides (NHR)								94
N–C		1.434	1.429	0.035	1.404	1.470	4	
Mo–N	See ADASMO (2.058), MPBMOE10 (1.955, 1.964)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
4.10.2 Primary amides (NHR)—(*continued*)								94
Os–N	See BOSRUW (1.896)							
4.10.3.1 Secondary amides [NR_2, R = C (sp^3)]								94
N–C		1.464	1.463	0.017	1.455	1.472	162	
Ti–N	(4,5), (IV): all	1.939	1.943	0.016	1.928	1.947	11	
Zr–N	See TBIAZR (2.058, 2.062)							
Mo–N	(4,5), (III): (mainly Mo_2)	1.955	1.952	0.020	1.945	1.967	44	
Tc–N	See CEWZIN10 (1.908, 1.916)							
Ta–N	(5,6), (V)	1.964	1.963	0.017	1.954	1.978	12	
W–N	(4), (III,VI)	1.952	1.955	0.015	1.937	1.967	7	
U–N	(4,5), (IV)	2.206	2.212	0.033	2.172	2.235	4	
4.10.3.2 Secondary amides (μ-NR_2)								
N–C	All C(sp^3)	1.479	1.482	0.036	1.470	1.493	10	
Ti–N	See BUNKEA (2.147, 2.191)							
Cu–N	See CIDBAS (1.901, 1.907)							
Mo–N	See PAIDMO (2.178, 2.250)							
Au–N	See CASPIV (2.142, 2.139)							
U–N	See URDEAM10 (2.456, 2.571)							
4.11.1.1 Amidinates [σ-RNC(R)NR, R = any C]								
(None)								
4.11.1.2 Amidinates [chelating, RNC(R)NR, R = any C]								84
N–C		1.315	1.311	0.021	1.300	1.324	12	
Mo–N	(7), (II)	2.171	2.177	0.021	2.148	2.188	10	
Re–N	See BIYWUB (2.215, 2.217)							
4.11.1.3 Amidinates (bridging, μ-RNC(R)NR, R = any C)								
N–C		1.340	1.336	0.022	1.323	1.352	22	
Cr–N	All MBZACR	2.032	2.031	0.009	2.024	2.041	4	
Mo–N	(5), (II)	2.149	2.151	0.016	2.134	2.161	12	
Re–N	All PBARTC	2.077	2.076	0.015	2.063	2.092	4	
4.12 Schiff bases (σ-RN=CR_2, R = any C)†								95
N=C		1.287	1.286	0.021	1.275	1.300	768	
N–C		1.471	1.473	0.022	1.461	1.485	765	
Ti–N	See ESALTJ (2.136, 2.139)							
V–N	(5,6), (IV): all	2.047	2.041	0.024	2.036	2.054	7	
Cr–N	(5,6), (0,I,III): all	2.079	2.028	0.073	2.018	2.152	9	
	(5,6), (0)	2.153	2.152	0.032	2.123	2.182	4	
	(6), (I,III)	2.019	2.019	0.006	2.014	2.025	5	
Mn–N	(6,7), (II,III): all	2.163	2.116	0.143	2.051	2.292	10	96,97
Fe–N	(5—7), (0,II,III): all	2.038	1.992	0.103	1.942	2.109	78	30
	(5), (0): all	1.953	1.932	0.039	1.926	1.997	6	
	(5,6), (II): all	2.044	2.031	0.098	1.950	2.119	32	30
	: low spin	1.958	1.954	0.021	1.938	1.977	16	
	: high spin	2.131	2.115	0.057	2.086	2.162	16	
	(5,6), (III): all	2.022	1.991	0.086	1.937	2.108	36	30
	: low spin	1.949	1.944	0.024	1.931	1.973	20	
	: high spin	2.113	2.108	0.029	2.094	2.123	16	
	(7), (II)	2.258	2.260	0.014	2.244	2.270	4	
Co–N	(4—6), (I—III): all	1.943	1.917	0.084	1.891	1.946	142	30
	(4), (II)	1.907	1.876	0.065	1.871	1.921	25	86
	(5,6), (II)	2.015	2.036	0.109	1.897	2.128	44	30
	: short < 1.95	1.897	1.894	0.023	1.881	1.916	18	
	: long > 1.99	2.097	2.115	0.054	2.048	2.140	26	
	(5,6), (III): all	1.914	1.917	0.021	1.897	1.931	71	
Ni–N	(4—6,*), (0,II,IV): all	1.929	1.906	0.080	1.860	2.000	136	
	(4), (0): all	1.924	1.924	0.006	1.922	1.930	7	
	(4), (II)	1.888	1.871	0.048	1.855	1.917	77	86
	(5), (II): all	1.922	1.889	0.084	1.853	2.031	16	30
	: short < 1.925	1.869	1.859	0.028	1.843	1.898	11	
	: long > 2.025	2.038	2.039	0.010	2.029	2.048	5	
	6, (II): all	2.051	2.055	0.034	2.022	2.075	27	
	6, (IV)	1.872	1.872	0.004	1.869	1.876	4	
Cu–N	(3—6,*), (I,II): all	1.969	1.964	0.053	1.936	1.990	227	86
	(3,4), (I)	2.005	1.989	0.073	1.947	2.075	18	
	(4), (II)	1.954	1.947	0.043	1.921	1.977	97	
	(5), (II)	1.966	1.965	0.039	1.936	1.986	88	
	(6), (II): all	2.010	2.005	0.049	1.966	2.049	14	
Zn–N	(4—6,*), (II): all	2.122	2.120	0.049	2.114	2.167	11	
Zr–N	All SAZPZR	2.428	2.435	0.021	2.406	2.443	4	
Mo–N	(5—7), (0—VI): all	2.189	2.181	0.065	2.131	2.237	31	
	(6), (0)	2.244	2.254	0.042	2.203	2.274	6	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
4.12 Schiff bases (σ-RN=CR_2, R = any C)—(*continued*)								95
Mo–N	(7), (II)	2.216	2.221	0.028	2.204	2.233	10	
	(−), (V,VI): excluding two >2.30	2.124	2.130	0.013	2.113	2.133	12	
Tc–N	(5,6), (V)	2.034	2.023	0.029	2.002	2.066	7	
Ru–N	See BAVSIA (2.190), COGXRU (2.138)							
Rh–N	(4,6), (I,III): all	2.053	2.039	0.046	2.013	2.103	8	
	(6), (III)	2.023	2.026	0.019	2.005	2.039	5	
Pd–N	(4,5,*), (II): all	2.037	2.032	0.040	2.017	2.046	26	
Ag–N	(4—6), (I,II): all	2.403	2.429	0.112	2.311	2.447	9	
Cd–N	See BEHMOQ (2.399, 2.457)							
La–N	All EPAILA	2.714	2.721	0.025	2.688	2.734	4	
Ce–N	(8), (IV)	2.615	2.614	0.025	2.608	2.638	8	
W–N	See ALBCIW (2.219)							
Re–N	(6), (V)	2.121	2.122	0.023	2.099	2.143	6	
Os–N	All μ-N(R)=C(R) clusters	2.145	2.150	0.025	2.125	2.161	18	
Ir–N	See SCLIRA10 (2.098)							
Pt–N	See BISIPT (2.171, 2.176), BZHXDB (2.021, 1.995)							
Au–N	See MEAZAU (1.976, 1.980)							
Hg–N	See BOCWEV (2.158)							
Th–N	(8), (IV): all	2.641	2.654	0.022	2.618	2.659	5	
U–N	(7), (VI): excluding COKPIB (2.710)	2.572	2.568	0.012	2.565	2.586	6	
4.13.1 Pyrroles†								
$N–C^1$		1.375	1.376	0.022	1.363	1.388	168	
$C^1–C^2$		1.429	1.434	0.039	1.399	1.453	168	
$C^2–C^{2'}$		1.368	1.371	0.025	1.350	1.384	83	
Ti–N	See CPYRTI10 (2.067, 2.100)							
Mn–N	(6), (−): all	2.126	2.141	0.041	2.095	2.148	5	
Fe–N	(5,6), (II,III): all	2.020	1.995	0.075	1.948	2.107	8	
	(5,6), (III)	1.969	1.985	0.031	1.936	1.995	5	
Co–N	(5), (II)	2.044	2.063	0.033	2.009	2.065	6	
Ni–N	(4), (II)	1.906	1.897	0.030	1.877	1.937	18	
Cu–N	(4,5), (II)	1.908	1.899	0.023	1.890	1.929	13	
Zn–N	(4,5), (II)	1.999	1.990	0.040	1.975	2.004	13	
	(4), (II)	1.980	1.976	0.009	1.974	1.990	10	
Zr–N	See CYPRZR10 (2.167, 2.170)							
Mo–N	See BOXHUR (2.151)							
Tc–N	See TPPTCC (2.161)							
Rh–N	(4,*), (I, II)	2.067	2.065	0.017	2.052	2.083	4	
Pd–N	See BESFOU (2.010, 2.071)							
Hf–N	See CESJOZ (2.164, 2.178)							
Pt–N	See CAFFIY (2.045)							
Hg–N	See FMTPHG (2.016), TAMPHG (2.325)							
U–N	See CIMINU10 (2.490, 2.527, 2.533)							
4.13.2 Porphyrinates†								98
N–C		1.380	1.379	0.011	1.373	1.385	564	
Ti–N	(5), (IV)	2.112	2.115	0.016	2.098	2.124	8	
V–N	(5,6), (II,IV)	2.085	2.098	0.027	2.051	2.104	6	
Cr–N	(4,5), (II,V)	2.037	2.036	0.005	2.033	2.042	6	
Mn–N	(4—6), (II—IV): all	2.024	2.013	0.046	1.998	2.030	34	
	(4—6), (II)	2.057	2.029	0.053	2.009	2.124	14	
	(5,6), (III,IV)	2.001	2.002	0.020	1.992	2.016	20	
Fe–N	(4—6), (II,III): all	2.031	2.038	0.036	1.995	2.062	88	30,98,99
	(4—6), (II)	2.009	2.000	0.035	1.987	2.006	22	
	(4—6), (III)	2.034	2.050	0.034	1.999	2.067	66	
	(4—6), (II,III): short <2.014	1.995	1.995	0.009	1.991	2.003	41	
	(4—6), (II,III): long >2.022	2.063	2.062	0.017	2.051	2.074	47	
Co–N	(4—6), (II,III): all	1.969	1.983	0.022	1.947	1.988	19	
Ni–N	(4), (II)	1.943	1.949	0.014	1.931	1.954	16	
Cu–N	(4), (II)	1.991	1.992	0.009	1.985	1.996	6	
Zn–N	(4,5), (II)	2.068	2.063	0.024	2.058	2.074	18	
Nb–N	(6,7), (V)	2.234	2.239	0.037	2.209	2.247	16	
Mo–N	(5,6), (II,IV): excluding OTPHMO	2.086	2.090	0.017	2.075	2.097	28	44
Ru–N	(5,6), (II,III)	2.047	2.047	0.007	2.043	2.055	24	
Rh–N	(5,6), (III)	2.034	2.031	0.010	2.026	2.042	6	
Cd–N	All PHPNCD	2.145	2.150	0.029	2.115	2.169	4	
Pt–N	See CEZKEX (2.005)							
4.13.3 Phthalocyanines†								
N–C		1.380	1.381	0.011	1.379	1.389	70	
Ti–N	(5), (IV): all BITSAY	2.066	2.064	0.013	2.055	2.080	4	
V–N	(5), (IV): all VPHTHC	2.026	2.029	0.013	2.012	2.037	4	
Mn–N	See MNPHCY03 (1.938, 1.939)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
4.13.3 Phthalocyanines†—(*continued*)								
Fe–N	(4,6), (II)	1.934	1.931	0.009	1.927	1.941	6	
Co–N	(4,6), (II)	1.921	1.915	0.017	1.910	1.938	4	
Ni–N	See NIPHTI (1.887)							
Zn–N	See PTHCZN (1.978, 1.980)							
Nb–N	(6), (IV): all BEJTIT	2.144	2.144	0.015	2.129	2.159	4	
Nd–N	All CIZGIB02	2.471	2.471	0.009	2.463	2.479	4	
Os–N	(6), (II): all PCPCOS	2.016	2.015	0.041	1.980	2.055	4	
4.14.1.1 Pyrazolates (σ-$C_3R_3N_2$)†								
N^1–N^2	(1.361, 1.369, 1.367)							
N^1–C^5	(1.347, 1.350, 1.345)							
N^2–C^3	(1.340, 1.332, 1.327)							
C^3–C^4	(1.376, 1.386, 1.383)							
C^4–C^5	(1.384, 1.368, 1.373)							
Mo–N	See CAFLEA (2.157, 2.166)							
Ir–N	See BIXBUF10 (2.080)							
4.14.1.2 Pyrazolates (μ-$C_3R_3N_2$)†								
N–N		1.367	1.368	0.014	1.360	1.375	34	
N–C		1.345	1.345	0.020	1.338	1.350	68	
C–C		1.378	1.377	0.017	1.370	1.385	68	
Ti–N	See PZCPTI (2.205, 2.183)							
Fe–N	All DMPZFE	2.005	2.007	0.004	2.001	2.009	4	
Co–N	All DMPZCO	1.988	1.988	0.007	1.982	1.995	4	
Ni–N	(3,4), (0—II)	1.957	1.971	0.044	1.917	1.997	16	
Cu–N	(3,5), (I,II)	1.929	1.934	0.035	1.892	1.958	8	
Rh–N	(4—6), (I,III): all	2.080	2.084	0.017	2.065	2.094	24	
Pd–N	All PZALPD10	2.073	2.071	0.006	2.069	2.079	4	
Ir–N	(4,5), (I,II)	2.070	2.078	0.022	2.053	2.091	7	
4.14.2.1 Imidazolates (σ-$C_3R_3N_2$)†								
N^1–C^2		1.344	1.345	0.023	1.329	1.360	21	
N^1–C^5		1.376	1.369	0.026	1.355	1.398	21	
C^2–N^3		1.336	1.338	0.017	1.322	1.346	21	
N^3–C^4		1.356	1.355	0.024	1.340	1.372	21	
C^4–C^5		1.380	1.382	0.021	1.373	1.393	21	
Co–N	See ACNTCC (2.005), CTENCO20 (1.956)							
Cu–N	(4,5), (II): all	1.994	1.992	0.024	1.980	2.009	6	
Pd–N	See ADBPPD (2.015)							
Ag–N	See IMDZAG (2.074, 2.098)							
Ir–N	See CEXZIO (2.321, 2.116), CEXZOU (2.081), CEYBEN (2.081)							
Pt–N	(4), (II)	2.035	2.030	0.035	2.005	2.070	4	
Hg–N	See ADMEHH (2.070), CIRMAR (2.081)							
4.14.2.2 Imidazolates (μ-$C_3R_3N_2$)†								
N^1–C^2		1.332	1.332	0.012	1.325	1.341	49	
N^1–C^5		1.372	1.373	0.016	1.363	1.381	49	
C^4–C^5		1.358	1.354	0.015	1.348	1.368	25	
Mn–N	All IMIDZA	2.154	2.114	0.078	2.099	2.250	6	30
Fe–N	(4,6), (II)	2.065	2.043	0.070	2.012	2.137	8	
Cu–N	(4—6), (II): excluding BIMTCU (2.323)	1.966	1.967	0.022	1.957	1.979	19	
Zn–N	See IMZZNN (1.986, 1.993)							
Rh–N	(4,5), (–)	2.104	2.104	0.034	2.071	2.138	8	
Ir–N	See CEYBEN (2.087, 2.094)							
Hg–N	(2,3), (II)	2.086	2.084	0.008	2.079	2.094	4	
4.14.3 *N*-Alkylpyrazoles†								
N^1–N^2		1.360	1.360	0.015	1.350	1.368	53	
N^1–C^5		1.331	1.333	0.015	1.324	1.340	53	
N^2–C^3		1.349	1.350	0.012	1.342	1.358	53	
C^3–C^4		1.356	1.358	0.020	1.344	1.371	53	
C^4–C^5		1.387	1.387	0.015	1.377	1.396	53	
N^2–C(R)		1.452	1.452	0.023	1.439	1.469	53	
Cr–N	All CEYBIR	2.101	2.097	0.023	2.082	2.128	6	
Co–N	See DPPTCC (2.021, 2.036)							
Ni–N	(5,6), (II)	2.057	2.047	0.031	2.034	2.089	4	
Cu–N	(2,4,5,*), (I,II): all	1.973	1.979	0.072	1.927	1.994	19	
	(2), (I)	1.876	1.878	0.009	1.867	1.884	4	
	(4), (I)	1.991	1.990	0.039	1.963	2.030	8	
	(4,5), (II): excluding BENDED (2.173)	1.985	1.985	0.007	1.979	1.992	5	
Mo–N	See CAFLAW (2.123)							
Rh–N	See COSTIN (2.102, 2.111)							
Pd–N	(4), (II)	2.026	2.031	0.018	2.007	2.040	4	
Ag–N	See PMPZAG10 (2.243)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
4.14.3 *N*-Alkylpyrazoles†—(*continued*)								
Pt–N	(4,6), (II,IV): all	2.189	2.210	0.064	2.121	2.236	4	
Au–N	See BOFCEE (2.130, 2.141)							
Th–N	All FAPZTH10	2.637	2.633	0.017	2.624	2.655	4	
U–N	All UHXAPY10	2.574	2.582	0.024	2.549	2.593	4	
4.14.4 *N*-Alkylimidazoles†								
N^1–C^2		1.346	1.344	0.014	1.337	1.353	103	
C^2–N^3		1.320	1.320	0.017	1.310	1.328	104	
N^3–C^4		1.382	1.380	0.016	1.370	1.393	104	
N^1–C^5		1.369	1.369	0.015	1.361	1.380	104	
C^4–C^5		1.359	1.362	0.023	1.342	1.375	104	
N^1–C(R)		1.468	1.468	0.020	1.458	1.480	104	
Mn–N	See MNTPPI10 (2.191)							
Fe–N	(6), (II): excluding BERTAT (2.021)	2.199	2.191	0.018	2.183	2.218	5	
Co–N	(4—6), (II,III): all	2.058	2.036	0.065	2.015	2.096	21	8
	(4), (II)	2.019	2.016	0.008	2.013	2.026	6	
	(5,6), (II)	2.100	2.096	0.067	2.031	2.161	10	
	(6), (III)	2.021	2.042	0.053	1.970	2.062	5	
Ni–N	See CESKIU (2.102, 2.110)							
Cu–N	(4—6), (I,II): all	2.022	2.004	0.051	1.995	2.046	33	
	(4), (II)	1.974	1.970	0.019	1.959	1.995	7	
	(5), (II)	2.040	2.007	0.061	1.996	2.092	16	
	(6), (II)	2.023	2.022	0.021	2.006	2.041	9	
Zn–N	See CEPGUZ (2.083), MADCZB10 (2.040)							
Mo–N	See COFZEC (2.141, 2.273)							
Ru–N	See BAKDUM (2.094)							
Rh–N	See RACCAF (2.316)							
Pd–N	See COHCUX (1.988), ENGUPD (2.013), TCMIPD10 (2.011)							
Ag–N	(2,3), (I)	2.141	2.139	0.016	2.126	2.155	8	
Cd–N	See BEGNAC (2.358)							
Pt–N	(4), (II): all	2.017	2.015	0.014	2.008	2.027	20	
Hg–N	See BEJGIG (2.132), CAGSIM (2.125), MEGUHG (2.087)							
4.14.5 Pyrazole†								
N^1–N^2		1.352	1.353	0.015	1.345	1.356	43	
N^2–C^3		1.329	1.329	0.009	1.325	1.336	42	
N^1–C^5		1.339	1.338	0.010	1.333	1.345	43	
C^4–C^5		1.357	1.357	0.019	1.350	1.367	43	
C^3–C^4		1.388	1.387	0.017	1.376	1.396	43	
Mn–N	(6), (I,II): all	2.209	2.240	0.071	2.168	2.249	6	
	(6), (II)	2.237	2.243	0.021	2.219	2.252	5	
Fe–N	See MEPZFE (2.068)							
Co–N	See FMPZCO (2.032, 2.040, 2.042)							
Ni–N	(6), (II): excluding PYRZNI (1.905, 1.908)	2.102	2.098	0.016	2.089	2.118	4	
Cu–N	(5,6), (II)	1.988	1.995	0.030	1.964	2.011	12	
Zn–N	See CIRVOO (2.016, 2.017)							
Mo–N	(6,7), (0,II,III): all	2.193	2.174	0.059	2.142	2.251	6	
Ru–N	See CIZBES (2.211)							
Rh–N	(4,6), (I,III)	2.102	2.100	0.016	2.088	2.118	4	
Pd–N	See BABTUT (2.101)							
Pt–N	See CEZMUP (2.027)							
4.14.6 Pyrazolylborates†								
N^1–N^2		1.366	1.366	0.012	1.360	1.372	210	
N^2–C^3		1.339	1.339	0.014	1.329	1.347	211	
N^1–C^5		1.347	1.347	0.011	1.340	1.354	209	
C^4–C^5		1.366	1.368	0.016	1.360	1.375	211	
C^3–C^4		1.383	1.382	0.015	1.373	1.391	210	
N^1–B		1.546	1.543	0.019	1.535	1.555	211	
Cr–N	(4), (II)	2.061	2.060	0.006	2.057	2.067	4	
Fe–N	(6,7), (II,III): all	2.129	2.147	0.055	2.102	2.169	22	
Co–N	(4,6), (II,III): all	1.948	1.951	0.048	1.916	1.979	6	30
Ni–N	All PYZBNI excluding PPZBNI (1.891)	2.092	2.090	0.007	2.087	2.099	6	
Cu–N	(2—6), (I,II): all	2.035	2.002	0.134	1.949	2.052	29	86
	(2—5), (I)	2.001	1.987	0.075	1.946	2.041	23	
	(3), (I)	1.936	1.941	0.028	1.913	1.958	5	
Zr–N	See CEFHEA (2.387, 2.438, 2.430)							
Mo–N	(5—7), (0—VI): all	2.218	2.219	0.042	2.188	2.245	90	
Tc–N	See CHBPTC (2.088, 2.089, 2.259)							
Ru–N	See PZBZRU10 (2.101, 2.112)							
Rh–N	(4—6), (I,III): all	2.098	2.083	0.043	2.071	2.123	12	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
4.14.6 Pyrazolylborates†—(*continued*)								
Ag–N	See PRZBAG (2.194, 2.412)							
Yb–N	All BORVIN	2.469	2.453	0.074	2.405	2.530	8	
Ta–N	See CEXHUI (2.227, 2.273, 2.294)							
W–N	(6), (−)	2.215	2.213	0.028	2.200	2.218	9	
Pt–N	(4,5), (II)	2.098	2.121	0.050	2.054	2.129	9	
Au–N	See CEPMAL (2.119, 2.127)							
4.14.7 Pyrazolylgallates†								
N^1–N^2		1.370	1.368	0.009	1.362	1.377	40	
N^2–C^3		1.336	1.339	0.014	1.334	1.344	40	
N^1–C^5		1.344	1.344	0.011	1.339	1.352	40	
C^4–C^5		1.363	1.364	0.017	1.355	1.372	40	
C^3–C^4		1.380	1.381	0.012	1.373	1.386	40	
N^1–Ga		1.966	1.975	0.029	1.942	1.989	40	
Mn–N	See BATZIF (2.077), BEWVEE (2.076, 2.080)							
Fe–N	See MEPGFE (2.107)							
Ni–N	(4—6), (0—II): all	1.986	1.981	0.075	1.920	2.068	11	
	(4), (0—II)	1.932	1.922	0.038	1.898	1.976	6	
Cu–N	(4), (I,II)	1.982	1.979	0.026	1.960	2.006	5	
Mo–N	(5—7), (0—II): all	2.252	2.264	0.048	2.221	2.288	13	
	(7), (−)	2.267	2.270	0.033	2.237	2.289	11	
Rh–N	(4,6), (I,II): all	2.168	2.173	0.038	2.168	2.188	7	
4.14.8 Imidazole†								
N^3–C^2		1.324	1.324	0.012	1.316	1.330	194	
N^3–C^4		1.381	1.380	0.015	1.372	1.391	197	
C^2–N^1		1.340	1.339	0.014	1.332	1.347	196	
N^1–C^5		1.369	1.366	0.018	1.358	1.379	196	
C^4–C^5		1.361	1.356	0.021	1.347	1.373	197	
Cr–N	See BOPPIF10 (2.062, 2.050), LDHPCR10 (2.057)							
Mn–N	(5,6), (I,II): all	2.237	2.248	0.057	2.196	2.276	10	
	(5,6), (II)	2.251	2.266	0.042	2.205	2.279	9	
Fe–N	(4,6), (−): all	2.157	2.152	0.091	2.107	2.235	7	
Co–N	(4—6), (II,III): all	2.010	2.013	0.077	1.930	2.089	22	8
	(4), (II)	2.022	2.019	0.011	2.013	2.034	4	
	(5,6), (II)	2.103	2.097	0.028	2.088	2.112	7	
	(6), (III)	1.946	1.930	0.036	1.916	1.958	11	
Ni–N	(4,6), (II): all	2.103	2.099	0.024	2.082	2.128	30	
Cu–N	(3—6), (I,II): excluding IMZCUN (2.593)	1.988	1.981	0.050	1.961	2.008	82	
	(4), (II)	1.982	1.981	0.024	1.963	2.001	19	
	(5), (II): all	1.984	1.975	0.038	1.961	1.997	35	86
	(5), (II): excluding two >2.07	1.976	1.974	0.020	1.961	1.994	33	
	(6), (II): excluding three >2.13	1.996	2.009	0.038	1.954	2.029	23	
Zn–N	(4—6), (II)	2.043	2.056	0.044	1.997	2.076	21	
	(4), (II)	2.023	2.010	0.033	1.995	2.056	11	
	(6), (II)	2.084	2.076	0.027	2.066	2.098	8	
Mo–N	See MOSHIS10 (2.238, 2.245)							
Ru–N	See BAKDOG (2.087)							
Pd–N	See BOLRID (2.005), HISTPD (2.029)							
Ag–N	Sdd ADAGPC (2.154), AGIMHN01 (2.118, 2.132)							
Cd–N	(6,8), (II)	2.302	2.290	0.054	2.255	2.349	11	
Os–N	See CASVIB (2.153)							
Ir–N	See CEYBEN (2.081)							
4.15.1 Pyridine†								
N–C^2		1.341	1.339	0.018	1.331	1.348	612	
C^2–C^3		1.382	1.380	0.020	1.371	1.393	613	
C^3–C^4		1.372	1.372	0.021	1.360	1.384	610	
Ti–N	See ESALTJ (2.279)							
V–N	See TPYCLV (2.188)							
Cr–N	(6), (−): all	2.178	2.158	0.076	2.147	2.171	11	100
	(6), (−)	2.146	2.158	0.030	2.122	2.168	9	85
Mn–N	See BANVUH10 (2.018), COTGEX (2.377), FACMNB (2.086, 2.109)							
Fe–N	(5,6), (0,II,III): all	2.224	2.242	0.102	2.148	2.270	14	87,96
Co–N	(4—6), (II,III): all	2.082	2.066	0.084	2.004	2.172	50	8
	(6), (III): excluding CORHOG (2.214)	2.034	2.040	0.044	1.992	2.071	29	
	(6), (II): excluding BACREC10 (1.953, 1.963)	2.185	2.183	0.037	2.170	2.214	15	
Ni–N	(4,6), (−): all	2.111	2.116	0.059	2.085	2.150	33	
	(6), (−)	2.122	2.117	0.042	2.096	2.152	31	
Cu–N	(−), (−): all	2.070	2.046	0.072	2.033	2.061	32	86
	(4), (−)	2.024	2.023	0.019	2.007	2.043	4	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
4.15.1 Pyridine†—(*continued*)								
Cu–N	(5), (–)	2.113	2.060	0.105	2.024	2.183	11	
	(6), (–)	2.054	2.046	0.032	2.039	2.055	16	
Zn–N	(4—6), (–)	2.095	2.081	0.063	2.051	2.149	16	
	(4), (–)	2.064	2.064	0.057	2.027	2.115	6	
	(5), (–)	2.116	2.121	0.069	2.046	2.178	6	
	(6), (–)	2.111	2.099	0.058	2.063	2.173	4	
Mo–N	(5—7), (–): all	2.300	2.279	0.078	2.252	2.336	25	15,100
	: excluding HPHOMO10 (2.446)	2.282	2.278	0.046	2.249	2.329	23	85
Ru–N	(6), (I—III): all	2.124	2.108	0.049	2.095	2.138	28	100
		2.114	2.107	0.031	2.094	2.121	26	85
Rh–N	(6), (II—III): all	2.119	2.066	0.090	2.056	2.222	13	30,100
		2.063	2.062	0.016	2.050	2.075	9	85
Pd–N	(4), (–)	2.089	2.085	0.061	2.033	2.149	4	
Ag–N	(–), (–)	2.299	2.322	0.056	2.228	2.331	7	
Cd–N	(6,7), (–)	2.381	2.368	0.042	2.355	2.413	5	
Ta–N	See PCTATL10 (2.423)							
W–N	(5,6): all	2.284	2.283	0.098	2.201	2.323	11	
	: excluding CAKTUD (2.528)	2.260	2.263	0.059	2.196	2.322	10	
Re–N	(5,6), (IV—VII): all	2.235	2.176	0.114	2.142	2.339	13	87
Os–N	(6), (–): all	2.165	2.169	0.053	2.106	2.217	6	
Ir–N	See PCHIRH10 (2.140), PHPCIR10 (2.176)							
Pt–N	(4,6), (–): all	2.085	2.061	0.078	2.036	2.125	11	
	(4)	2.050	2.045	0.048	2.014	2.091	8	
Hg–N	Excluding ETACHG (2.656)	2.164	2.146	0.054	2.127	2.198	6	26
4.15.2 2,2′-Bipyridyl (chelating, bipy)†								
N–C		1.352	1.351	0.017	1.343	1.359	329	
C^2–$C^{2'}$		1.471	1.474	0.021	1.462	1.481	166	
V–N	(5,6), (–): all	2.186	2.151	0.075	2.126	2.280	12	30
	: short < 2.2	2.137	2.133	0.028	2.114	2.153	8	
Cr–N	(6), (III): all	2.085	2.076	0.037	2.059	2.088	20	30
Mn–N	See BPYMNA (2.291, 2.311), TNBPMN (2.087, 1.996)							
Fe–N	(5,6), (0,II,III): all	2.008	1.964	0.089	1.958	2.123	23	30
	(5,6), (II,III): low spin	1.961	1.962	0.012	1.954	1.967	16	
	(6), (III): high spin	2.151	2.153	0.024	2.123	2.172	6	
Co–N	(6), (II,III): all	2.098	2.129	0.093	2.072	2.147	10	8,30
	(6), (II)	2.141	2.133	0.023	2.126	2.152	8	
Ni–N	(4,5,6), (–): all	1.956	1.948	0.044	1.934	1.960	12	9
	(4)	1.944	1.939	0.033	1.921	1.959	9	
Cu–N	(4,5,6), (–): all	2.031	2.007	0.057	1.991	2.071	108	12,86
	(4), (II)	2.002	1.997	0.025	1.986	2.018	12	
	(5), (–)	2.038	2.010	0.062	1.992	2.081	70	86
	(6), (–)	2.024	2.003	0.053	1.990	2.053	22	86
Zn–N	(–), (–): all	2.088	2.090	0.034	2.056	2.117	4	
Zr–N	See TCBPZR (2.412)							
Nb–N	See TCBPNB (2.319)							
Mo–N	(5,6,7), (–): all	2.260	2.251	0.074	2.210	2.314	32	15
Ru–N	(6), (–): all	2.064	2.063	0.028	2.044	2.087	34	
Rh–N	See BIHJORH10 (2.020, 2.029)							
Pd–N	(3,4,6), (0,II,IV): all	2.088	2.086	0.087	2.014	2.169	8	
Ag–N	See BPYAGN (2.179, 2.153)							
Cd–N	(6), (–): all	2.369	2.367	0.033	2.339	2.396	14	
Re–N	See DPCLRE10 (2.245)							
Os–N	See CIXLIE (2.071, 2.112)							
Ir–N	(6), (–)	2.071	2.049	0.042	2.039	2.115	20	
Pt–N	See BIBFUN (2.107, 2.103), BPYCPT (2.001)							
Hg–N	(5,6,7), (–): all	2.307	2.293	0.057	2.276	2.358	8	
U–N	(9), (–): all	2.627	2.623	0.018	2.612	2.646	4	
4.15.3 Phenanthroline (chelating, phen)†								
N–C		1.361	1.360	0.014	1.353	1.367	157	
C^2–$C^{2'}$		1.428	1.429	0.017	1.419	1.439	84	
Ti–N	See PNOLTI (2.147, 2.223)							
Cr–N	See BUWYIB (2.055, 2.057)							
Mn–N	(6), (I,II): all	2.106	2.069	0.070	2.055	2.190	6	
	(6), (I)	2.062	2.052	0.013	2.055	2.075	4	
Fe–N	(6), (II): all	2.059	1.982	0.122	1.968	2.182	25	
	: tris-phen only	1.969	1.970	0.015	1.958	1.979	15	
Co–N	(6), (I—III): all	2.027	1.998	0.096	1.943	2.133	16	30
	(6), (I,II)	2.141	2.137	0.020	2.124	2.156	6	
	(6), (III)	1.958	1.947	0.033	1.938	1.992	10	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
4.15.3 Phenanthroline (chelating, phen)†—(*continued*)								
Ni–N	(4—6), (II): all	2.053	2.063	0.047	2.009	2.092	16	9
	(4), (II)	1.989	1.985	0.011	1.982	2.001	4	
	(5), (II)	2.034	2.033	0.011	2.024	2.045	4	
	(6), (II)	2.093	2.092	0.015	2.080	2.104	8	
Cu–N	(4—6), (I,II): all	2.059	2.023	0.069	2.009	2.087	51	12,86
	(4), (I)	2.083	2.078	0.040	2.056	2.122	14	
	(5), (II): excluding three > 2.21	2.021	2.015	0.027	2.009	2.021	18	
	(6), (II): short < 2.05	2.008	2.005	0.016	1.998	2.012	10	
	: long > 2.09	2.129	2.124	0.025	2.111	2.149	5	
Zn–N	(4), (II)	2.063	2.063	0.007	2.057	2.069	4	
Nb–N	See OPENBO10 (2.280, 2.332)							
Mo–N	(5,6), (0,IV,VI)	2.276	2.273	0.076	2.205	2.351	4	
Ru–N	See MPTBRH (2.083, 2.092)							
Rh–N	(6), (III): all CELLAG	1.934	1.933	0.009	1.925	1.934	4	
Cd–N	(6,*), (II)	2.369	2.368	0.018	2.354	2.384	5	
Ir–N	See CAYGAK (2.085, 2.122)							
Pt–N	See BOVLED (2.165, 2.175), CNPLPT (2.053, 2.762; 2.063, 2.007)							
Hg–N	(4,6,8), (II): all	2.486	2.408	0.147	2.391	2.669	11	30
4.16.1.1 Pyrazines (σ-$C_4R_4N_2$)†								
N^1–C^2		1.340	1.336	0.016	1.330	1.344	36	
C^2–C^3		1.390	1.387	0.022	1.376	1.403	37	
C^3–N^4		1.334	1.334	0.018	1.325	1.342	38	
Cr–N	See ACPCRB (2.315)							
Fe–N	See PYZTCI (2.031)							
Co–N	(6), (II): all	2.145	2.125	0.054	2.104	2.190	6	
Cu–N	(5,6), (II): excluding PYZCUA01 (2.167)	2.011	2.004	0.041	1.975	2.053	4	
Zn–N	See AZNPYD (2.145)							
Ru–N	See CABYIN (2.129, 2.152), PYZRUA (2.006)							
Rh–N	See PRNRHC (2.363)							
Ir–N	See CLPZIR (2.018)							
4.16.1.2 Pyrazines (μ-$C_4R_4N_2$)†								
N–C		1.337	1.333	0.022	1.326	1.345	18	
C–C		1.383	1.380	0.015	1.369	1.398	9	
Cu–N	(4,5), (II)	2.024	2.016	0.021	2.009	2.046	4	
Rh–N	See BUZZAX (2.100)							
Pd–N	See BENDAZ (2.051)							
Yb–N	See CPPYYB01 (2.614)							
Hg–N	See PAZHGN (2.263)							
4.16.2.1 Pyridazines (σ-$C_4R_4N_2$)†								
N^1–N^2		1.334	1.334	0.006	1.328	1.340	4	
N^1–C^6		1.325	1.327	0.007	1.318	1.330	4	
N^2–C^3		1.335	1.334	0.005	1.329	1.337	4	
C^3–C^4		1.374	1.377	0.026	1.349	1.397	4	
C^4–C^5		1.347	1.351	0.012	1.334	1.356	4	
C^5–C^6		1.388	1.387	0.017	1.373	1.405	4	
Fe–N	See TAZCFE (2.013)							
Cu–N	See BEJNIN (2.052, 2.071), PYAZCU10 (2.122)							
4.16.2.2 Pyridazines (μ-$C_4R_4N_2$)†								
N^1–N^2		1.352	1.357	0.028	1.333	1.373	14	
N^1–C^6		1.319	1.316	0.020	1.303	1.335	28	
C^3–C^4		1.417	1.415	0.027	1.392	1.442	28	
C^4–C^5		1.373	1.380	0.038	1.337	1.406	14	
Fe–N	See DAZHCF (1.955, 1.956)							
Ni–N	See HPCXNI (2.075, 2.060)							
Cu–N	(4—6,*), (II): all	2.015	2.013	0.029	1.988	2.039	22	
Ru–N	See DAZRUC10 (2.132, 2.136)							
4.16.3.1 Pyrimidines (σ-$C_4R_4N_2$)†								
N^1–C^2		1.360	1.361	0.026	1.346	1.377	95	
N^1–C^6		1.361	1.357	0.022	1.349	1.374	95	
N^3–C^2		1.345	1.342	0.033	1.321	1.374	95	
N^3–C^4		1.359	1.356	0.024	1.341	1.377	95	
C^4–C^5		1.372	1.375	0.030	1.351	1.395	95	
C^5–C^6		1.401	1.397	0.029	1.378	1.422	95	
Co–N	(4), (II) or (6), (III): excluding CICYAO (2.158)	1.981	1.981	0.006	1.976	1.987	4	
Ni–N	See URCLNI (2.144)							
Cu–N	(3—6), (I,II): excluding CLPRCV	2.006	1.992	0.047	1.981	2.020	19	
	(4—6), (II)	1.999	1.992	0.027	1.981	2.016	16	
Zn–N	(4,6), (II): all	2.065	2.065	0.013	2.056	2.074	6	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
4.16.3.1 Pyrimidines (σ-$C_4R_4N_2$)†—(*continued*)								
Mo–N	(5,6), (II,V): all	2.203	2.183	0.058	2.158	2.243	10	
	(5), (II)	2.178	2.173	0.026	2.157	2.198	8	
Pd–N	See BUCBUW (2.086), DCMCPD (2.031)							
Ag–N	(2—5), (I): all	2.188	2.188	0.026	2.167	2.209	5	
Cd–N	(4—6,8), (II): all	2.295	2.295	0.065	2.239	2.324	7	
	(4—6), (II)	2.275	2.289	0.042	2.232	2.304	6	
W–N	(5,8), (II,IV): all	2.161	2.163	0.010	2.156	2.169	8	
Pt–N	(4,5), (II): all	2.033	2.033	0.015	2.024	2.044	26	
Hg–N	(2,5), (II): all	2.117	2.100	0.033	2.092	2.151	5	
4.16.3.2 Pyrimidines (μ-$C_4R_4N_2$)†								
N^1–C^2		1.349	1.351	0.019	1.328	1.367	6	
N^1–C^6		1.330	1.322	0.024	1.310	1.353	6	
C^4–C^5		1.378	1.375	0.044	1.354	1.406	6	
Ti–N	See PMDTTI10 (2.174, 2.239)							
Cu–N	See COPFOC (2.007, 2.011)							
Ag–N	See SULPMS (2.205, 2.460)							
4.17.1 Hydrazido(1−)(σ-$NRNR_2$)								80
N–N	(1.318),(1.388)							
Re–N	See CEXKAR (1.949)							
Ir–N	See NPHZIR (1.912)							
4.17.2 Hydrazido(2−)(σ-NNR_2, R = C, H)								80
N–N		1.300	1.293	0.032	1.282	1.324	16	
Fe–N	See CESTOJ (1.811)							
Mo–N	(5,6), (II,IV,VI)	1.768	1.764	0.024	1.748	1.794	9	77
W–N	(6,7), (IV,V)	1.751	1.752	0.014	1.738	1.763	5	
Re–N	See BILMUE (1.937)							
4.17.3.1 Diazenes (σ-RNNR)†								
N–N	(1.235, 1.240, 1.131)							
Pd–N	See DCAZPD (2.023, 2.023)							
Au–N	See AZTLAW (2.151)							
4.17.3.2 Diazenes (η^2-RNNR)†								
N–N	(1.340)							
Ti–N	See AZBCTI10 (1.965, 1.971)							
4.17.4.1 Hydrazines (σ-NR_2NR_2)								
N–N		1.424	1.421	0.020	1.411	1.433	81	
Mn–N	See PHYZMN (2.345)							
Fe–N	See BEPZIF (2.273, 2.276)							
Co–N	(5,6), (II,III): all	2.105	2.173	0.115	1.980	2.208	7	30
	(5,6), (II)	2.196	2.194	0.024	2.175	2.220	4	
Ni–N	(4,6), (II): all	2.100	2.119	0.064	2.093	2.133	21	
	(6), (II)	2.118	2.120	0.027	2.101	2.133	19	
Cu–N	(4—6), (I,II): all	2.019	2.011	0.033	2.004	2.033	15	
Zn–N	(6), (II)	2.158	2.167	0.022	2.130	2.175	7	
Ru–N	See DMHERU01 (2.166, 2.279, 2.203)							
Rh–N	(6), (III)	2.118	2.115	0.023	2.098	2.136	10	
Cd–N	(6), (II)	2.451	2.469	0.070	2.367	2.502	6	
Sm–N	See ISNHSM (2.628, 2.651, 2.719)							
Dy–N	See CECLIF10 (2.570)							
Er–N	All CECLEB10	2.540	2.537	0.010	2.533	2.550	4	
4.17.4.2 Hydrazines (μ-NR_2NR_2)								
N–N	(1.423)							
Fe–N	See HZBTFE (2.245)							
4.18.1.1 Triazenido (terminal, σ-RNNNR)†								84,101
(M)N–N	(1.336, 1.333, 1.339)							
N–N	(1.286, 1.282, 1.274)							
Pd–N	See CTAZPD10 (2.033)							
Pt–N	See PAZPPT10 (2.084, 2.089)							
4.18.1.2 Triazenido (chelating, RNNNR)†								101
N–N		1.308	1.313	0.024	1.298	1.322	6	
Mo–N	See TLTZMO (2.232, 2.270)							
Ru–N	See TAZRUP10 (2.149, 2.179)							
Hg–N	See MNAZHG (2.313, 2.434)							
4.18.1.3 Triazenido (μ-RNNNR)†								101
N–N		1.308	1.303	0.020	1.295	1.318	46	
Cu–N	All CUDPTZ10	2.019	2.008	0.044	1.980	2.061	8	
Zn–N	All BISPAU	2.002	2.003	0.012	1.992	2.013	6	
Mo–N	(5), (III): asymmetric	2.212	2.210	0.056	2.159	2.261	6	
Rh–N	(5), (−)	2.117	2.117	0.022	2.095	2.138	8	
Pd–N	(5), (II)	2.078	2.079	0.042	2.034	2.123	16	
W–N	See MOPAZW (2.107, 2.096)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
4.19 Hydrazones and related ligands (σ-$NR_2N{=}CR_2$)								
N–N		1.382	1.380	0.021	1.367	1.397	137	
N=C		1.294	1.293	0.017	1.281	1.308	137	
Cr–N	(7), (III): see COHTOI (2.196, 2.259), DAPSCR10 (2.023, 2.397)							
Mn–N	(5—7), (II)	2.293	2.289	0.030	2.274	2.316	12	
Fe–N	(6,7), (II,III): all	2.100	2.124	0.126	1.957	2.202	14	96
Co–N	(5—7), (I,II)	2.171	2.169	0.049	2.148	2.198	30	
Ni–N	(5—7,*), (II): all	2.102	2.095	0.060	2.071	2.126	38	
	(6), (II)	2.092	2.093	0.049	2.065	2.111	32	
Cu–N	(4—6), (II): excluding two > 2.40	1.986	1.982	0.047	1.938	2.036	20	
Zn–N	(4,6,7), (II): all	2.232	2.234	0.069	2.187	2.293	6	
	(6,7), (II)	2.255	2.247	0.043	2.216	2.299	5	
Mo–N	See CLOSMO (2.194)							
Pd–N	(4), (II)	2.043	2.030	0.031	2.020	2.068	6	
Yb–N	See PCPHYB (2.534)							
Pt–N	See BHZEPT (2.221), COPGAP (2.249), HAPZPT10 (2.166)							
4.20 *vic*-Dioximes [chelating, N(O)CRCRN(O)]†								
N–C		1.299	1.299	0.014	1.291	1.308	548	
N–O		1.356	1.352	0.026	1.339	1.369	550	
C–C		1.467	1.466	0.019	1.456	1.482	268	
Fe–N	(6), (II)	1.901	1.901	0.018	1.886	1.918	4	
Co–N	(4,6), (II,III): all	1.893	1.889	0.030	1.882	1.897	363	102
	(6), (II): excluding FLDXCO10 (2.12—2.15)	1.903	1.897	0.026	1.887	1.928	12	
	(6), (III)	1.890	1.888	0.014	1.881	1.896	332	
Ni–N	(4,6), (II): all	1.939	1.872	0.103	1.864	2.067	45	9,30
	(4), (II)	1.869	1.868	0.013	1.860	1.872	30	
	(6), (II)	2.079	2.082	0.035	2.054	2.105	15	
Cu–N	(4—6), (I,II): all	2.012	1.992	0.072	1.961	2.034	38	30
	(4,5), (I)	2.135	2.137	0.022	2.110	2.156	10	
	(4—6), (II)	1.974	1.980	0.027	1.951	1.998	28	
Rh–N	(6), (III)	2.009	1.998	0.034	1.988	2.023	34	
Pd–N	(4,5,*), (II)	1.991	1.983	0.023	1.973	2.002	28	
Pt–N	(4,6,*), (II,IV)	1.994	1.991	0.019	1.980	2.010	38	
4.21 *N*-Nitrite (σ-NO_2) (see also 5.12.1)								103,104
N–O		1.221	1.227	0.027	1.212	1.236	172	91
Cr–N	See HMTZCR (2.203)							
Co–N	(6), (III): excluding BISHUG (2.105)	1.932	1.932	0.023	1.920	1.943	67	
Ni–N	(4,6), (0,II): all	2.118	2.125	0.071	2.084	2.153	6	9
	(6), (II)	2.143	2.129	0.043	2.118	2.174	5	
Cu–N	See PMPDCU (2.052)							
Ru–N	See BUPMOO (2.099)							
Pd–N	(4), (II)	2.020	2.020	0.021	2.001	2.035	6	
Pt–N	(4,6), (II–IV): all	2.132	2.171	0.076	2.038	2.188	6	
	(6), (III,IV)	2.181	2.179	0.013	2.169	2.195	4	
4.22.1 Ammonia (NH_3)								105
Cr–N	(6), (III)	2.069	2.069	0.008	2.063	2.076	5	
Co–N	(6), (III)	1.965	1.963	0.021	1.953	1.974	119	
Ni–N	(4,6), (II): all	2.074	2.115	0.093	1.941	2.141	7	30
	(6), (II)	2.128	2.130	0.019	2.109	2.146	5	
Cu–N	(4—6), (II)	1.987	1.988	0.017	1.977	1.996	11	
Zn–N	See CAXPUM (2.036, 2.051)							
Mo–N	See MEKTMO (2.217)							
Ru–N	(6), (II,III): all	2.126	2.123	0.024	2.109	2.145	37	
	(6), (II)	2.151	2.150	0.012	2.142	2.162	14	
	(6), (III)	2.110	2.111	0.016	2.104	2.122	19	
Rh–N	(4,6), (I,III): all	2.114	2.120	0.018	2.111	2.124	7	
	(4), (I)	2.120	2.121	0.007	2.113	2.126	6	
Pd–N	See APDPZC (2.026, 2.038)							
Re–N	See ATCTPR (2.253)							
Os–N	See TCTPOS (2.136)							
Pt–N	(4—6,*), (II—IV): all	2.050	2.048	0.021	2.036	2.059	102	
	(4), (II)	2.049	2.046	0.017	2.035	2.060	40	
	(6), (III,IV)	2.050	2.051	0.009	2.045	2.056	25	
	(5), (II)	2.052	2.053	0.023	2.038	2.069	23	
	(*), (–)	2.032	2.036	0.013	2.019	2.045	12	
4.22.2 Primary amines [NH_2R, R = C (sp^3)]								
N–C		1.484	1.484	0.019	1.474	1.494	1 577	
Cr–N	(6), (III)	2.078	2.080	0.021	2.068	2.089	138	
Mn–N	(5), (II)	2.198	2.199	0.007	2.192	2.204	6	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
4.22.2 Primary amines [NH_2R, R = C (sp^3)]—(*continued*)								
Fe–N	(6), (II): all picolylamine	2.067	2.030	0.070	2.019	2.084	15	30
	(6), (II): excluding FEPICA	2.035	2.027	0.027	2.012	2.063	12	
Co–N	(4—6), (II, III): all	1.966	1.964	0.025	1.952	1.977	716	
	(6), (III)	1.965	1.964	0.021	1.952	1.976	710	
Ni–N	(4—6,*), (−): all	2.074	2.089	0.064	2.071	2.115	130	30
	(4), (II): excluding BIHFAZ, NETNIP02	1.917	1.918	0.008	1.912	1.922	16	
	(4), (II): only BIHFAZ, NETNIP02	2.084	2.086	0.008	2.075	2.091	6	
	6, (II)	2.097	2.096	0.024	2.078	2.117	99	
Cu–N	(4—6,*), (−): all	2.019	2.013	0.039	1.996	2.030	274	12, 86
	(4), (II)	2.011	2.009	0.026	1.995	2.025	61	
	(5), (−)	2.024	2.014	0.040	1.998	2.033	132	86
	(6), (II): excluding three >2.150	2.014	2.016	0.023	1.997	2.029	62	
Zn–N	(4—6), (II): all	2.114	2.102	0.065	2.063	2.152	51	
	(5), (II)	2.064	2.063	0.034	2.043	2.074	18	
	(6), (II)	2.152	2.139	0.054	2.103	2.206	30	
Mo–N	(6—8), (II,IV—VI): all	2.290	2.271	0.067	2.237	2.355	13	30
	(6—8), (II,IV,V)	2.243	2.251	0.030	2.224	2.267	8	
	(6), (VI)	2.364	2.362	0.023	2.343	2.387	5	
Tc–N	(6), (V)	2.171	2.173	0.026	2.144	2.191	6	
Ru–N	(6), (II,IV): all	2.123	2.120	0.025	2.108	2.141	27	
Rh–N	(6), (III)	2.061	2.062	0.009	2.053	2.068	12	85
Pd–N	(4,5), (II): all	2.037	2.041	0.022	2.027	2.050	42	
Ag–N	See AGENPC10 (2.169, 2.171)							
Cd–N	(6), (II)	2.291	2.292	0.013	2.279	2.298	13	
Nd–N	All BILSIY	2.628	2.627	0.020	2.613	2.638	6	
W–N	See BOWLUU (2.407), CACRIH (2.213)							
Re–N	(6), (V)	2.164	2.161	0.018	2.149	2.179	8	
Os–N	(6), (IV,VI)	2.128	2.114	0.037	2.109	2.155	5	
Pt–N	(4—6,*), (II,IV): all	2.049	2.048	0.030	2.034	2.065	107	
	(4), (II)	2.043	2.046	0.026	2.033	2.061	65	
	(6), (II,IV)	2.069	2.065	0.034	2.047	2.079	27	
Au–N	See ENSPAU (2.119, 2.134)							
Hg–N	See COKDUB (range 2.179—2.416)							
4.22.3 Primary amines [NH_2R, R = C (sp^2)]								
N–C		1.437	1.440	0.025	1.429	1.449	43	
Co–N	(5,6), (II,III): all	2.012	2.009	0.051	1.977	2.042	13	
	(5,6), (II)	2.016	2.014	0.009	2.008	2.025	4	
	(6), (III)	2.010	2.001	0.062	1.947	2.066	9	
Ni–N	See MAQUNI10 (2.057, 2.063)							
Cu–N	(4—6,*), (II): excluding BZBCUA (2.216)	2.036	2.027	0.028	2.012	2.066	5	12
Zn–N	(4—6), (II)	2.095	2.085	0.053	2.049	2.150	4	
Mo–N	See ABTCMO (2.001, 2.009)							
Ru–N	See CANBRU (2.213)							
Rh–N	See BAYJAM (2.155), PRNRHD (2.324)							
Pd–N	See SULPDC10 (2.055)							
Cd–N	(5—7), (II)	2.402	2.423	0.039	2.359	2.435	9	
Nd–N	See BABNAT (2.743)							
Re–N	See ACANRE (2.246)							
Pt–N	See BATLPT10 (2.103), XAXASP (2.074)							
4.22.4 Secondary amines [NHR_2, R = C (sp^3)]								
N–C		1.488	1.487	0.021	1.476	1.499	1 718	
Ti–N	See BUNKIE (2.284, 2.301)							
V–N	See CAGSAE (2.328), CINKUF (2.150, 2.160, 2.328)							
Cr–N	(6), (0,II,III): all	2.090	2.086	0.033	2.071	2.100	40	
	(6), (II,III)	2.085	2.085	0.021	2.070	2.093	38	
Fe–N	(6,7), (II,III): all	2.158	2.164	0.078	2.133	2.181	44	
	(6), (III)	2.142	2.157	0.062	2.125	2.179	40	
	(7), (II)	2.316	2.306	0.042	2.283	2.360	4	
Co–N	(6), (II,III): all	1.976	1.970	0.050	1.949	1.991	229	
	(6), (II)	2.168	2.161	0.031	2.152	2.176	9	
	(6), (III)	1.968	1.967	0.030	1.947	1.986	216	
Ni–N	(4—6), (II): all	2.042	2.067	0.086	1.954	2.108	204	30
	(4), (II)	1.930	1.930	0.028	1.916	1.953	60	
	(6), (II)	2.097	2.098	0.042	2.072	2.121	124	
Cu–N	(4—6,*), (II): all	2.034	2.026	0.056	2.008	2.048	166	12,86
	(4), (II)	2.030	2.025	0.034	2.008	2.049	17	
	(5), (II): all	2.043	2.029	0.067	2.010	2.055	97	86
	: excluding five >2.23	2.029	2.027	0.032	2.008	2.049	92	
	(6), (II): all	2.022	2.022	0.027	2.002	2.048	35	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
4.22.4 Secondary amines [NHR_2, R = C (sp^3)]—(*continued*)								
Zn–N	(4—6), (II): all	2.143	2.162	0.079	2.066	2.214	17	
	(4), (II): all MAMPZN	2.039	2.039	0.006	2.032	2.045	4	
	(5), (II): all	2.188	2.200	0.051	2.155	2.219	10	
Mo–N	(5—8), (0,II—VI)	2.271	2.259	0.054	2.219	2.329	32	81,87
Tc–N	All BAPPIR	2.126	2.125	0.011	2.115	2.137	4	
Ru–N	(6), (II,III): all	2.127	2.085	0.085	2.071	2.238	10	30
	(6), (III)	2.075	2.083	0.018	2.064	2.085	7	
Rh–N	(4,6), (I,III): all	2.116	2.094	0.084	2.044	2.201	14	30
	(4), (I)	2.202	2.202	0.036	2.163	2.236	6	
	(6), (III)	2.051	2.051	0.032	2.019	2.084	8	
Pd–N	(4,6), (II,IV): all	2.043	2.053	0.035	2.007	2.060	28	
	(4), (II)	2.041	2.047	0.036	2.003	2.059	25	
Ag–N	(5,6), (I): excluding TZTDAG01 (2.159, 2.162)	2.483	2.476	0.054	2.443	2.536	10	
Cd–N	(4—7), (II): all	2.318	2.329	0.051	2.267	2.370	10	
W–N	See CAPSOB (2.333, 2.338)							
Re–N	(6), (I)	2.248	2.250	0.021	2.230	2.268	6	
Pt–N	(4,6), (II,IV): all	2.054	2.046	0.052	2.020	2.075	31	
	(4), (II)	2.060	2.052	0.059	2.003	2.122	21	
	(6), (IV)	2.049	2.048	0.013	2.036	2.063	8	
Hg–N	See BUPSUA (2.275, 2.439), HGTXZO (2.724)							
U–N	See SDAPOU20 (2.589)							
4.22.5 Secondary amines [NHR_2, $R_2 \neq C(sp^3)_2$]								
N–C	R = C (sp^2)	1.452	1.452	0.021	1.436	1.468	14	
	R = C (sp^3)	1.488	1.484	0.015	1.497	1.478	14	
Ni–N	(4,6), (II): all	2.070	2.090	0.084	2.018	2.143	10	
	(6), (II)	2.105	2.091	0.045	2.066	2.156	8	
Zn–N	See CAKGAW (2.213, 2.214)							
Mo–N	See BESJOY (2.357, 2.379)							
4.22.6 Tertiary amines (NR_3, R = any C)								
N–C		1.487	1.487	0.021	1.475	1.500	2 246	
Ti–N	(6), (IV)	2.296	2.294	0.025	2.273	2.317	6	
V–N	(6,7), (III—V)	2.277	2.279	0.056	2.262	2.294	12	
Cr–N	(5,6), (0,II,III): all	2.152	2.138	0.106	2.066	2.209	20	
	(6), (0)	2.207	2.209	0.016	2.192	2.221	4	
	(6), (III): excluding BILDIJ (2.355)	2.093	2.089	0.044	2.046	2.138	13	
Mn–N	(4—6), (I—III): all	2.306	2.338	0.120	2.197	2.384	9	
	(5,6), (II)	2.393	2.354	0.076	2.341	2.465	5	
Fe–N	(5—7), (II,III): all	2.215	2.199	0.112	2.090	2.317	36	
	(5), (II): all	2.155	2.162	0.079	2.080	2.191	11	96
	(5—7), (III): all	2.241	2.292	0.115	2.099	2.319	25	30,96
	(5—7), (III): Fe–N < 2.18	2.101	2.089	0.031	2.085	2.105	9	
	(5—7), (III): Fe–N > 2.26	2.321	2.316	0.044	2.294	2.338	16	
Co–N	(4—6), (I—III): all	2.080	2.040	0.135	1.961	2.199	91	86
	(4), (II)	2.075	2.068	0.026	2.062	2.102	7	
	(6), (II)	2.216	2.218	0.039	2.187	2.237	25	
	(6), (III)	1.961	1.960	0.027	1.938	1.977	43	
Ni–N	(4—6), (0—III): all	2.112	2.115	0.109	2.062	2.177	95	
	(4), (II)	1.957	1.973	0.048	1.894	1.996	11	
	(6), (II)	2.144	2.147	0.057	2.101	2.177	59	
	(6), (III): all CEXHAO	1.924	1.926	0.012	1.912	1.939	7	
Cu–N	(4—6,*), (I,II): all	2.098	2.071	0.093	2.045	2.112	260	12,86
	(4), (I)	2.139	2.135	0.053	2.099	2.178	44	
	(4), (II)	2.057	2.055	0.039	2.045	2.073	35	
	(5), (—)	2.099	2.067	0.112	2.043	2.095	125	86
	(6): all	2.091	2.049	0.095	2.034	2.105	43	30,86
	(6): short < 2.12	2.046	2.042	0.028	2.021	2.062	34	
	(6): long > 2.19	2.260	2.244	0.056	2.213	2.299	9	
Zn–N	(4—6), (II): excluding CMPORZ (2.530)	2.159	2.147	0.071	2.105	2.197	24	
	(4)	2.111	2.106	0.031	2.086	2.143	11	
	(5)	2.234	2.205	0.059	2.191	2.300	6	
	(6): all	2.171	2.147	0.068	2.110	2.244	7	
Mo–N	(5,6,*), (II—IV): all	2.372	2.387	0.094	2.273	2.450	33	
	(*), (IV): clusters only	2.252	2.255	0.016	2.242	2.265	6	
	(6), (II)	2.398	2.410	0.054	2.344	2.447	6	
	(6), (IV)	2.419	2.409	0.046	2.382	2.462	5	
	(6), (VI)	2.430	2.428	0.078	2.354	2.514	6	81
Tc–N	(6), (—)	2.196	2.200	0.029	2.170	2.220	5	
Ru–N	See CIYTUZ01 (2.306)							
Rh–N	(6), (I,III): all	2.087	2.083	0.066	2.032	2.152	9	
	(6), (III)	2.050	2.052	0.040	2.020	2.086	6	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
4.22.6 Tertiary amines (NR_3, R = any C)—(*continued*)								
Pd–N	(4,5,*), (−): all	2.111	2.098	0.052	2.097	2.147	66	
	(4), (−)	2.110	2.093	0.053	2.077	2.145	61	81
Ag–N	(3,4,*), (I)	2.372	2.380	0.031	2.342	2.406	9	
Cd–N	(5—8), (II)	2.437	2.428	0.074	2.379	2.499	18	
La–N	See HETALA11 (2.804, 2.835)							
Pr–N	See BIFYUK (2.696, 2.731)							
Nd–N	See BILSIY (2.701, 2.717)							
Sm–N	(9,10), (III)	2.715	2.716	0.059	2.659	2.771	4	
Eu–N	(7,9), (−): excluding CEXHUL (2.899)	2.606	2.627	0.062	2.540	2.651	4	
Gd–N	See BIFZEV (2.625, 2.677)							
Dy–N	(8,9), (−)	2.602	2.596	0.031	2.577	2.634	4	
Er–N	See HENAEB (2.523, 2.561)							
Yb–N	(8,9), (−)	2.571	2.555	0.054	2.529	2.628	4	
Lu–N	See CILCUV (2.588, 2.478, 2.468)							
W–N	See CEPLUE (2.492, 2.325)							
Re–N	See BOTFOF (2.326), COLWAB (2.242, 2.269)							
Os–N	See CHDQOS (2.231)							
Ir–N	(4,6), (I,II): all	2.095	2.078	0.049	2.066	2.134	5	
	(6), (III)	2.074	2.077	0.013	2.061	2.085	4	
Pt–N	(4—6), (II): all	2.137	2.116	0.083	2.082	2.146	18	86
	(4), (II)	2.108	2.116	0.035	2.078	2.126	13	
Hg–N	See CEFCUL (2.888)							
U–N	See EMASOU10 (2.692)							
4.23 Borazines (see also 2.3)								
V–N	See BOKXEE (2.218)							
Cr–N	See BRNOCR (2.067, 2.069), BUZPIV (2.205, 2.211), EMABOB (2.133, 2.159)							
Fe–N	See BEHLOP (2.090), BEMLAG10 (2.008), BUCZOO (2.012)							
Ni–N	See CIDBOG (2.495)							
5.1.1.1 Oxo (terminal, O)								106
V–O	(5—7), (−)	1.607	1.606	0.026	1.588	1.622	79	107
Cr–O	(4,5), (−)	1.616	1.598	0.041	1.590	1.651	11	7
Nb–O	(5—7), (−)	1.720	1.731	0.030	1.695	1.745	17	
Mo–O	(4—7), (−)	1.693	1.694	0.021	1.678	1.707	346	77,108
Tc–O	(5—6), (−): all	1.676	1.660	0.051	1.632	1.743	14	30
	(5,6), (−): not *trans* to O	1.647	1.652	0.022	1.626	1.664	10	44
	(6), (V): *trans* to O	1.749	1.751	0.006	1.743	1.754	4	
W–O	(−), (−)	1.692	1.697	0.020	1.674	1.706	22	
Re–O	(4—6), (−)	1.709	1.709	0.032	1.695	1.723	54	90
Os–O	(4—6), (−)	1.718	1.722	0.022	1.711	1.732	17	110
U–O	(6—8), (−)	1.763	1.762	0.026	1.748	1.776	161	
5.1.1.2 Oxo (μ-O)								106
Ti–O	(5—8), (−)	1.820	1.824	0.028	1.794	1.841	44	
V–O	See BIGVAO (1.697, 1.884; 1.694, 1.874), BUPCEU (1.763, 1.875)							
Cr–O	See CEYBIR (1.812, 1.818), HMTCRC10 (1.764)							
Fe–O	(4—7), (−): all	1.794	1.779	0.065	1.770	1.791	22	
	: excluding CEFVOY	1.775	1.774	0.017	1.769	1.787	20	
Zr–O	(4,8), (IV)	1.957	1.958	0.008	1.950	1.964	11	
Nb–O	(6—8), (IV,V)	1.946	1.926	0.036	1.913	1.983	21	
Mo–O	(5—7,*), (−): excluding CABHIW	1.924	1.927	0.028	1.910	1.941	239	
Tc–O	(6), (−)	1.914	1.914	0.008	1.907	1.923	6	
Hf–O	See OXMCHF (1.941)							
Ta–O	(6,7), (V)	1.924	1.923	0.027	1.900	1.951	4	
W–O	(5,6,*) (−)	1.916	1.920	0.023	1.899	1.933	64	
Re–O	(6), (II—VII)	1.926	1.920	0.026	1.907	1.945	16	
Os–O	(5,6), (IV,VI)	1.859	1.830	0.061	1.811	1.922	5	87
U–O	See PAUELI10 (2.161, 2.197)							
5.1.1.3 Oxo (μ_3-O)								
Ti–O	All CPTIOO	1.972	1.971	0.006	1.968	1.977	20	
V–O		1.946	1.985	0.061	1.872	1.995	20	30
Cr–O		1.937	1.936	0.008	1.933	1.944	13	
Mn–O	See OACPMN (1.942)							
Fe–O	All COCNAJ	1.929	1.956	0.056	1.863	1.968	6	
Co–O	See OXCFOR (2.039, 2.055, 2.114)							
Nb–O		2.062	2.039	0.046	2.027	2.118	12	30
Mo–O		2.015	2.003	0.035	1.990	2.048	47	
Ru–O	See BAHPEF (2.056, 2.067, 2.114)							
Rh–O		1.959	1.965	0.040	1.920	1.996	6	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
5.1.1.3 Oxo (μ_3-O)—(*continued*)								
W–O		1.994	1.999	0.019	1.981	2.007	28	
U–O	See BIHCUQ (2.229, 2.231, 2.243)							
5.2.1.1 Hydroxy (terminal, OH)								
Cr–O	Including H · · · O(H)–Cr	1.929	1.926	0.013	1.919	1.936	6	
Co–O	See CHXPCO (1.895), HGXIMC (2.190)							
Zn–O	See ACBZNM (2.268)							
Mo–O		1.988	1.976	0.043	1.957	1.032	4	
Re–O	See BAXJOZ (1.795)							
Pt–O		2.006	2.002	0.017	1.992	2.023	9	
5.2.1.2 Hydroxy (μ-OH)								
V–O	See CINKUF (1.955, 1.968)							
Cr–O	(6), (II,III)	1.959	1.960	0.023	1.946	1.972	55	
Fe–O	(5,6,*), (III): dominated by COCNAJ	1.967	1.965	0.039	1.951	1.989	34	
Co–O	(6), (III)	1.905	1.908	0.019	1.895	1.924	11	
Cu–O	(4,5,*), (II)	1.918	1.913	0.029	1.897	1.931	55	111
Zr–O	See COSROR (2.091, 2.167)							
Mo–O	(6—8), (III,IV)	2.061	2.081	0.068	2.040	2.098	10	87
Ru–O	(6,*), (II,III)	2.093	2.112	0.049	2.031	2.132	13	87
Rh–O	(6), (III)	2.110	2.108	0.046	2.090	2.135	10	
Yb–O	See PCPHYB (2.188, 2.216)							
Ta–O	See BUCLUG (2.024, 2.041)							
Re–O	(6), (I,VII)	2.100	2.070	0.054	2.060	2.165	6	87
	(6), (VII)	2.065	2.065	0.006	2.059	2.070	4	
Os–O	See CIRNUM (2.120, 2.133)							
Ir–O	All BAHVAH	2.120	2.119	0.004	2.117	2.125	4	
Pt–O	All HEPPTB	2.130	2.130	0.041	2.094	2.167	4	
U–O	See BUFFUD (2.336, 2.346)							
5.2.1.3 Hydroxy (μ_3-OH)								
Ni–O	All TACNIH10	2.087	2.091	0.011	2.079	2.096	7	
Cu–O	(*), (II)	1.995	1.988	0.033	1.969	2.024	10	
Zn–O	See ACBZNM (1.990, 2.089, 2.096)							
Mo–O	All CHPMOC	2.100	2.074	0.067	2.055	2.172	12	30
Ru–O	(*), (−)	2.146	2.141	0.028	2.123	2.173	4	
W–O	All DPEPOW	2.211	2.229	0.048	2.161	2.247	12	
Re–O	See BALZUJ (2.210)							
5.3.1.1 Alkoxy [terminal, O–C (sp^3)]								
O–C		1.426	1.427	0.030	1.411	1.443	287	
Ti–O	(6—8), (IV)	1.847	1.855	0.055	1.812	1.883	6	
V–O	See PRXHQV (1.774)							
Cr–O	(4,5), (III,IV)	1.816	1.824	0.045	1.773	1.855	5	
Mn–O	See BOPWAE (1.838)							
Fe–O	See LIBCRC (1.806, 1.829), MPORFE10 (1.815)							
Co–O	(6), (−): dominated by (III)	.921	1.931	0.026	1.897	1.939	9	
Ni–O	See BIBSAG (1.853), FMPHNI (1.840, 1.842)							
Cu–O	(4,5), (II): excluding one > 2.46	1.899	1.908	0.025	1.875	1.917	17	
Zr–O	(7,8), (IV)	1.924	1.921	0.020	1.905	1.944	5	
Nb–O	(6), (V)	1.869	1.877	0.048	1.818	1.910	15	
Mo–O	(4—6,*), (−)	1.911	1.908	0.046	1.885	1.935	114	15
Tc–O	See ASMETE (1.963, 1.936)							
Rh–O	See INDRHA (2.081), INDRHB (2.013)							
Ce–O	See FLMECE (2.196, 2.203, 2.230)							
W–O		1.900	1.901	0.044	1.868	1.934	85	
Re–O	(6), (V,VI)	1.890	1.886	0.028	1.869	1.901	8	
Os–O	(5,6), (VI)	1.914	1.896	0.047	1.873	1.970	8	
Pt–O	(4,6), (II,IV)	2.028	2.029	0.031	2.000	2.056	4	
U–O	(7,8), (IV,VI)	2.122	2.121	0.084	2.047	2.199	4	
5.3.1.2 Alkoxy [μ-OC (sp^3)]								
O–C		1.433	1.429	0.029	1.410	1.455	42	
Cr–O	(6), (I,II)	1.980	1.980	0.026	1.957	2.005	4	
Fe–O	See BIGPOW (1.998, 1.948)							
Cu–O	(4,5,*), (II)	1.929	1.934	0.018	1.918	1.944	20	111
Zn–O		1.958	1.969	0.027	1.929	1.975	4	
Zr–O	All BUXLEL	2.156	2.158	0.026	2.130	2.180	6	
Nb–O	All NBPMOX	2.149	2.151	0.023	2.127	2.170	4	
Mo–O		2.094	2.105	0.054	2.032	2.154	12	
Rh–O	See BUHTON (2.051, 2.063)							
Pd–O	All BIJPAL	1.996	1.999	0.010	1.985	2.004	4	
W–O		2.081	2.087	0.057	2.029	2.114	16	
Re–O	All MXOXRE10	2.113	2.109	0.021	2.095	2.135	4	
Pt–O	See MODIPT (2.040, 2.161)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
5.3.1.3 Alkoxy [μ_3-OC (sp^3)]								
O–C		1.445	1.441	0.026	1.429	1.459	49	
Fe–O	See BOWCAR10 (1.985, 1.989, 1.941)							
Co–O	(−), (II, III): all (many asymmetric)	2.044	2.091	0.104	1.911	2.135	20	30
	(−), (III): all are < 1.93	1.899	1.903	0.019	1.886	1.911	6	
	(−), (II): all are > 2.02	2.106	2.101	0.042	2.082	2.143	14	
Ni–O		2.066	2.062	0.035	2.032	2.084	18	
Cu–O	(−), (I,II): all	2.147	1.986	0.260	1.959	2.422	68	30
	(−), (II): short < 2.12	1.968	1.963	0.026	1.954	1.977	41	
	(−), (II): long > 2.22	2.518	2.540	0.116	2.428	2.596	21	
Zn–O	All BOYTOY	2.017	2.064	0.017	2.056	2.086	12	
Mo–O		2.186	2.166	0.049	2.154	2.221	13	111
Ru–O	See IPVRUB (2.127, 2.145, 2.210)							
W–O	See HXETOW10 (2.174, 2.201, 2.160)							
5.3.2.1 Aryloxy (terminal, OC_{aryl})†								
O–C^1		1.321	1.318	0.022	1.307	1.333	442	
C^1–C^2		1.410	1.411	0.018	1.399	1.422	888	
C^2–C^3		1.394	1.393	0.026	1.375	1.411	890	
C^3–C^4		1.381	1.379	0.024	1.367	1.394	890	
Ti–O	(5,6,8), (III,IV): all	1.873	1.898	0.064	1.828	1.920	9	
V–O	(5,6), (IV,V): all	1.917	1.925	0.043	1.906	1.945	13	
Cr–O	(6), (III)	1.921	1.924	0.007	1.914	1.926	6	
Mn–O	(6), (III)	1.914	1.896	0.064	1.866	1.953	8	
Fe–O	(4—6,*), (II,III)	1.913	1.905	0.043	1.882	1.937	66	
Co–O	(4—6), (I—III): all	1.907	1.896	0.051	1.873	1.919	93	86
	(4), (II)	1.867	1.860	0.028	1.847	1.880	22	
	(5), (II)	1.923	1.925	0.039	1.879	1.953	15	
	(6), (II)	1.977	1.995	0.062	1.906	2.030	17	30
	(6), (III)	1.894	1.895	0.014	1.886	1.903	34	
Ni–O	(4—6), (II): all	1.915	1.865	0.085	1.847	2.006	37	30
	(4), (II)	1.865	1.856	0.049	1.824	1.888	16	
	(5), (II): excluding two > 1.97	1.848	1.849	0.007	1.842	1.853	8	
	(6), (II)	2.023	2.023	0.021	2.005	2.045	11	
Cu–O	(2—6), (I,II): all	1.908	1.898	0.039	1.887	1.927	89	111
	(4), (II)	1.893	1.892	0.015	1.884	1.900	48	
	(5), (II)	1.920	1.918	0.034	1.892	1.940	25	
	(6), (II)	1.940	1.943	0.022	1.928	1.957	12	
Zn–O	See CPZHZN (1.953), MPZHZN (1.957), SALEZN (1.937)							
Y–O	All BIRJUH	2.298	2.297	0.013	2.287	2.310	4	
Zr–O	(8), (IV)	2.074	2.086	0.033	2.030	2.099	7	
Mo–O	(4—6), (II—VI)	1.964	1.956	0.080	1.915	1.974	29	15
	(4—6), (III,IV)	1.927	1.926	0.026	1.902	1.954	11	
Tc–O	See CEPHUA (1.987), COKZAD (1.949)							
Ru–O	See CESNAP (2.080, 2.129)							
Rh–O	(4,6), (I,III)	2.035	2.035	0.010	2.024	2.041	7	
Pd–O	(4), (II)	2.016	1.992	0.041	1.984	2.056	12	
Ce–O	All CEZYUB	2.215	2.219	0.021	2.194	2.233	4	
Ta–O	See BUNKAW (1.909), COLVII (1.836)							
W–O	(5—7), (II,V,VI): all	1.955	1.936	0.063	1.919	1.962	18	
	(5,6), (V,VI)	1.935	1.931	0.031	1.916	1.956	16	
Re–O	(6), (III–V)	1.971	1.975	0.021	1.951	1.992	8	
Os–O	(6), (II)	1.988	1.987	0.016	1.973	2.005	5	
Ir–O	See MICPIR10 (2.062, 2.050), SCLIRA10 (2.004)							
Pt–O	(4), (II)	1.996	2.003	0.020	1.978	2.010	5	
Th–O	(8,9), (IV)	2.321	2.335	0.026	2.301	2.344	7	
U–O	(7,8), (VI)	2.235	2.234	0.023	2.213	2.238	7	
5.3.2.2 Alkenoxy/aryloxy [μ-OC (sp^2)]								
O–C		1.330	1.331	0.029	1.315	1.344	68	
Ti–O	See CIGVET (2.041, 2.080), CLPHTI (1.911, 2.121)							
V–O	See BUVNUB (1.963, 2.269)							
Fe–O	(5,6), (I,III)	2.009	2.003	0.048	1.965	2.057	6	
Co–O	(6), (II)	2.077	2.085	0.062	2.016	2.130	14	
Ni–O	(4,6), (II): all	2.003	2.010	0.072	1.982	2.054	14	
	(6), (II)	2.031	2.039	0.041	1.988	2.061	12	
Cu–O	(3—6,*), (I,II): all	2.021	1.977	0.145	1.923	2.069	78	30
	(4—6,*), (II): short < 2.14	1.956	1.949	0.055	1.916	1.985	58	
	: long > 2.26	2.357	2.348	0.067	2.299	2.413	10	
Mo–O	See BCATMO (2.038, 2.324), PXTCMO10 (2.048, 2.052)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
5.3.2.2 Alkenoxy/aryloxy [μ-OC (sp^2)]—(*continued*)								
Ru–O	See CIYTUZ01 (2.203, 2.211)							
Cd–O	See PYXCDC (2.306, 2.317)							
Re–O	See PHCORE (2.152, 2.149)							
Hg–O	See PHGMQU (2.161, 2.790)							
U–O	All BIHCUQ	2.522	2.531	0.033	2.497	2.548	6	
5.4.1 Ketones (terminal, OCR_2, R = any C)								
O–C		1.264	1.264	0.022	1.252	1.272	24	
V–O	See DPKEVB (2.081)							
Fe–O	See MEOBFE (1.997)							
Ru–O	See ACSNRU (2.194)							
Cd–O	(7), (II): all CIHNEM	2.283	2.285	0.009	2.276	2.289	6	
Er–O	(7), (III): all MPYOER10	2.280	2.299	0.044	2.252	2.321	7	
Re–O	See PXBURE (2.159)							
Ir–O	See CEXLUM (2.234, 2.220)							
U–O	(6,7), (VI)	2.336	2.341	0.059	2.228	2.396	6	
5.4.2 Urea [terminal, $OC(NH_2)_2$]								112
O–C		1.266	1.266	0.014	1.254	1.277	52	
C–N		1.330	1.328	0.016	1.319	1.342	103	
Sc–O	(8), (III): all URSCNI	2.105	2.099	0.021	2.089	2.126	4	
Ti–O	See TIUREA01 (2.014)							
Cr–O	(6), (III): all $Cr[OC(NH_2)_2]_6^{3+}$	1.971	1.973	0.007	1.964	1.976	8	
Mn–O	See BOPWEI (1.985)							
Co–O	(6), (II)	2.091	2.094	0.010	2.081	2.099	4	
Cu–O	(6), (II)	2.127	2.130	0.022	2.105	2.148	5	82
Zn–O	See UREAZN (2.147, 2.073, 2.091)							
Mo–O	See BOHYEC (2.135)							
Pr–O	See ACURLB (2.479, 2.504)							
Nd–O	See CEFHOK (2.472, 2.500)							
U–O	(7), (VI)	2.356	2.360	0.034	2.332	2.382	21	
5.5.1.1 Formate (σ-O_2CH)								
(M)O–C		1.257	1.260	0.022	1.249	1.270	22	
C–O		1.234	1.230	0.021	1.220	1.250	22	
Fe–O	See FEFRMT (2.167)							
Ni–O	See CESGAI10 (1.936)							
Cu–O		1.966	1.956	0.030	1.949	1.988	5	
Zn–O	See AQNCZN (2.089)							
Y–O		2.343	2.364	0.046	2.296	2.370	7	
Cd–O	See AFNICD (2.284)							
U–O		2.352	2.328	0.052	2.309	2.408	5	
5.5.1.2 Formate (chelating, O_2CH)								
O–C	(1.253, 1.261, 1.188)							
Cu–O	See CAXMIX (2.352)							
Y–O	See CAVYON (2.414, 2.425)							
5.5.1.3 Formate (μ-O_2CH)								
O–C		1.262	1.263	0.014	1.251	1.272	47	
Cr–O	(6), (II)	2.021	2.023	0.005	2.015	2.026	8	
Co–O	See COKCIO (1.912)							
Mo–O	(5,6), (II): all	2.121	2.123	0.013	2.106	2.132	12	
Ru–O	(6,*), (0,II,III): all	2.042	2.026	0.046	2.021	2.033	14	
	(6), (II,III)	2.024	2.023	0.007	2.020	2.030	12	
Rh–O	See BIHJOR10 (2.040, 2.049)							
Re–O	(6), (III) all CLFORE10	2.041	2.053	0.026	2.012	2.058	6	
Os–O	All BIYXAI	2.167	2.166	0.008	2.159	2.174	4	
5.5.2.1 Acetate (terminal, O_2CMe)								
(M)O–C		1.264	1.263	0.028	1.252	1.280	46	
C–O		1.236	1.237	0.031	1.229	1.250	46	
C–C		1.512	1.510	0.026	1.499	1.523	46	
Cr–O	See ACETCR (2.306)							
Fe–O	See CIRDAI (1.898)							
Co–O	(4—6), (II)	1.990	1.970	0.059	1.947	2.049	10	8
Ni–O	See ACATEN (2.063, 2.080), NIAQAC03 (2.072)							
Cu–O	(4—6), (II)	1.957	1.957	0.015	1.949	1.966	10	12
Zn–O	(4), (II)	1.966	1.967	0.019	1.947	1.984	4	
Mo–O	See PNPMOA (2.208)							
Rh–O	See CESYAA (2.342)							
Pd–O	See AMXPPD (2.115), SFSTPD (2.164)							
Ag–O	See CELJEI (2.686)							
Cd–O	See ETNTCD (2.281)							
W–O	(6,7), (0,IV): all	2.124	2.125	0.100	2.030	2.214	6	30
Os–O	See BOWLII (2.018, 2.032)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
5.5.2.1 Acetate (terminal, O_2CMe)—(*continued*)								
Au–O	See CILYAX (2.063)							
Hg–O	See ACHPHG (2.454, 2.410), PHHGAC01 (2.083)							
5.5.2.2 Acetate (chelating, O_2CMe)								113
O–C		1.257	1.263	0.024	1.244	1.270	66	
C–C		1.496	1.497	0.025	1.480	1.514	34	
Co–O	See BIHYEW (2.086, 2.109)							
Cu–O	(6), (II)	2.306	2.259	0.208	2.172	2.477	6	12
Ru–O	See ACMPRU, ACTFIR, MPRUAC (in range 2.173—2.279)							
Rh–O	See AZBRHA10 (2.240, 2.219), BOXNEH (2.235, 2.162)							
Cd–O	See ACCDSC10, CDACET (in range 2.303—2.544)							
Pr–O	See ACURLB (2.538, 2.536)							
Nd–O	See CEFHOK (2.527, 2.516)							
Sm–O	See BEDZAL (2.513, 2.421)							
Gd–O	See ACAQGD (in range 2.427—2.484)							
Re–O	See ACTPRE (2.233, 2.197)							
Os–O	See BOWLII (2.169, 2.127)							
Hg–O	See ETACHG, TBPAHG10 (in range 2.244—2.666)							
U–O	(7,8), (VI): all	2.467	2.465	0.025	2.452	2.484	20	
5.5.2.3 Acetate (μ-O_2CMe)								
O–C		1.263	1.263	0.019	1.255	1.273	373	
C–C		1.509	1.507	0.023	1.495	1.524	187	
Cr–O	(5,6), (II): all Cr≡Cr	2.010	2.007	0.014	2.001	2.021	26	7
Co–O		1.927	1.926	0.014	1.915	1.941	6	8
Ni–O	See BAPHAB (2.033, 2.052)							
Cu–O	(6), (II)	1.971	1.970	0.013	1.963	1.980	38	12
Mo–O	(5—7), (II—IV)	2.110	2.110	0.021	2.096	2.122	97	
Tc–O	(5,6), (II,III)	2.068	2.066	0.009	2.060	2.072	10	
Ru–O	(6), (II,III)	2.036	2.020	0.033	2.013	2.062	22	
Rh–O	(5,6), (I—III)	2.038	2.035	0.025	2.026	2.046	97	83,86
Pd–O	(5,6), (I,II)	2.095	2.106	0.051	2.050	2.127	18	
W–O	(6,7), (II—IV)	2.092	2.089	0.029	2.072	2.111	22	
Re–O	(5,6), (III)	2.025	2.025	0.009	2.015	2.031	10	
Os–O	See CESXUT, COHNUI (in range 2.005—2.223)							
Pt–O	(6), (II): all	2.087	2.117	0.081	2.004	2.161	18	30
	: long > 2.075	2.155	2.160	0.026	2.141	2.175	10	
	: short < 2.025	2.003	2.003	0.016	1.993	2.016	8	
5.5.3.1 Alkylcarboxylates [terminal, O_2CC (sp^3)]								
(M)O–C		1.278	1.279	0.021	1.266	1.291	769	
C–O		1.234	1.233	0.017	1.224	1.244	768	
C–C		1.521	1.521	0.019	1.510	1.532	768	
Ti–O	(6), (IV)	2.000	1.983	0.043	1.967	2.015	15	
V–O	(6,7), (III–V): all	2.019	2.006	0.042	1.991	2.035	36	
	(6), (IV,V): exluding BUPCIY	2.002	2.003	0.017	1.990	2.010	23	
Cr–O	(5,6), (III,V): all	1.963	1.963	0.019	1.952	1.975	52	8
	(6), (III)	1.965	1.965	0.016	1.954	1.975	50	
Mn–O	(6), (I—III): all	2.059	2.040	0.121	1.913	2.165	35	
	(6), (II)	2.161	2.164	0.022	2.146	2.180	15	
	(6), (III): all	1.974	1.913	0.114	1.903	2.013	17	86
	: excluding two > 2.23	1.937	1.909	0.050	1.902	1.998	15	86
Fe–O	(6,7), (II,III): all	2.033	2.038	0.069	1.974	2.094	40	
	(6), (III)	2.018	2.012	0.057	1.971	2.048	15	
	(7), (III)	2.041	2.046	0.068	1.976	2.099	22	
Co–O	(4—6), (II,III): all	1.938	1.911	0.071	1.896	1.942	195	8,86
	(4), (II)	1.966	1.955	0.022	1.948	1.989	10	
	(6), (II)	2.088	2.075	0.050	2.062	2.097	26	
	(6), (III)	1.906	1.904	0.019	1.894	1.918	153	
Ni–O	(4—6), (II,III): all	2.051	2.055	0.056	2.038	2.087	72	
	(6), (II)	2.065	2.059	0.034	2.044	2.089	66	
Cu–O	(4—6), (II,III): all	2.015	1.961	0.145	1.946	1.982	123	86,114
	(4), (II)	1.948	1.947	0.026	1.931	1.964	25	
	(5), (II): all	1.991	1.957	0.108	1.947	1.976	44	86
	: excluding four > 2.2	1.960	1.952	0.036	1.945	1.973	40	
	(6), (II): all	2.074	1.977	0.184	1.957	2.205	51	30
	: short < 2.14	1.962	1.967	0.024	1.947	1.978	36	
	: long > 2.2	2.342	2.351	0.106	2.303	2.401	15	
Zn–O	(4—6), (II): all	2.038	2.050	0.059	1.978	2.079	29	
	(4), (II)	1.946	1.952	0.022	1.923	1.963	4	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
5.5.3.1 Alkylcarboxylates [terminal, O_2CC (sp^3)]—(*continued*)								
Zn–O	(5), (II)	2.018	1.997	0.059	1.967	2.080	8	
	(6), (II)	2.070	2.071	0.034	2.048	2.092	17	
Nb–O	See CNBPAC (2.161)							
Mo–O	(5—8), (o—VI): all	2.130	2.118	0.063	2.093	2.151	38	
Tc–O	(6), (−): all	2.050	2.025	0.070	2.011	2.063	8	86
	: excluding PCLTCA10 (2.215)	2.027	2.019	0.023	2.009	2.036	7	
Ru–O	(6), (II)	2.091	2.095	0.014	2.086	2.102	8	
Rh–O	(6), (III)	2.023	2.027	0.018	2.003	2.038	9	
Pd–O	(4,5), (II)	2.023	2.019	0.024	2.006	2.029	16	
Cd–O	(6,7), (II)	2.372	2.358	0.048	2.338	2.389	8	
La–O	(10), (III)	2.503	2.497	0.019	2.486	2.526	6	
Ce–O	(9), (III)	2.483	2.480	0.021	2.472	2.489	7	
Pr–O	(9), (III): all BIFYUK	2.458	2.447	0.027	2.441	2.484	4	
Nd–O	See ODACND (2.428)							
Sm–O	(9), (III): all NSMEDT02	2.421	2.421	0.021	2.400	2.441	4	
Eu–O	(9), (III)	2.394	2.395	0.096	2.317	2.470	5	
Gd–O	(9), (III): all BIFZEV	2.399	2.395	0.022	2.381	2.421	4	
Dy–O	(8,9), (III)	2.363	2.365	0.064	2.295	2.415	8	
Er–O	See HENAEB (2.240, 2.262, 2.265)							
Yb–O	(8,9), (III)	2.286	2.282	0.035	2.252	2.308	10	
W–O	See CIFNIO (2.132)							
Os–O	See BABWAC (2.038), FATBOS10 (2.207)							
Ir–O	(6), (III)	2.066	2.055	0.032	2.042	2.093	6	
Pt–O	(4,6), (II,IV)	2.031	2.014	0.040	2.003	2.045	13	
Hg–O	See FAHGME10 (2.064), PHGTFA (2.121)							
Th–O	(9,10), (IV)	2.402	2.402	0.012	2.393	2.413	5	
U–O	(7), (VI)	2.356	2.359	0.032	2.325	2.366	7	
5.5.3.2 Alkylcarboxylates [chelating, O_2CC (sp^3)]								
O–C		1.256	1.256	0.013	1.246	1.263	44	
C–C		1.516	1.521	0.024	1.501	1.529	22	
Ti–O	(8), (IV)	2.163	2.163	0.005	2.161	2.166	6	
Co–O	See BIYHOG (2.145, 2.223)							
Cu–O	See CEJPEM (2.528, 2.037)							
Zn–O	(6), (II)	2.205	2.191	0.072	2.162	2.244	6	
Mo–O	See FAMPMO (2.296, 2.338)							
Cd–O	See ABPENC (2.262, 2.716), BAYDIO (2.378, 2.350)							
Nd–O	See BODZEZ (2.535, 2.510)							
Sm–O	See BOTWUC (2.495, 2.455; 2.495, 2.585)							
U–O	See BIMAOU10 (2.526, 2.578)							
5.5.3.3 Alkylcarboxylates [μ-O_2CC(sp^3)]								
O–C		1.258	1.257	0.020	1.246	1.270	434	
C–C		1.519	1.519	0.026	1.504	1.536	222	
Cr–O	(6), (II)	2.018	2.017	0.003	2.015	2.021	5	
Cu–O	(6), (−)	1.966	1.968	0.014	1.956	1.975	95	
Nb–O	All CIPNEU	2.151	2.145	0.014	2.141	2.163	10	
Mo–O	(5,6,*), (−)	2.114	2.114	0.018	2.104	2.128	126	
Ru–O	(6), (−)	2.134	2.132	0.009	2.128	2.142	8	
Rh–O	(6), (−)	2.035	2.034	0.010	2.029	2.041	90	115
Pd–O	All BXCAPD	2.040	2.039	0.022	2.021	2.061	4	
Cd–O	All CIFGON	2.266	2.259	0.020	2.251	2.289	8	
Nd–O	All CIGRAL	2.422	2.422	0.018	2.406	2.439	4	
W–O	(5,6,*), (−)	2.092	2.091	0.016	2.082	2.103	66	
Re–O	See OCPPRE (2.093, 2.097)							
Os–O	(6), (III)	2.014	2.015	0.010	2.007	2.021	8	
5.5.4.1 Carboxylates [terminal, O_2CC (sp^2)]								
(M)O–C		1.277	1.277	0.017	1.266	1.288	74	
C–O		1.234	1.239	0.015	1.227	1.247	73	
C–C(sp^2)		1.508	1.507	0.014	1.499	1.513	74	
V–O	See BIGFAY01 (1.896, 1.912)							
Cr–O	See CAKCIA (1.946, 1.958)							
Mn–O	See ABZAMN (2.187), ZEGPEG (2.111)							
Co–O	See BELLEJ (2.130), CEBDIW (2.102), CUCOES (1.996), FSCUCO (1.941, 1.954)							
Ni–O	(4,6), (II): all	2.049	2.053	0.084	1.984	2.123	14	
	(6), (II): mononuclear	2.100	2.118	0.044	2.053	2.135	9	
Cu–O	(4—6,*), (II): all	1.992	1.947	0.170	1.930	1.967	38	86
	(4), (II)	1.927	1.934	0.032	1.896	1.951	13	
	(5), (II)	1.953	1.950	0.027	1.937	1.967	17	
	(6), (II): excluding three > 2.45	1.964	1.954	0.041	1.931	2.007	4	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
5.5.4.1 Carboxylates [terminal, O_2CC (sp^2)]—(*continued*)								
Zn–O	(4,6), (II)	2.033	2.010	0.053	1.989	2.090	5	
Cd–O	See CITDEO (2.253)							
Sm–O	See COSLEB (2.273), SALASM10 (2.488)							
Er–O	See COSLIF (2.198)							
Au–O	See CIYMEC (2.073, 2.074)							
5.5.4.2 Carboxylates [chelating, O_2CC (sp^2)]								
O–C		1.266	1.265	0.019	1.253	1.278	39	
C–C		1.481	1.482	0.022	1.474	1.493	20	
Ti–O	All BUCBEG	2.148	2.150	0.009	2.138	2.155	4	
Cu–O	See MESACV (1.976, 2.596)							
Ru–O	See BAWZUU (2.118), BZCPRU (2.166, 2.130)							
Cd–O	(7), (II): excluding CDMALD	2.409	2.427	0.058	2.351	2.445	10	
La–O	See ALANIC (2.568, 2.646)							
Nd–O	See BABNAT (2.529, 2.517), COSLAX (2.559, 2.512)							
Sm–O	See COSLEB (2.467, 2.521), SMNICD (2.486, 2.567)							
Dy–O	See AMAQDY (2.353, 2.517; 2.418, 2.502)							
U–O	See BAWRIA (2.452, 2.543)							
5.5.4.3 Carboxylates [μ-O_2CC (sp^2)]								
O–C		1.267	1.267	0.018	1.252	1.280	97	
C–C		1.493	1.492	0.024	1.476	1.508	49	
Co–O	(6), (II): excluding PYMCXC	2.037	2.030	0.021	2.020	2.056	8	8
Cu–O	(4—6,*), (I,II)	1.972	1.972	0.016	1.964	1.979	28	
Zn–O	See ACBZNM (1.979, 2.018)							
Mo–O	(5,6), (II,III)	2.110	2.107	0.017	2.099	2.119	22	
Rh–O	(6), (II)	2.038	2.036	0.011	2.027	2.050	16	
W–O	(5), (II)	2.079	2.079	0.012	2.070	2.087	12	
Re–O	(5,6), (III)	2.015	2.016	0.010	2.006	2.025	8	
5.5.5 Carbamates (chelating, O_2CNR_2)								
O–C		1.297	1.298	0.002	1.296	1.299	4	
C–N	(1.298, 1.319)							
N–C		1.462	1.457	0.011	1.456	1.473	4	
Ta–O	All BOBXUL	2.131	2.131	0.018	2.114	2.147	4	
5.5.6 Thiocarbamates (chelating, $OSCNR_2$) (see also 9.6.2)								
O–S		1.274	1.274	0.010	1.267	1.281	15	
S–C		1.728	1.731	0.009	1.725	1.733	15	
C–N		1.336	1.338	0.014	1.325	1.345	15	
N–C	Excluding one > 1.6	1.478	1.474	0.027	1.461	1.496	29	
Ti–O	See EMTCTJ (2.088, 2.077, 2.075)							
Co–O	See TMTCPC (2.157)							
Zr–O	See BUWMAH (2.249), EMTCZR (2.180, 2.200)							
U–O		2.408	2.402	0.040	2.381	2.439	5	
5.5.7.1 Thiocarboxylates (chelating, OSCR) (see also 9.5.2.1)								
O–C		1.236	1.246	0.035	1.234	1.255	9	
S–C		1.705	1.702	0.012	1.698	1.716	9	
C–C		1.521	1.522	0.025	1.501	1.531	9	
Ni–O	(6), (II)	2.142	2.135	0.035	2.119	2.171	9	
5.5.7.2 Thiocarboxylates (μ-OSCR) (see also 9.5.2.2)								
O–C		1.255	1.255	0.025	1.239	1.267	15	
S–C		1.694	1.696	0.018	1.681	1.703	15	
C–C		1.510	1.501	0.028	1.487	1.535	15	
Mn–O	(7), (II)	2.315	2.313	0.036	2.283	2.342	8	
Rh–O	See TACDRH10 (2.099, 2.114)							
Ag–O	See CEFMIJ (2.510)							
Eu–O	All BOTVIP10	2.511	2.508	0.032	2.483	2.541	4	
5.6 Oxalate [chelating, $(O_2C)_2$]								
(M)O–C		1.279	1.279	0.015	1.269	1.288	222	
C–C		1.546	1.546	0.018	1.536	1.556	111	
C–O		1.224	1.224	0.015	1.216	1.234	222	
Ti–O	(6—8), (III,IV): all	2.041	2.031	0.054	1.992	2.086	30	81
V–O	(5,6), (IV,V): all	2.083	2.036	0.090	2.015	2.164	18	81,86
	: short < 2.1	2.020	2.022	0.021	2.006	2.036	11	44
Cr–O	(6), (III)	1.969	1.975	0.019	1.959	1.981	24	
Mn–O	(6), (III): all ZZZCCG10	2.000	2.018	0.077	1.911	2.074	6	
Co–O	(6), (III)	1.911	1.912	0.011	1.903	1.920	22	
Cu–O	(4—6), (II)	1.951	1.949	0.018	1.934	1.964	29	
Y–O	(8), (III): all CIBZAO	2.335	2.340	0.018	2.329	2.344	6	
Zr–O	(8), (IV)	2.202	2.195	0.034	2.183	2.219	10	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
5.6 Oxalate [chelating, $(O_2C)_2$]—(*continued*)								
Mo–O	(6,7,*), (−)	2.119	2.101	0.038	2.092	2.140	22	
Rh–O	(6), (III): all CAZCIP	2.021	2.021	0.015	2.006	2.037	6	
Nd–O	All CICBOF	2.474	2.457	0.042	2.448	2.518	4	
Gd–O	All CICBUL	2.429	2.406	0.055	2.395	2.485	4	
Er–O	(8), (III): all CIBYOB	2.333	2.336	0.011	2.321	2.342	6	
Hf–O	(8), (IV): all KOXHFP10	2.190	2.184	0.022	2.171	2.211	8	
Re–O	(6), (IV): all KXOXRE	2.063	2.060	0.029	2.038	2.085	8	
Pt–O	(*), (−)	2.003	1.999	0.014	1.990	2.019	8	
U–O	(7,10), (IV,VI)	2.412	2.428	0.031	2.373	2.436	10	
5.7 Acetylacetonates [chelating, RC(O)CRC(O)R]†								
O–C_α		1.270	1.270	0.019	1.258	1.280	484	
C_α–C_β		1.387	1.387	0.020	1.377	1.397	488	
C_α–R		1.518	1.514	0.025	1.501	1.533	489	
Sc–O	(6), (III): all ACACSC	2.070	2.068	0.010	2.061	2.080	6	
Ti–O	(6), (IV)	1.979	1.964	0.052	1.941	2.032	12	81
V–O	(5,6), (III,IV)	1.981	1.984	0.015	1.966	1.993	8	107
Cr–O	(6), (III)	1.959	1.961	0.008	1.954	1.965	39	7
Mn–O	(5,6), (II,III)	2.034	2.026	0.119	1.915	2.145	20	30
	(6), (II)	2.158	2.149	0.021	2.144	2.180	8	
	(5,6), (III): all	1.952	1.924	0.075	1.910	1.940	12	
	: excluding two > 2.1	1.921	1.916	0.013	1.910	1.933	10	
Fe–O	(6), (II,III)	2.002	1.999	0.024	1.980	2.025	8	
Co–O	(6), (II,III)	1.939	1.894	0.074	1.884	2.012	64	86,87
	(6), (II)	2.033	2.034	0.035	2.003	2.062	23	
	(6), (III)	1.887	1.887	0.013	1.879	1.892	41	
Ni–O	(4,6), (II): all	1.999	2.015	0.050	1.969	2.035	10	9
	(6), (II)	2.020	2.021	0.023	2.000	2.044	8	
Cu–O	(4—6), (II): all	1.961	1.947	0.068	1.920	1.980	42	86,116
	(4,5), (II): excluding one > 2.1	1.931	1.922	0.032	1.906	1.953	22	
Zn–O	See ZNACAT10 (2.002, 1.971)							
Y–O	All CYSFAC10	2.324	2.318	0.017	2.311	2.341	4	
Zr–O	(8,9), (IV)	2.164	2.161	0.066	2.108	2.228	16	109,116
	(8), (IV)	2.123	2.118	0.041	2.084	2.160	10	
	(9), (IV)	2.232	2.238	0.033	2.205	2.254	6	
Nb–O	(8), (IV): all PIVMNB10	2.132	2.133	0.009	2.125	2.142	8	
Mo–O	(5—7), (II—V): all	2.096	2.077	0.052	2.068	2.110	24	81
		2.087	2.075	0.034	2.068	2.105	23	44
Tc–O	All TCACT01	2.015	2.013	0.006	2.010	2.021	4	
Ru–O	All BISKOD	2.031	2.036	0.011	2.019	2.041	8	
Rh–O	(4—6,*), (I,III)	2.041	2.046	0.032	2.014	2.061	32	
Pd–O	(4), (II)	2.049	2.061	0.051	2.002	2.092	49	30,109
		2.007	1.995	0.048	1.973	2.024	18	
		2.073	2.077	0.035	2.059	2.096	31	
Cd–O	See CAYJAN (2.223, 2.274)							
La–O	All AQACAL	2.472	2.480	0.024	2.453	2.489	6	
Pr–O	All CAZGUF	2.443	2.459	0.032	2.425	2.460	6	
Sm–O	All CAZHAM	2.392	2.401	0.027	2.380	2.407	6	
Eu–O	(7,8), (III)	2.348	2.354	0.024	2.325	2.364	24	
Er–O	(6,8), (III)	2.285	2.295	0.073	2.221	2.351	10	116
	(6), (III)	2.212	2.214	0.046	2.167	2.255	4	
	(8), (III)	2.333	2.331	0.038	2.301	2.368	6	
Re–O	All PASACR	2.007	2.009	0.009	1.997	2.015	4	
Ir–O	(4,6), (I,III)	2.064	2.041	0.063	2.021	2.099	6	
Pt–O	(4,6), (II,IV)	2.042	2.052	0.039	1.996	2.067	10	
Th–O	All TACTHB	2.402	2.405	0.019	2.391	2.416	8	
U–O	(7), (VI)	2.387	2.375	0.031	2.362	2.414	26	
5.8.1 *o*-Quinones (chelating, *o*-$O_2C_6R_4$)†								117
O–C_α	All	1.323	1.339	0.037	1.291	1.348	132	30
		1.270	1.274	0.022	1.252	1.287	38	118,119
		1.343	1.345	0.011	1.338	1.350	93	120
C_α–C_α	All	1.423	1.413	0.042	1.402	1.429	66	
		1.439	1.438	0.014	1.429	1.452	12	118,119
	μ-Chloranilates	1.529	1.530	0.009	1.522	1.536	7	
		1.404	1.404	0.017	1.400	1.415	47	120
Ti–O	(6), (IV)	1.978	1.980	0.048	1.940	2.009	12	120
V–O	(5,6), (III,IV)	1.973	1.966	0.036	1.942	1.999	18	118,119
Cr–O	(6), (0,III)	1.962	1.952	0.023	1.944	1.986	14	118,119
Mn–O	(6), (IV)	1.880	1.872	0.034	1.853	1.916	4	
Fe–O	(6), (III)	2.026	2.024	0.023	2.011	2.037	20	119,120
Ni–O	(6), (II)	2.068	2.063	0.043	2.027	2.107	6	118,119

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
5.8.1 *o*-Quinones (chelating, *o*-$O_2C_6R_4$)†—(*continued*)								117
Cu–O	See BAKPUY (1.945, 2.454), PMECAC (1.955, 2.196)							
Mo–O	(6,*), (–): excluding PHQUMO	1.992	1.955	0.062	1.940	2.050	18	8,120
Rh–O	(5), (I,III)	2.031	2.037	0.026	2.003	2.051	4	
Pd–O	See TCATPD (2.030, 2.039)							
Ce–O	See CECATI (2.357, 2.362)							
Pr–O	All CAZZAE	2.488	2.490	0.016	2.471	2.501	6	
Hf–O	See HFCATH (2.194, 2.220)							
Ir–O	See BRNPIR (2.008, 1.905)							
Pt–O	See CINREW (2.017, 1.994)							
Th–O	See CATETH (2.418, 2.421)							
U–O	See SCATUR (2.362, 2.389)							
5.8.2 *o*-Tropolonates (chelating, *o*-$O_2C_7R_5$)†								
O–C_α		1.286	1.286	0.016	1.274	1.299	26	
C_α–$C_{\alpha'}$		1.464	1.465	0.009	1.459	1.469	14	
Sc–O	(6,8), (III)	2.189	2.179	0.064	2.163	2.209	7	
Co–O	See COTROP (2.050, 2.068), COTROQ (1.888, 1.885, 1.882)							87
Cu–O	See CUTROP01 (1.913, 1.914)							
Rh–O	See TROPRH (2.034, 2.081)							
Th–O	(9), (IV): all TROPTH	2.450	2.444	0.018	2.438	2.463	8	
U–O	See TROPUE (2.393, 2.373)							
5.9.1.1 Carbonates (chelating, CO_3)								121
(M)O–C		1.300	1.301	0.031	1.297	1.324	16	
C–O		1.237	1.237	0.022	1.215	1.261	8	
Co–O	(6), (III): excluding CAIMCO	1.905	1.906	0.015	1.893	1.916	6	
Zr–O	See COMPEZ (2.198)							
Pt–O	See BUPPUX (2.059)							
U–O	All BANDAV	2.428	2.431	0.021	2.407	2.446	4	
5.9.1.2 Carbonates (μ-CO_3)								121
(M)O–C		1.264	1.256	0.027	1.252	1.288	9	
C–O		1.278	1.283	0.027	1.250	1.300	4	
Cu–O	(5), (II)	1.991	1.978	0.036	1.972	2.038	7	
Pt–O	See CIXHEW (2.085)							
5.9.1.3 Alkyl carbonates (μ-O_2COR)								
O–C		1.272	1.273	0.019	1.254	1.289	4	
C–O(R)	(1.294, 1.328)							
Mo–O	All BCBXMO	2.127	2.127	0.015	2.113	2.141	4	
5.10.1 Amine oxides (σ-ONR_3)								
O–N	(1.409, 1.408)							
Cu–O	See AQOXCU (1.948)							
Re–O	See BUTTOZ (2.149)							
5.10.2 Pyridine *N*-oxides (terminal, C_5R_5NO)								
O–N		1.335	1.333	0.017	1.324	1.345	49	
N–C		1.352	1.347	0.022	1.340	1.362	96	
Mn–O	See BIVWIM (2.155)							
Fe–O	See FEHPYO (2.111)							
Co–O	(6), (II)	2.086	2.090	0.035	2.050	2.119	5	
Ni–O	(6), (II)	2.054	2.049	0.022	2.036	2.076	4	
Cu–O	(4—6), (II): all	2.066	1.976	0.171	1.949	2.115	18	86
	(4—6), (II): short < 2.10	1.987	1.958	0.067	1.946	2.077	14	
Zn–O	(5,6), (II)	2.076	2.076	0.031	2.049	2.103	4	
Cd–O	See CITDEO (2.329)							
Th–O	(9), (IV)	2.422	2.419	0.040	2.392	2.438	10	
U–O	(7), (VI)	2.329	2.331	0.017	2.311	2.344	4	
5.10.3 Hydroxamates [σ-ON(=CR_2)R]†								
O–N		1.365	1.366	0.017	1.350	1.377	54	
N=C		1.315	1.311	0.018	1.303	1.322	55	
N–C		1.456	1.462	0.017	1.442	1.469	55	
Cr–O	See CRMTBH (1.965, 1.967, 1.976)							
Mn–O	See MNMTBH (1.959, 1.941, 2.132)							
Fe–O	(6), (III)	1.981	1.985	0.023	1.957	2.001	12	
Co–O	See COMTBH (1.937, 1.925, 1.943)							
Mo–O	(5,6), (VI)	2.047	2.025	0.053	2.010	2.065	15	
Rh–O	See BIWLAU (2.037)							
Hf–O	(8), (IV)	2.132	2.130	0.023	2.117	2.143	8	
Pt–O	See CACMIC (2.059)							
Th–O	(8), (IV)	2.352	2.342	0.023	2.336	2.373	5	
U–O	See CIBHAW (2.418, 2.379)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
5.11.1.1 Nitrate (terminal, NO_3)								104
(M)O–N		1.267	1.266	0.030	1.250	1.260	64	
N–O		1.227	1.229	0.023	1.216	1.240	127	
Ti–O	See BASSAP (2.059, 2.086)							
Mn–O	See MALCDB (2.251), TNBPMN (1.865)							
Fe–O	See CNOFEA (1.973)							
Co–O	(5,7), (II)	2.103	2.102	0.029	2.080	2.127	5	
Ni–O	(6), (II)	2.082	2.061	0.055	2.040	2.135	5	
Cu–O	(4—6,*), (II)	2.285	2.284	0.259	2.027	2.532	26	
	(4,5), (II): short < 2.055	1.996	1.996	0.037	1.964	2.037	9	
Zn–O	See CATKOX (2.179)							
Rh–O	(6), (III)	2.117	2.124	0.037	2.078	2.148	4	
Pd–O	See CAYXAB (1.995, 1.989)							
Ag–O	See MCYTAG10 (2.469), NTPAAG (2.259)							
Cd–O	(6,7), (II)	2.385	2.402	0.056	2.317	2.437	6	
Nd–O	See BAWDIM10 (2.525)							
Pt–O	(4,6), (II,III)	2.143	2.168	0.063	2.098	2.174	5	
Hg–O	See PYHGAN10 (2.702, 2.723)							
5.11.1.2 Nitrate (chelating, NO_3)								104
(M)O–N		1.255	1.259	0.027	1.239	1.273	290	
N–O		1.217	1.218	0.016	1.207	1.226	147	
Sc–O	All URSCNI	2.351	2.336	0.061	2.303	2.415	4	
Ti–O	All BEYGAN	2.146	2.145	0.036	2.113	2.179	4	
Mn–O	See TNBPMN (2.102, 2.386; 2.225, 2.183)							
Fe–O	See CALGAX (2.323, 2.019)							
Co–O	(6,7), (II): many asymmetric	2.212	2.200	0.131	2.108	2.297	18	
Ni–O	(6), (II)	2.166	2.156	0.052	2.132	2.210	12	
Cu–O	(5,6,*), (II): all	2.298	2.416	0.276	1.993	2.554	44	12,30
	: short < 2.05	1.993	1.992	0.021	1.985	2.007	18	
	: long > 2.17	2.509	2.532	0.132	2.455	2.575	26	
Zn–O	See CATKOX (2.228, 2.253), CEMWEW (2.301, 2.500)							
Zr–O	(8,9), (IV)	2.310	2.302	0.043	2.277	2.320	10	
Rh–O	See NCPRHB (2.188, 2.184)							
Ag–O	(4,5), (I): many asymmetric	2.555	2.552	0.102	2.462	2.658	6	
Cd–O	(6—8), (II): many asymmetric	2.460	2.408	0.159	2.342	2.596	18	
La–O	(11,12), (III)	2.664	2.665	0.051	2.627	2.686	36	
Ce–O	(10,11), (III,IV)	2.629	2.641	0.096	2.551	2.699	10	45,87
Nd–O	(10—12), (III)	2.584	2.576	0.063	2.549	2.613	32	
Sm–O	All SMHXAZ10	2.543	2.528	0.055	2.503	2.578	12	
Eu–O	(10,11), (III)	2.504	2.498	0.050	2.477	2.513	12	
Gd–O	(9,10), (III)	2.483	2.490	0.047	2.446	2.520	10	
Hg–O	(5,6,8), (II)	2.558	2.675	0.270	2.245	2.771	12	
Th–O	(12), (IV)	2.586	2.572	0.040	2.560	2.598	16	122
U–O	(8), (VI)	2.528	2.527	0.027	2.509	2.538	24	122
5.11.1.3 Nitrate (μ-NO_3)								104
(M)O–N		1.257	1.258	0.023	1.240	1.279	12	
N–O		1.229	1.227	0.017	1.215	1.241	6	
Cu–O	See CERCUX (2.790, 2.534), COLDOW (2.331, 2.421), NTPHCU (2.335, 1.995)							12
Ag–O	See CIXYAJ (2.381, 2.481)							
Hg–O	See BIPYHG (2.705, 2.535)							
5.12.1.1 *O*-Nitrite (terminal, ONO) (see also 4.21)								103,104
(M)O–N		1.293	1.293	0.028	1.265	1.312	6	
N–O		1.196	1.197	0.035	1.174	1.223	7	
Cr–O	See NTPYCR (1.963)							
Co–O	See EINICI (1.915)							
Ni–O	See HPNONI (2.112), NMEDNI10 (2.114)							9
Cu–O	See BPNICU (2.074), CEZNIE (1.969)							
Zn–O	See BEKPUC (2.220)							
5.12.1.2 *O*-Nitrite (chelating, O_2N) (see also 4.21)								103,104
O–N		1.247	1.249	0.019	1.235	1.258	29	
Ni–O	(6), (II)	2.151	2.143	0.020	2.136	2.173	6	
Cu–O	(6), (II): all	2.272	2.277	0.217	2.057	2.466	10	30
	: short < 2.25	2.081	2.072	0.083	2.007	2.160	5	
	: long > 2.35	2.463	2.462	0.090	2.388	2.539	5	
Zn–O	(6),(II): all	2.221	2.251	0.145	2.072	2.331	13	30
	: short < 2.1	2.063	2.072	0.024	2.046	2.077	5	
	: long > 2.2	2.319	2.298	0.085	2.254	2.356	8	
5.13.1 Dioxygen (terminal, O_2)								123,124
O–O	(1.301, 1.276, 1.283)							118

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
5.13.1 Dioxygen (terminal, O_2)—(*continued*)								123,124
Co–O	See FSMICO (1.881), MESOCO (1.888), OAMSCO (1.885)							8
5.13.2 Dioxygen (η^2-O_2)								123—125
O–O		1.460	1.463	0.026	1.442	1.472	44	120
Ti–O	(5,6), (IV)	1.852	1.850	0.024	1.832	1.867	10	120,126
V–O	(5,6), (IV—V)	1.895	1.884	0.034	1.868	1.913	22	86,120
Co–O	See MPASCO (1.862, 1.868)							8
Nb–O	(5,6), (V)	1.980	1.980	0.017	1.969	1.985	8	120
Mo–N	(5,6), (VI)	1.932	1.929	0.019	1.915	1.951	36	77,120
Rh–O	(5), (I)	2.034	2.026	0.033	2.009	2.067	4	
Ir–O	(5), (I)	2.058	2.057	0.020	2.039	2.078	4	
U–O	See BANDAV (2.219, 2.250)							
5.13.3 Dioxygen (μ-O_2)								125
O–O		1.482	1.487	0.019	1.463	1.496	4	120
Co–O		1.894	1.889	0.018	1.882	1.908	5	120
5.13.4 Peroxy (OOR)								125
O–O	Excluding CEMMIQ (1.215)	1.467	1.465	0.023	1.445	1.489	5	
V–O(η^2)	See CAMXOD (1.872, 1.999)							
Co–O (σ)	See CUMPCO (1.897), SCQUCO (1.854)							8
Pt–O (σ)	See BOVLED (2.032), BULTEH (2.051), CEMMIQ (1.989)							
5.14 Tertiary phosphine oxides (terminal, OPR_3)								
O–P		1.506	1.505	0.018	1.496	1.522	28	
P–C		1.791	1.794	0.026	1.777	1.807	87	
Mn–O	See CONTEE (2.084, 2.147)							
Co–O	See BIRXIJ (1.990), CLTPOC01 (1.940)							
Cu–O	(4,*), (II)	1.947	1.948	0.013	1.934	1.959	5	
Zn–O	See BIJWEW (1.966), CLPOZN (1.983)							
Nb–O	See COJYEF (2.135)							
Rh–O	See CXPORH (2.049)							
Ce–O	See NTPOCE (2.215, 2.222)							
W–O	See CXPHOW (2.163, 2.175), PMYPCW (2.198)							
Re–O	See CADMAV (2.092)							
U–O	(6—8), (IV,VI): excluding CAMCUO	2.279	2.265	0.049	2.243	2.321	10	
5.15.1.1 Phosphate (chelating, PO_4)								
(None)								104
5.15.1.2 Hydrogenphosphate (μ-PO_4H)								
Mo–O	See PYMOPH (2.001, 2.007)							
Pt–O	See CAJFAU (1.987—2.020)							
5.15.1.3 Alkyl phosphates (PO_4R)								
(M)O–P		1.519	1.521	0.016	1.511	1.534	8	
Co–O		1.963	1.964	0.033	1.931	1.994	4	8
Cd–O		2.238	2.252	0.046	2.189	2.273	4	
5.16.1.1 Dialkylphosphinates (σ-O_2PR_2)								104
(M)O–P	(1.506)							
P–O	(1.508)							
P–C	(1.834, 1.778)							
Mn–O	See AMPMNC (2.140)							
5.16.1.2 Dialkylphosphinates (μ-O_2PR_2)								
O–P		1.509	1.512	0.013	1.505	1.519	23	
P–O		1.798	1.801	0.017	1.788	1.808	24	
Mn–O	All AMMPMN	2.163	2.155	0.037	2.133	2.204	4	
Cu–O	(4,5), (II)	1.919	1.918	0.010	1.914	1.923	14	
Zn–O	See BISCEL (1.926)							
Re–O	All DPINRE	2.167	2.153	0.034	2.147	2.202	4	
5.17 *O*-Dialkyl sulphoxides (terminal, OSR_2) (see also 9.16)								127
O–S		1.525	1.520	0.021	1.516	1.621	40	
S–C		1.787	1.788	0.020	1.775	1.799	77	
Fe–O	(6), (III)	2.016	2.012	0.013	2.006	2.029	5	
Cu–O	See CEBREG (2.525), TMSCCU (1.945, 1.950)							
Mo–O	(6), (–)	2.256	2.258	0.082	2.202	2.335	12	87
Ru–O	See BESXRU (2.051), CDMSOR (2.142)							
Rh–O	See BEGFEY (2.234, 2.262), MSORHB (2.240)							82
Cd–O	See BEGNAC (2.291)							
Eu–O	See MTXPVE (2.404)							
Re–O	See ACMRHD (2.302)							
Pt–O	See BINJEN (2.126)							
Hg–O	See DMSOHG (2.318, 2.320; 2.377, 2.576)							
Th–O	See CPHSTH (2.459, 2.460)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
5.17 *O*-Dialkyl sulphoxides (terminal, OSR_2) (see also 9.16)—(*continued*)								127
U–O	See BOZDID (2.432), CEMCUS (2.317), FDMSON (2.352)							
5.18.1.1 Sulphate (terminal, SO_4)								104
(M)O–S		1.479	1.479	0.022	1.459	1.501	9	
S–O		1.465	1.463	0.025	1.457	1.482	27	
Mn–O	See AQSUMN (2.129)							
Cu–O	(5), (II): short; see AXEXAC (1.948), PYRCUD (1.909), TIMCUS (2.015)							
	(5,6), (II): long; see AENCUS (2.492), DAPRCX (2.496)							
Th–O	See BOHPUJ (2.378)							
U–O	See BEMPOY10 (2.377), TURURS01 (2.408)							
5.18.1.2 Sulphate (chelating, SO_4)								
(None)								
5.18.1.3 Sulphate (μ-SO_4)								
(M)O–S		1.507	1.500	0.031	1.476	1.538	10	
S–O		1.457	1.459	0.023	1.437	1.478	10	
Fe–O	See CNOFEB (1.983)							
Cu–O	See HETXCU (2.441)							
Cd–O		2.407	2.391	0.087	2.333	2.497	4	
Pt–O	All BINJEN	2.010	2.009	0.010	2.005	2.015	4	
5.18.1.4 Sulphate (μ_3-SO_4)								
(M)O–S		1.486	1.492	0.014	1.475	1.492	9	
Co–O	See EFASCO01 (2.005)							
Cu–O	See COLDUC (2.168, 2.060, 2.346)							
U–O	See URSDUR03 (2.374, 2.389)							
5.19.1.1 Alkyl sulphonates (terminal, OSO_2R)								
(M)O–S		1.453	1.450	0.015	1.443	1.456	8	
S–O		1.446	1.449	0.021	1.432	1.464	16	
S–C		1.785	1.780	0.022	1.767	1.806	8	
Fe–O	See CAWTAV (2.007)							
Cu–O	(6), (II)	2.358	2.356	0.022	2.338	2.380	4	
Pd–O	See FMSEPD (2.272)							
Au–O	See MAUFMS (2.201)							
5.19.1.2 Alkyl sulphonates [chelating, $O_2S(O)R$]								
(None)								
5.19.1.3 Alkyl sulphonates [μ-$O_2S(O)R$]								
(M)O–S		1.452	1.452	0.013	1.440	1.465	8	
S–O		1.452	1.452	0.010	1.443	1.462	4	
S–C		1.784	1.780	0.034	1.754	1.819	4	
Cu–O (μ_3)	See CAWJAL (2.068, 2.049), COMMAS (2.060, 2.385)							
Cd–O (μ)	See CAMSOB (2.404, 2.412)							
U–O (μ)	See URMSUL (2.363, 2.399)							
5.19.2 Alkyl sulphites (terminal, SO_2R)								
O–S	(1.501, 1.533)							
Fe–O	See FEBUTS10 (2.004)							
Cu–O	See PYSLCU (1.957)							
5.20 *O*-Sulphur dioxide (σ-OSO) (see also 9.14.1)								104
O–S	(1.448)							
S–O	(1.410)							
Mn–O	See CONTEE (2.282)							
5.21.1.1 Perchlorate (terminal, ClO_4)								128
(M)O–Cl		1.430	1.437	0.026	1.409	1.447	33	
Cl–O		1.407	1.414	0.031	1.393	1.429	99	
Co–O	See PNENCO10 (2.360)							
Ni–O	See ZEGCET (2.221, 2.235)							
Cu–O	(4—6), (I,II)	2.496	2.517	0.119	2.425	2.568	26	91
	(5,6), (II)	2.508	2.532	0.115	2.485	2.570	24	91
La–O	See APXLAP (2.494)							
Sm–O	See HBHOSM (2.364)							
Hg–O	See OTPCHG (2.726), TTHPHG (2.757)							
5.21.1.2 Perchlorate (chelating, ClO_4)								
(M)O–Cl		1.437	1.450	0.029	1.406	1.462	5	
Cl–O		1.397	1.401	0.030	1.475	1.418	5	
Ag–O	See CAMROX (2.291, 2.754)							
La–O	See APXLAP (2.683, 2.291)							
Sm–O	See HBHOSM (2.642)							
5.21.1.3 Perchlorate (μ-ClO_4)								
(M)O–Cl		1.400	1.417	0.055	1.359	1.436	6	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
5.21.1.3 Perchlorate (μ-ClO_4)—(*continued*)								
Cu–O	See BAMCIB10 (2.541, 2.569), OXMCUA (2.552, 2.428)							
Ag–O	See BUZMUE (2.581, 2.342)							
5.22.1 Aquo (terminal, OH_2)								
Ti–O	(6—8), (III—IV)	2.066	2.063	0.052	2.024	2.122	8	
V–O	(6), (−): all	2.129	2.063	0.131	2.013	2.250	14	30
	: short < 2.1	2.024	2.025	0.030	1.996	2.047	8	44
	: long > 2.2, *trans* to O	2.268	2.260	0.048	2.228	2.317	6	129
Cr–O	(6,7), (−): all	1.997	1.979	0.070	1.955	2.007	33	86
	: excluding five > 2.06	1.997	1.986	0.052	1.966	2.008	28	85
	: excluding Cr(II)	1.987	1.982	0.036	1.965	2.003	26	
Mn–O	(6,7), (−): all	2.189	2.183	0.040	2.162	2.216	88	130
Fe–O	(6,7), (−): all	2.085	2.108	0.066	2.043	2.135	29	
	: excluding MAZCOC	2.099	2.109	0.046	2.054	2.136	27	
Co–O	(4—7), (−): all	2.085	2.090	0.064	2.059	2.123	121	
	: excluding TAZOCO	2.081	2.090	0.055	2.058	2.122	119	91
Ni–O	(6,7), (−): all	2.079	2.078	0.038	2.050	2.105	126	9
Cu–O	(4—6), (−): all	2.186	2.208	0.215	1.965	2.355	219	30
	(4), (II)	1.942	1.946	0.016	1.931	1.954	10	
	(5), (−): all	2.209	2.257	0.187	2.000	2.344	116	
	: short < 2.08	1.986	1.974	0.038	1.961	2.010	41	
	: long > 2.14	2.331	2.316	0.103	2.259	2.372	75	
	(6), (−): all	2.189	2.125	0.246	1.960	2.408	87	30
	: short < 2.01	1.963	1.960	0.019	1.950	1.973	42	
	: long > 2.12	2.399	2.399	0.154	2.275	2.520	45	
Zn–O	(4—7), (−): all	2.090	2.092	0.061	2.051	2.137	56	
	(4), (−)	2.006	2.001	0.017	1.994	2.020	5	
	(5), (−)	2.078	2.091	0.079	2.007	2.159	7	
	(6), (−)	2.097	2.093	0.049	2.059	2.145	40	
Y–O	(7—9)	2.398	2.412	0.068	2.335	2.440	9	
Nb–O	(6—8), (−): all	2.248	2.188	0.137	2.158	2.368	6	
		2.167	2.177	0.030	2.135	2.189	4	44
Mo–O	All	2.201	2.187	0.094	2.146	2.263	37	85
	Clusters	2.142	2.151	0.052	2.109	2.176	21	131
Tc–O	See CEPHOU (2.282)							
Ru–O	(6), (−)	2.074	2.066	0.051	2.031	2.119	12	85
Rh–O	(4—6), (I—III): all	2.190	2.178	0.096	2.108	2.296	14	
		2.105	2.108	0.035	2.100	2.129	7	85
		2.274	2.295	0.045	2.227	2.309	7	82
Pd–O	See BQAPPD (2.200)							
Ag–O	See CERFAG (2.334), COVBIY (2.367)							
Cd–O	(5—8), (−)	2.318	2.299	0.065	2.272	2.345	73	86
La–O	(8—10), (−)	2.556	2.564	0.062	2.511	2.610	17	
Ce–O	(9,11), (−)	2.565	2.601	0.063	2.497	2.615	5	
Pr–O	(8,9), (−)	2.518	2.519	0.038	2.482	2.537	13	
Nd–O	(7,11), (−)	2.533	2.528	0.058	2.478	2.582	25	
Sm–O	(8,9), (−)	2.459	2.447	0.050	2.420	2.477	24	86
Eu–O	(9), (−)	2.441	2.412	0.055	2.400	2.486	8	
Gd–O	(9), (−)	2.443	2.418	0.074	2.392	2.526	13	
Tb–O	See ZZZARD01 (2.382, 2.527)							
Dy–O	(8,9), (−)	2.409	2.374	0.074	2.356	2.469	12	
Ho–O	(7—9), (−)	2.407	2.392	0.069	2.354	2.477	10	
Er–O	(7—9), (−)	2.404	2.372	0.083	2.352	2.427	15	
Yb–O	(8,9), (−)	2.353	2.342	0.066	2.311	2.388	12	
Lu–O	(9), (−): all	2.404	2.408	0.116	2.298	2.507	4	
W–O	(−), (−): all	2.115	2.106	0.065	2.072	2.148	14	
		2.101	2.092	0.045	2.072	2.142	13	44
Re–O	(6), (−): all	2.199	2.214	0.091	2.106	2.276	4	
Os–O	See CIBKED (2.166)							
Au–O	See MAUFMS (2.157)							
Hg–O	(4,6), (−): all	2.690	2.680	0.083	2.612	2.773	5	
Th–O	(9,10), (−): all	2.483	2.483	0.032	2.452	2.513	4	
U–O	(7,8), (−): all	2.455	2.464	0.047	2.430	2.478	15	
5.22.2 Aquo (μ-OH_2)								
Mn–O	See MNPROP (2.223, 2.369)							
Co–O	(6), (II,III)	2.151	2.156	0.021	2.132	2.167	5	
Ni–O	(6), (II)	2.102	2.103	0.030	2.072	2.133	8	
Cu–O	See AXEXAC (2.300, 2.487), CESYII (2.755)							
Zn–O	See CITKIZ (2.100, 2.326)							
Ru–O	See COCXOH (2.159, 2.168)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
5.22.2 Aquo (μ-OH_2)—(*continued*)								
Ag–O	See BUGFUE (2.437, 2.451)							
U–O	See AQOURI (2.354, 2.375)							
5.23.1 Alkyl alcohols [ROH, R = C (sp^3)]								
O–C		1.436	1.435	0.022	1.425	1.448	196	
V–O	See CIJDAA (1.918, 2.233)							
Mn–O	(4,6), (II,III): all	2.223	2.202	0.055	2.184	2.248	19	
	: excluding one > 2.39	2.213	2.201	0.035	2.182	2.246	18	
Fe–O	(6), (II,III)	2.133	2.157	0.052	2.078	2.175	5	
Co–O	(5,6), (II,III): all	2.089	2.085	0.091	2.068	2.108	28	
	(6), (III)	1.951	1.953	0.017	1.934	1.967	4	
	(6), (II)	2.098	2.086	0.042	2.076	2.108	23	
Ni–O	(4,6,*),(II): all	2.101	2.093	0.073	2.065	2.140	31	
	(6), (II)	2.099	2.089	0.043	2.071	2.128	25	
Cu–O	(4—6), (I,II): all	2.162	2.039	0.206	1.991	2.375	61	30
	(4), (II)	1.973	1.977	0.027	1.948	1.996	8	
	(5,6), (II): short < 2.07	2.003	2.000	0.031	1.978	2.029	24	
	(5,6), (II): long > 2.16	2.384	2.404	0.102	2.290	2.474	26	
Zn–O	(5,6), (II)	2.122	2.105	0.041	2.085	2.166	10	
Mo–O	(5,6), (V,VI)	2.326	2.326	0.035	2.308	2.358	6	
Rh–O	(4,6), (I,II)	2.259	2.273	0.047	2.223	2.296	6	
	(6), (II): all $Rh_2(O_2CR)_4 \cdot L_2$	2.276	2.277	0.023	2.255	2.296	5	
La–O	(9—11), (III)	2.574	2.579	0.025	2.547	2.595	6	
Pr–O	(8,9), (III)	2.539	2.533	0.033	2.513	2.568	5	
Nd–O	See BAWDIM10 (2.480, 2.547)							
Eu–O	See CEYRON (2.433, 2.470)							
Er–O	See BUHVOP (2.468), HENAEB (2.240)							
Yb–O	See GEIAYB10 (2.386, 2.420)							
Hg–O	See TESTHG (2.487)							
Th–O	See BURPEJ (2.579)							
U–O	(6,7), (VI)	2.439	2.460	0.052	2.387	2.481	5	
5.23.2 Alkenyl, aryl alcohols [ROH, R = C (sp^2)]								
O–C		1.378	1.365	0.034	1.361	1.397	9	
Fe–O	See CAYGOY (2.317)							
Co–O	See APIMCO (2.154), BAVJOX10 (1.937, 1.937)							
Ni–O	See APIMNI (2.102)							
Cu–O	See CAXYOP (2.600)							
Mo–O	See CETGIR (2.601, 2.645)							
Sm–O	See SALASM10 (2.434)							
5.24.1 Tetrahydrofuran (thf)								
O–C		1.453	1.453	0.025	1.438	1.466	167	
Ti–O	(7—8), (II—IV): all	2.205	2.219	0.069	2.166	2.257	8	
V–O	(6), (II—IV): all	2.128	2.132	0.063	2.070	2.153	14	
	Excluding BUXTAP	2.115	2.131	0.042	2.070	2.151	13	
Cr–O	(6), (0—III): all	2.125	2.084	0.137	2.002	2.279	6	
		2.042	2.023	0.058	2.000	2.104	4	85
Mn–O	See CLTIMN (2.227), HFURMN (2.100)							
Fe–O	See PTHFFE (2.352)							
Ni–O	See BECXIQ (1.964)							
Y–O	(9,10), (III)	2.405	2.413	0.054	2.350	2.457	5	
Zr–O	See COTZRH (2.446), COTZRF (2.274)							
Mo–O	(6), (II—VI): all	2.430	2.432	0.148	2.307	2.570	6	30
Cd–O	See PHPNCD (2.643)							
La–O	See CEYPEB (2.555, 2.509, 2.490)							
Ce–O	See COCTCE (2.577, 2.588)							
Sm–O	(8), (II): all CALCEX	2.634	2.628	0.018	2.620	2.652	4	
Eu–O	See CIFCAV (2.602, 2.641)							
Gd–O	See CPTHGD10 (2.494)							
Er–O	See BOBWAQ (2.351, 2.365, 2.452)							
Yb–O	See CPFYBA10 (2.412), CPYBHF (2.525)							
Ta–O	See ACTHTA (2.282), BEHHIF (2.379), BEJGAY (2.308)							
Re–O	See BOJSUO (2.486, 2.469)							
Hg–O	See BIYPAA (2.645)							
Th–O	See COCTFT10 (2.573, 2.525)							
U–O	(8—10), (III,IV)	2.471	2.470	0.045	2.439	2.494	6	
5.24.2 Ethers [OR_2, R = C (sp^3)]								
O–C		1.432	1.434	0.033	1.415	1.450	383	
Ti–O	All TCXNTI	2.134	2.124	0.026	2.118	2.161	4	
Cr–O	(5), (II): excluding FACCRE (2.244)	2.133	2.132	0.007	2.128	2.138	6	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
5.24.2 Ethers [OR_2, R = C (sp^3)]—(*continued*)								
Mn–O	(8), (II): predominantly ODMNBR	2.319	2.325	0.051	2.274	2.369	6	
Co–O	(6,7), (II)	2.230	2.207	0.092	2.142	2.327	20	8,30
Ni–O	(6), (II)	2.147	2.151	0.063	2.089	2.187	14	
Cu–O	(6,7), (II)	2.431	2.404	0.187	2.299	2.608	22	
Zn–O	See CEPMOZ (2.093)							
Y–O	See BUWBAW (2.385)							
Mo–O	(5,6), (II,V): excluding CETGEN	2.263	2.269	0.027	2.242	2.285	6	
Ag–O	All CIJWIB	2.575	2.575	0.015	2.561	2.588	4	
Cd–O	(6—8,*), (II)	2.569	2.541	0.120	2.466	2.697	11	
La–O	(10—12), (III)	2.685	2.693	0.053	2.641	2.730	42	20
Nd–O	(10,12), (III)	2.665	2.646	0.076	2.600	2.719	11	
Sm–O	(9,10), (III)	2.504	2.503	0.046	2.473	2.537	14	
Eu–O	(6,10,11), (II,III)	2.618	2.638	0.088	2.529	2.680	9	
	(10,11), (III)	2.596	2.601	0.080	2.508	2.665	7	
Ta–O	See BUBKUE (2.462, 2.166; 2.411, 2.176)							
Hg–O	See CESZOP (2.825), HGTXZO (2.909, 2.935)							
U–O	See BAMVUG (2.602, 2.586)							
5.24.3 Ethers [OR_2, R_2 ≠ C (sp^3)$_2$]								
O–C (sp^2)		1.390	1.389	0.014	1.380	1.400	51	
O–C (sp^3)		1.444	1.446	0.020	1.429	1.455	51	
V–O	See BUCTOI (2.196, 2.219, 2.229)							
Cr–O	(5), (II): all Cr≡Cr	2.131	2.131	0.009	2.127	2.135	7	
Co–O	See BXZPCO (2.325)							
Ni–O	(6), (II)	2.176	2.175	0.052	2.141	2.201	11	
Cu–O	(6,7), (II)	2.393	2.371	0.096	2.310	2.472	8	
Mo–O	All DMXPMO10	2.269	2.269	0.019	2.252	2.287	4	
Ru–O	See CEFNOQ (2.472), CPASRU (2.257, 2.299)							
Pd–O	See BUWJUY (2.236)							
Cd–O	See CATKUD (2.614, 2.731)							
La–O	(10), (III)	2.697	2.699	0.031	2.679	2.729	8	22
Sm–O	See HBHOSM (2.417, 2.537, 2.591)							22
5.25.1 η^2-Acyl [η^2-C(O)R] (see also 3.12.1.2)								
Zr–O	See BOPSII (2.249, 2.251)							
Mo–O		2.267	2.289	0.050	2.214	2.300	6	
W–O	See BUSYIX (2.223), COSSOS (2.167)							
5.25.2 η^2-CO_2 (see also 3.22.1)								
(None)								
5.25.3.1 *O*-Isocyanate (terminal, OCN) (see also 4.5.1.1)								
(None)								
5.25.3.2 Isocyanate (μ-NCO) (see also 4.5.1.2)[+]								
Cu–O	See CNPRCV (2.607), ICNPCU10 (2.663)							
5.25.4 Borates (all types)								132
O–B	(1.437, 1.405, 1.431)							
Ni–O	See CECWEM (2.038, 2.056, 2.057)							
O–B	(1.527, 1.547)							
Mo–O	See BAXHEN (2.129, 2.145)							
6.1.1.1 Fluoro (terminal, F)								
Ti–F	See FPOTIP (1.853, 1.887)							
V–F	(5,6), (IV,V): all	1.856	1.876	0.059	1.790	1.908	8	
Cr–F	(6), (III)	1.870	1.872	0.027	1.847	1.892	5	
Mn–F	See TMAFMN (1.809, 1.867)							
Ni–F	See FACTNI (2.081, 2.093)							
Cu–F	See BIPTAV (1.935)							
Zr–F	(7,8), (−): all	2.043	2.051	0.037	2.024	2.063	22	133
Nb–F	(6), (V): all	1.957	1.941	0.069	1.906	1.982	11	
		1.940	1.936	0.041	1.903	1.980	10	44
Mo–F	See AFXPCM (2.058), TCMOFM (1.922, 1.845)							
W–F	See COBXOG (2.081)							
Re–F	See COLWAB (2.036)							
Pt–F	See TEPPTB (2.043)							
U–F	(7,10), (−): all	2.240	2.268	0.077	2.178	2.289	5	
	(7), (−)	2.274	2.276	0.020	2.254	2.293	4	
6.1.1.2 Fluoro (μ-F)								134
Cu–F	See CASYEA (1.927, 1.919)							
Mo–F	(6), (VI): all	2.168	2.147	0.046	2.134	2.212	6	
Ag–F	See BIWVEI (2.548, 2.550)							
U–F	(10,7), (IV,VI): all	2.316	2.325	0.041	2.273	2.350	4	
6.2.1 BF_4 (terminal)								
(M)F–B	All	1.366	1.357	0.044	1.330	1.391	6	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
6.2.1 BF_4 (terminal)—(*continued*)								
(M)F–B	Excluding one > 1.43	1.349	1.357	0.019	1.330	1.365	5	
B–F	All	1.331	1.347	0.058	1.305	1.378	18	
	Excluding four < 1.25	1.360	1.357	0.023	1.337	1.378	14	
Cu–F	See BUWWOF10 (2.560)							
Ir–F	See BEVYIK (2.272)							
U–F	See CISZOT (2.420, 2.403)							
6.2.2 PF_6 (terminal)								
(None)								
7.1 Silicon ligands (all types)								
Mn–Si	See BOTGAS (2.351), CATSUL (2.254), DPSCMN (2.402), MSISMN (2.564)							
Fe–Si	SiR_3, SiX_3, SiX_2, *etc.*: all	2.329	2.348	0.066	2.264	2.367	15	
	: X = halide	2.263	2.258	0.014	2.251	2.280	6	
	: X ≠ halide	2.374	2.363	0.045	2.349	2.411	9	
Mo–Si	See FBSIMO (2.603, 2.608)							
Ru–Si	SiX_3, SiR_3, μ-SiR_2	2.423	2.439	0.057	2.365	2.463	9	
	Excluding SiX_3	2.447	2.451	0.037	2.414	2.465	7	
Rh–Si	See CONFEQ01 (2.379)							
W–Si	See ESITCO (2.586)							
Re–Si	All ESICRE, HETSRE	2.543	2.547	0.007	2.536	2.549	5	
Os–Si	See BEGKAZ (2.400, 2.421), CAFCUH (2.429)							
Ir–Si	See HTSIXI10 (2.398, 2.417)							
Pt–Si	SiR_3, μ-SiR_2	2.336	2.318	0.060	2.313	2.382	7	
Hg–Si	(6), (II): SiR_3	2.533	2.544	0.026	2.506	2.549	4	
8.1 Phosphorus								
Co–P	(μ_3-P): all CPCOPT	2.233	2.218	0.022	2.216	2.256	7	
Ru–P	(μ_5-P): see BUTKUW (range 2.327—2.623)							
Rh–P	(μ_8-P): all BEAMRH	2.425	2.421	0.026	2.402	2.451	8	
8.2.1.1 Phosphinidenes (terminal, PR)								
(None)								
8.2.1.2 Phosphinidenes (μ-PR)								136
P–C	(1.897)							
Cr–P	See CIHXIA (2.288, 2.315)							
8.2.1.3 Phosphinidenes (μ_3-PR)								136
P–C	Predominantly R = Ph	1.808	1.809	0.013	1.799	1.816	23	
Fe–P	(*), (−)	2.204	2.204	0.030	2.179	2.223	42	
Co–P	See COTSEJ (2.156, 2.163, 2.170)							
Ru–P	(*), (−)	2.302	2.292	0.039	2.277	2.327	21	
Ir–P	See BUNMEC (2.255, 2.279, 2.285)							
8.2.1.4 Phosphinidenes (μ_4-PR)								136
P–C	R = aryl	1.812	1.817	0.018	1.801	1.825	16	
	R = Me: all BUZRAP	1.862	1.863	0.007	1.855	1.867	4	
Fe–P	(*), (−)	2.261	2.254	0.051	2.235	2.287	52	
Co–P	All PPCOCO01	2.240	2.240	0.014	2.229	2.245	8	
Ru–P	Asymmetrics included	2.408	2.353	0.089	2.343	2.483	12	
Rh–P		2.388	2.397	0.032	2.358	2.415	8	
8.3.1.1 Phosphino (terminal, PR_2, R = alkyl)								
P–C		1.865	1.865	0.012	1.861	1.877	20	
Fe–P	See CPFMPI10 (2.265)							
Mo–P	All CEHTUE	2.274	2.276	0.007	2.267	2.279	4	
Hf–P	(5,8), (IV): planar at P	2.500	2.496	0.025	2.478	2.526	4	
	See CAKSOW (2.682): not planar at P							
8.3.1.2 Phosphino (μ-PR_2)								
P–C	All but R = Bu^t; mostly R = Ph	1.831	1.830	0.016	1.821	1.839	264	
	R = Bu^t	1.909	1.919	0.020	1.899	1.921	25	
V–P	All DMPCOV	2.357	2.357	0.005	2.352	2.361	6	
Cr–P	All MPCRCO	2.318	2.318	0.001	2.317	2.319	4	
Mn–P	(5,6), (0,I)	2.289	2.282	0.039	2.260	2.290	12	
Fe–P	(4—6,*), (−)	2.222	2.217	0.030	2.204	2.233	67	
Co–P	(4,5,*), (−)	2.189	2.188	0.036	2.160	2.224	44	
Ni–P	(3,4), (−)	2.189	2.185	0.039	2.161	2.228	15	
Cu–P	See PHPECU01 (2.357, 2.370)							
Mo–P	(6,7), (−)	2.390	2.381	0.030	2.364	2.419	12	
Ru–P	(5,*), (−)	2.333	2.327	0.041	2.310	2.355	62	
Rh–P	(4,*), (−)	2.307	2.299	0.037	2.285	2.327	22	
Os–P	(5,6,*), (−)	2.379	2.391	0.051	2.341	2.415	8	
Ir–P	All CEFVIS	2.355	2.358	0.046	2.312	2.395	4	
Pt–P	(4,*), (−)	2.282	2.281	0.037	2.256	2.312	24	
8.3.2 Phosphavinyls (σ-PR=CR_2)								
P=C	(1.679, 1.651, 1.661)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
8.3.2 Phosphavinyls (σ-PR=CR_2)—(*continued*)								
P–C	(1.822, 1.818, 1.793)							
Cr–P	See MESTCR (2.356)							
Pt–P	See BESHAI (2.218), BEXLEV (2.199)							
8.3.3 Diaminophosphino [$P(NR_2)_2$]								
P–N		1.615	1.624	0.028	1.598	1.632	8	
Fe–P	All CINLAM	2.106	2.124	0.061	2.041	2.152	4	
8.4.1 P–P bonded ligands (σ-P–P)								137
P–P		2.211	2.205	0.034	2.193	2.220	54	
Cr–P	(6), (0)	2.385	2.383	0.036	2.361	2.403	11	
Mn–P	See COGSIA (2.355, 2.369), PDPMNC (2.215)							
Fe–P	(4,5), (−)	2.235	2.221	0.027	2.217	2.263	10	
Ni–P	See PSNIMO (2.221)							
Mo–P	(6), (0)	2.511	2.512	0.045	2.463	2.534	11	
Rh–P	See BUYKIP (2.285, 2.302)							
W–P	See BAVKAK (2.573), CIPGAJ (2.535)							
Re–P	See BTPCRE10 (2.478, 2.539)							
Ir–P	See CAYLAP (2.423, 2.433)							
Hg–P	See TMDPHG (2.490)							
8.4.2 $P_3(\eta^3\text{-}P_3)$								137
P–P		2.135	2.137	0.016	2.122	2.149	18	
Co–P	(5), (−)	2.311	2.309	0.011	2.302	2.321	4	
Ni–P	See CAFSOR (2.308, 2.309, 2.309)							9
Rh–P	See PPMERH (2.418)							
Pd–P	(5), (−)	2.452	2.450	0.045	2.411	2.497	6	
Ir–P	See PPMEIR (2.436)							
Pt–P	See BUSLEG (2.430, 2.433, 2.437)							
8.4.3 P–P bonded ligands (σ-P=P)								137,138
P=P		2.038	2.039	0.014	2.023	2.052	5	
Cr–P	See CEGHAX (2.360), CIKPUH (2.315)							
Fe–P	See BUPJAX (2.226), CAYFAJ (2.232), CEMXIB (2.215)							
8.4.4 P–P bonded ligands (η^2-P=P)								137,138
P=P		2.150	2.146	0.027	2.128	2.176	4	
Fe–P	See CEGHEB (2.346, 2.361)							
Ni–P	See EPMSPN11 (2.234, 2.259)							
Mo–P	See CPPYMO10 (2.536, 2.550)							
Pd–P	See BIHGOO (2.366)							
8.5.1 Trimethylphosphine (PMe_3)								137
P–C		1.824	1.824	0.023	1.811	1.837	1 243	
V–P		2.510	2.509	0.010	2.502	2.520	4	
Cr–P	All	2.389	2.370	0.069	2.328	2.460	5	87
Mn–P	(4—7), (−)	2.455	2.453	0.164	2.293	2.619	8	38
	(5,6), (−)	2.304	2.295	0.027	2.285	2.332	4	
	(4,7), (−)	2.605	2.605	0.042	2.566	2.645	4	
Fe–P	(5,6), (−): all	2.246	2.248	0.042	2.223	2.268	20	
	(5), (−)	2.230	2.228	0.037	2.215	2.252	11	
	(6), (−)	2.265	2.255	0.042	2.239	2.296	9	
Co–P	(4—6,*), (−): all	2.217	2.212	0.043	2.183	2.241	38	12,139
	(4—6), (−)	2.209	2.208	0.036	2.181	2.238	35	140
Ni–P	(3—5), (−): all	2.204	2.202	0.031	2.188	2.216	37	9,51
	(3), (−)	2.182	2.170	0.060	2.138	2.233	5	
	(4), (−)	2.200	2.200	0.020	2.184	2.208	20	
	(5), (−)	2.220	2.215	0.024	2.204	2.245	12	
Zr–P	See COPVIM (2.692)							
Mo–P	(5—7), (−): all	2.462	2.455	0.046	2.429	2.487	46	38
	(5), (−)	2.530	2.535	0.031	2.497	2.546	9	
	(6), (−)	2.459	2.457	0.031	2.432	2.481	16	
	(7), (−)	2.435	2.435	0.027	2.425	2.457	21	
Ru–P	All	2.307	2.307	0.050	2.271	2.335	65	
	Excluding MEPRUA, MPMYRU	2.298	2.303	0.037	2.268	2.329	58	
Rh–P	(4—6), (−): all	2.266	2.259	0.036	2.248	2.297	22	
	(4), (−)	2.284	2.296	0.037	2.256	2.308	12	
	(6), (−)	2.249	2.250	0.017	2.247	2.260	9	
Pd–P		2.287	2.281	0.018	2.273	2.305	6	
Ta–P	(5—8), (−): all	2.589	2.588	0.044	2.555	2.625	32	
	(5), (−)	2.564	2.565	0.027	2.535	2.591	13	
	(6), (−)	2.611	2.614	0.048	2.593	2.648	12	
	(8), (−)	2.611	2.627	0.047	2.563	2.651	5	
W–P	Excluding CIPDIO and PHIMDW	2.485	2.496	0.039	2.456	2.509	40	38,139
Re–P	All	2.369	2.374	0.065	2.324	2.407	29	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
8.5.1 Trimethylphosphine (PMe_3)—(*continued*)								137
Re–P	Excluding CACWOS, MEORHC, NOMPRE	2.348	2.335	0.050	2.321	2.383	24	
Os–P		2.328	2.323	0.029	2.297	2.359	15	
Ir–P		2.323	2.329	0.028	2.309	2.341	30	139
Pt–P		2.295	2.306	0.036	2.265	2.321	36	91,142
8.5.2 Triethylphosphine (PEt_3)								
P–C		1.832	1.831	0.021	1.820	1.843	557	
Ti–P	See BOZMIM (2.585)							
Cr–P		2.374	2.372	0.061	2.319	2.433	6	38,81
Mn–P	See COLDIQ (2.568), TEPPMN01 (2.253)							
Fe–P	See BDODFE (2.220), CATGEJ (2.234)							
Co–P	All	2.208	2.225	0.039	2.181	2.236	18	
	Cobaltacarbaboranes	2.224	2.226	0.021	2.215	2.241	11	
	$M(cp)L_2$	2.147	2.139	0.024	2.128	2.172	4	
Ni–P	(3,4), (−): all	2.196	2.189	0.036	2.173	2.233	10	9,51
	(3), (−)	2.169	2.176	0.023	2.145	2.187	4	
	(4), (−)	2.214	2.222	0.031	2.183	2.238	6	
Mo–P		2.507	2.513	0.042	2.477	2.545	9	38
Ru–P		2.356	2.355	0.006	2.351	2.362	4	
Rh–P		2.338	2.346	0.029	2.316	2.360	13	
Pd–P		2.315	2.321	0.022	2.294	2.336	18	139
Ta–P	See BEHHIF (2.667)							
W–P		2.537	2.539	0.015	2.522	2.551	4	38
Re–P	See CEVHOA (2.479)							
Os–P	See HETPOS (2.412)							
Ir–P	(6), (−)	2.334	2.332	0.013	2.325	2.341	6	139
Pt–P	All, mostly (4,5)	2.296	2.298	0.047	2.259	2.326	100	139,142
	(4,5), (−)	2.288	2.293	0.041	2.255	2.321	92	139
	(6), (−)	2.385	2.396	0.036	2.336	2.410	7	139
Au–P	See AGLPAU (2.259), CIMGEK (2.328), COSMOM (2.278)							
8.5.3 Triphenylphosphine (PPh_3)								
P–C		1.828	1.828	0.014	1.819	1.837	2 239	
V–P	See ALCPPV (2.486, 2.485), CPHSVB (2.472)							
Cr–P	See CEDHUO (2.315), HETCRB10 (2.321), MBZCRP (2.338)							38
Mn–P		2.305	2.304	0.044	2.277	2.340	9	
Fe–P		2.237	2.233	0.038	2.213	2.274	31	
Co–P	All	2.243	2.211	0.096	2.174	2.283	52	8
	(−), (0): clusters excluded	2.227	2.228	0.016	2.211	2.243	4	
	(6), (III)	2.392	2.397	0.046	2.362	2.423	9	
	(4—6), (I,III)	2.202	2.199	0.038	2.174	2.230	33	
Ni–P	All	2.225	2.208	0.069	2.159	2.309	21	9,30,51
	Short < 2.25	2.187	2.197	0.035	2.154	2.221	15	
	Long > 2.30	2.321	2.320	0.012	2.312	2.331	6	
Cu–P		2.252	2.256	0.044	2.226	2.273	53	12
Mo–P		2.524	2.528	0.042	2.511	2.560	15	38
Tc–P	See CETKUH (2.494, 2.525), TCACTC (2.433)							
Ru–P	(4—6,*), (−): all	2.370	2.367	0.044	2.337	2.408	59	
	(4), (−)	2.342	2.341	0.009	2.334	2.351	4	
	(5), (−)	2.372	2.382	0.040	2.343	2.395	13	
	(6), (−)	2.370	2.367	0.049	2.332	2.419	30	
	(*), (−)	2.379	2.377	0.041	2.362	2.408	12	
Rh–P	(4—6,*), (−): all	2.314	2.324	0.050	2.282	2.344	85	100
	(4), (−)	2.302	2.321	0.053	2.248	2.334	44	
	(5), (−)	2.331	2.335	0.048	2.288	2.370	20	
	(6), (−)	2.321	2.331	0.041	2.288	2.346	18	
Pd–P	Excluding TTPPDB (2.458)	2.308	2.320	0.038	2.281	2.337	51	91
Ag–P		2.419	2.414	0.046	2.388	2.455	27	
Cd–P	See CIFGON (2.524)							
W–P		2.535	2.558	0.069	2.479	2.590	6	38,100
Re–P	All	2.432	2.427	0.048	2.398	2.472	41	
	(−), (I—III)	2.411	2.413	0.036	2.381	2.433	29	
	(−), (IV,V,VII)	2.484	2.487	0.027	2.472	2.505	12	
Os–P		2.388	2.385	0.037	2.361	2.416	42	
Ir–P	(4—6,*), (−): all	2.345	2.341	0.039	2.319	2.374	91	143
	(4), (−)	2.328	2.325	0.025	2.314	2.344	36	
	(5), (−)	2.350	2.348	0.037	2.330	2.378	33	
	(6), (−)	2.365	2.378	0.048	2.328	2.408	20	
Pt–P	(−), (−): all	2.294	2.298	0.032	2.273	2.313	151	142
	(3), (−)	2.280	2.279	0.023	2.267	2.298	29	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
8.5.3 Triphenylphosphine (PPh_3)—(*continued*)								
Pt–P	(4), (−)	2.298	2.302	0.032	2.287	2.317	99	
Au–P	(2—4,*), (−): all	2.303	2.295	0.043	2.281	2.312	62	144
	(2), (−)	2.272	2.278	0.025	2.255	2.291	15	
	(4), (−)	2.377	2.398	0.055	2.347	2.411	8	
	(*), (−)	2.297	2.298	0.020	2.288	2.308	34	
Hg–P		2.453	2.457	0.034	2.429	2.483	8	26
8.5.4 Tri-isopropylphosphine (PPr^i_3)								
P–C		1.863	1.863	0.015	1.855	1.872	93	
Rh–P		2.309	2.300	0.047	2.274	2.355	22	
Pd–P	See BUPTEL (2.242), BUSHEC (2.275)							
W–P	See CEJDEA (2.487, 2.503)							38
Ir–P	See APRPIR (2.270), BUHIPI (2.300, 2.322)							
Pt–P	See BUPPUX (2.261)							
Au–P	See CEPYIF (2.266)							142
8.5.5 Tri-n-propylphosphine (PPr^n_3)								
P–C		1.827	1.829	0.028	1.817	1.847	27	
Pd–P	See CEKGOO (2.248, 2.248)							
Pt–P		2.245	2.257	0.024	2.219	2.265	5	142
Hg–P	See CIPTAW (2.425, 2.410)							145
8.5.6 Tri-t-butylphosphine (PBu^t_3)								
P–C		1.926	1.922	0.026	1.907	1.936	54	
Fe–P	See TBPCFE (2.363)							
Ni–P	See BPBRNI10 (2.494)							
Cu–P	See BOZRAJ (2.228, 2.228)							
Ru–P		2.574	2.476	0.057	2.521	2.624	4	
Rh–P	See BUPCRH (2.427, 2.433)							
Pt–P		2.275	2.267	0.027	2.262	2.276	7	142
Hg–P	See TBPAHG10 (2.370)							26
8.5.7 Tricyclohexylphosphine [$P(C_6H_{11})_3$]								
P–C		1.856	1.855	0.017	1.846	1.867	144	
Mn–P	See COBSOB (2.362)							
Co–P	See BECTIM (2.463)							
Ni–P		2.211	2.226	0.036	2.172	2.242	5	51
Cu–P	See CCHXPC (2.183), CHPCUP (2.262)							
Ru–P	See BOMMEV (2.419), CAVVEA (2.424, 2.420)							
Rh–P	See CIDHEC (2.256)							
Pd–P	See FMEACA10 (2.359, 2.363)							
Ir–P	See PCHIRH10 (2.287, 2.291, 2.281)							
Pt–P		2.323	2.327	0.034	2.306	2.343	23	142
Hg–P		2.413	2.412	0.034	2.379	2.444	7	26
8.5.8 Methyldiphenylphosphine (PPh_2Me)								
P–C(Ph)		1.823	1.822	0.013	1.813	1.833	112	
P–C(Me)		1.827	1.827	0.016	1.815	1.840	56	
V–P	See CAPFOO (2.459, 2.529)							
Mn–P	See CABZAG (2.684), COLNAS (2.612)							
Fe–P	See BOPPAX10 (2.260, 2.276)							
Co–P	See CNCOPP10 (2.254, 2.257)							
Ni–P	See MPFPNI (2.206)							51
Cu–P		2.266	2.260	0.018	2.250	2.285	5	
Mo–P		2.487	2.483	0.079	2.419	2.561	4	38,85
Ru–P		2.396	2.418	0.060	2.333	2.438	4	
Ag–P		2.438	2.445	0.031	2.406	2.464	4	
Re–P	See CAJGEZ (2.373, 2.397, 2.414)							
Os–P	See CEVFUE10 (2.315)							
Ir–P		2.334	2.322	0.035	2.315	2.365	10	
Pt–P	All	2.300	2.309	0.034	2.270	2.238	17	142
	Trans to P, CO	2.317	2.320	0.018	2.299	2.332	13	
	Trans to Cl, SR	2.246	2.246	0.002	2.244	2.248	4	
Au–P		2.331	2.303	0.081	2.275	2.416	4	
8.5.9 Dimethylphenylphosphine ($PPhMe_2$)								
P–C(Ph)		1.826	1.826	0.017	1.815	1.836	252	
P–C(Me)		1.825	1.824	0.021	1.813	1.837	502	
V–P	See BOBZUN (2.523)							
Fe–P		2.259	2.268	0.021	2.237	2.272	4	
Co–P	See BISNEW (2.161), CAHZAM (2.191), PCOPIM10 (2.230)							
Ni–P		2.227	2.223	0.037	2.188	2.261	1	9,51
Nb–P	See CIDBEW (2.697, 2.702)							
Mo–P	All	2.499	2.501	0.038	2.474	2.532	25	38
	Trans to P, good σ-donor	2.532	2.532	0.017	2.520	2.544	12	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
8.5.9 Dimethylphenylphosphine ($PPhMe_2$)—(*continued*)								
Mo–P	*Trans* to weak σ donors	2.468	2.475	0.022	2.457	2.479	13	
Tc–P	All	2.437	2.463	0.054	2.416	2.478	7	
	All CTMPTC	2.455	2.466	0.028	2.421	2.479	6	
Ru–P		2.342	2.346	0.046	2.316	2.365	20	
Rh–P	All	2.325	2.327	0.055	2.283	2.383	14	30,81,146
	Long > 2.35	2.373	2.383	0.020	2.352	2.388	7	146
	Short < 2.31	2.278	2.285	0.029	2.267	2.296	7	
Pd–P	All	2.293	2.275	0.052	2.247	2.350	12	30,81
	Long > 2.32	2.348	2.352	0.014	2.335	2.359	5	147
	Short < 2.30	2.253	2.258	0.022	2.227	2.265	7	
Cd–P	See MPPCDC (2.560)							
Ta–P	CPMPTA (2.633, 2.649)							
W–P		2.523	2.528	0.033	2.499	2.548	22	38
Re–P		2.393	2.393	0.057	2.353	2.435	31	
Os–P		2.326	2.329	0.030	2.297	2.349	38	
Ir–P		2.319	2.313	0.038	2.286	2.347	27	
Pt–P		2.299	2.303	0.037	2.281	2.323	54	142
Au–P	See MPAUSN (2.310, 2.318)							
8.5.10 Trifluorophosphine (PF_3)								148
P–F		1.542	1.542	0.020	1.529	1.551	39	
Ti–P	All CPFPTI10	2.344	2.344	0.003	2.342	2.347	4	
Cr–P	(6), (0)	2.143	2.140	0.016	2.129	2.159	4	
Rh–P	All PACPRH10	2.219	2.220	0.007	2.213	2.226	4	
Pt–P	See CEPFPP (2.142)							
8.6.1 1,2-Bis(dimethylphosphino)ethane (chelating, dmpe)†								
P–C(Me)		1.824	1.824	0.019	1.813	1.833	160	
P–C(CH_2)		1.841	1.842	0.021	1.827	1.851	80	
C–C		1.514	1.516	0.024	1.497	1.533	38	
Ti–P		2.604	2.608	0.049	2.570	2.637	8	
Mn–P	(−), (I), see also Mn(II) in COLNEW (2.674)	2.211	2.212	0.004	2.207	2.215	4	
Co–P	See BOHGAG (2.264, 2.248), CADHOE (2.205)							
Ni–P	See COFVIC (2.155, 2.179)							
Zr–P		2.797	2.796	0.049	2.752	2.850	6	
Mo–P	See CITCIR (2.541), NMSPEM (2.409, 2.395)							
Ru–P		2.296	2.297	0.017	2.280	2.311	4	
Pd–P	See CAWLIV (2.304)							
Hf–P		2.687	2.688	0.010	2.678	2.696	4	
Ta–P		2.591	2.602	0.047	2.532	2.629	14	
W–P		2.469	2.470	0.024	2.447	2.491	4	
Ir–P		2.343	2.342	0.005	2.340	2.348	4	
Pt–P	See COMSUS (2.262, 2.270)							
Th–P	See CEKGEE (3.156, 3.152)							
U–P	See CEKGII (3.020, 3.010)							
8.6.2 1,2-Bis(diphenylphosphino)ethane (chelating, dppe)†								
P–C(Ph)		1.827	1.826	0.016	1.816	1.838	287	
P–C(CH_2)		1.845	1.844	0.016	1.835	1.855	143	
C–C		1.527	1.527	0.028	1.513	1.541	72	
V–P	(7), (I)	2.458	2.460	0.025	2.434	2.481	4	
Fe–P	(5,6), (0,II)	2.199	2.201	0.016	2.185	2.210	8	
Co–P	(4,5), (0,III)	2.235	2.239	0.017	2.217	2.248	4	8
Ni–P	(5), (II,III)	2.212	2.209	0.021	2.194	2.232	4	9
Cu–P	(4), (I)	2.304	2.302	0.011	2.295	2.316	4	
Mo–P	(6,7), (0,II,IV)	2.524	2.530	0.048	2.493	2.556	16	38
Tc–P	(6), (II,III)	2.475	2.469	0.033	2.443	2.507	4	
Rh–P	(4,5), (I)	2.294	2.293	0.061	2.232	2.355	8	
Pd–P	(3,4), (0,II)	2.260	2.255	0.029	2.235	2.293	8	
W–P	(5,6), (II)	2.530	2.529	0.021	2.513	2.542	20	38
Re–P	Excluding CAFZUE	2.428	2.440	0.035	2.403	2.453	10	81
Ir–P	(5,6), (I,III)	2.353	2.349	0.036	2.327	2.375	22	
Pt–P	(4,5,*), (0,II)	2.278	2.274	0.033	2.256	2.302	18	
Au–P	(4), (I)	2.400	2.397	0.013	2.389	2.416	8	
8.6.3.1 Bis(diphenylphosphino)methane (chelating, dppm)†								
P–C(Ph)		1.818	1.817	0.013	1.809	1.830	58	
P–C(CH_2)		1.848	1.846	0.014	1.837	1.858	29	
Fe–P	(5,6), (0,II)	2.214	2.217	0.013	2.201	2.215	4	
Nb–P	See CEGGUQ (2.664, 2.660)							
Mo–P	See CEDXEO (2.527, 2.549)							
Ru–P	See CEZXAG (2.341, 2.367)							
Rh–P	(5,6), (I,III)	2.336	2.329	0.024	2.322	2.354	8	
Pd–P	(4), (II)	2.258	2.257	0.020	2.239	2.278	4	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
8.6.3.1 Bis(diphenylphosphino)methane (chelating, dppm)†—(*continued*)								
Os–P	All CEZWOT	2.320	2.322	0.022	2.299	2.339	4	
Pt–P	See CACLUN (2.249, 2.335)							
Au–P	See CACPIF (2.360)							
8.6.3.2 Bis(diphenylphosphino)methane (μ-dppm)†								
P–C(Ph)		1.822	1.822	0.015	1.813	1.831	174	
P–C(CH_2)		1.836	1.837	0.015	1.825	1.848	87	
Co–P	See BOHBIJ (2.176, 2.178)							
Mo–P	See CIKKAI (2.509, 2.510)							
Ru–P	(*), (−)	2.320	2.317	0.012	2.314	2.329	6	
Rh–P	(4—6,*), (−)	2.321	2.319	0.035	2.307	2.345	42	
Pd–P	See BOGFOS (2.324, 2.359)							
Ag–P	(4,5), (−)	2.427	2.425	0.026	2.406	2.454	6	
Re–P	(6), (−)	2.500	2.501	0.028	2.474	2.524	4	
Os–P	See CEMTIX (2.443, 2.452)							
Ir–P	See BUNMEC (2.310, 2.324), CTDPIR (2.319)							
Pt–P	(4,5), (−)	2.309	2.305	0.021	2.297	2.327	16	
Au–P	See PPEAUC (2.284, 2.325)							
8.7.1 Trimethyl phosphite [$P(OMe)_3$]								
P–O		1.595	1.595	0.019	1.582	1.608	311	
O–C		1.432	1.436	0.027	1.419	1.446	311	91
Cr–P	See CROPPH10 (2.269)							38
Mn–P		2.216	2.219	0.043	2.175	2.240	7	149
Fe–P		2.151	2.152	0.017	2.145	2.159	14	149
Co–P		2.156	2.153	0.042	2.124	2.174	19	149
Ni–P		2.189	2.187	0.020	2.171	2.208	4	8,149
Mo–P		2.400	2.395	0.053	2.358	2.425	28	38,149
Ru–P	All	2.291	2.284	0.043	2.273	2.345	16	81
	Not *trans* to $P(OMe)_3$	2.267	2.279	0.025	2.239	2.285	11	
	Trans to $P(OMe)_3$	2.346	2.346	0.002	2.344	2.347	5	
Rh–P	See BPHPRH10 (2.178)							
Pd–P	See COWGEA (2.281, 2.277)							
Ag–P	See MPNDAG (2.409)							
W–P	See CANHAA (2.453)							38
Os–P		2.283	2.283	0.002	2.281	2.285	4	
Ir–P		2.272	2.274	0.022	2.257	2.291	9	
8.7.2 Triphenyl phosphite [$P(OPh)_3$]								
P–O		1.600	1.602	0.011	1.593	1.610	45	
O–C		1.404	1.403	0.019	1.394	1.414	45	
Cr–P	See POTCDR (2.251)							
Mn–P	See COLZEI (2.198, 2.202, 2.207)							38
Rh–P	(4,5,*), (−): all	2.195	2.188	0.047	2.155	2.241	8	85
	(4,5), (−)	2.172	2.184	0.023	2.145	2.189	6	85
Pd–P	See DTCPPD10 (2.323)							
8.8.1 Aminophosphines and μ-phosphides [$P(NR_2)R'_2$, *etc.*]								
P–N		1.678	1.676	0.026	1.658	1.696	104	
Cr–P	See BUJNOJ (2.322)							
Mn–P	(6,7), (I,III)	2.331	2.330	0.028	2.310	2.354	5	
Fe–P	(5,6), (0,II)	2.183	2.192	0.049	2.128	2.212	11	
Co–P	(5,6), (0,I,III)	2.128	2.102	0.053	2.089	2.158	18	
Mo–P	(6), (0,I)	2.402	2.385	0.053	2.355	2.461	18	
Ag–P	See CEMSUI (2.394, 2.396)							
W–P	See BEGYAN (2.497), BUDBEH (2.437)							
Os–P	See BUPYOA (2.375, 2.399), BUPYUG (2.441)							
Pt–P	All BIYVIO	2.252	2.252	0.015	2.238	2.266	4	
8.8.2 Iminoaminophosphines [$P(NR)NR_2$]								
P=N		1.540	1.551	0.022	1.516	1.556	6	
P–N		1.669	1.674	0.015	1.655	1.678	6	
Cr–P	See PCBASC (2.304, 2.321)							
Re–P	See CECGUM (2.477)							
Pt–P	(3,4), (0)	2.248	2.246	0.021	2.228	2.268	4	
8.8.3 Cyclotriphosphazenyl† and related ligands								
P–N		1.644	1.642	0.014	1.636	1.656	13	
Cr–P	See COLPIC (2.349)							
Fe–P	(6), (II)	2.232	2.236	0.042	2.190	2.273	6	
Mo–P	See COLPOI (2.512)							
9.1.1.1 Sulphur (terminal, S)								150
V–S	See BAWBUW01 (2.060)							
Mo–S	(4—6,*), (IV—VI)	2.131	2.133	0.022	2.112	2.151	28	
Ta–S	See CIFMAF (2.204), STAETC (2.181)							
W–S	(4,*), (VI)	2.153	2.158	0.013	2.142	2.162	9	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
9.1.1.2 Sulphur (μ-S)								
V–S	(6,*), (−)	2.234	2.230	0.019	2.219	2.248	10	
Cr–S	All SCPDCC	2.074	2.074	0.003	2.071	2.077	4	
Fe–S	(4,*), (−)	2.225	2.224	0.019	2.210	2.241	50	90
Ni–S	See PMENIB20 (2.035)							
Nb–S	(6—8), (III,IV): all	2.479	2.523	0.129	2.343	2.579	18	
	(6), (III,IV)	2.324	2.338	0.029	2.290	2.343	6	
	(7,8), (III,IV)	2.557	2.556	0.075	2.522	2.631	12	
Mo–S	(4—7,*), (−)	2.317	2.320	0.022	2.306	2.328	102	
Rh–S	See TPPMRH10 (2.368)							
W–S	(6), (IV,V)	2.324	2.319	0.022	2.308	2.342	5	
Re–S	See COJDUA (2.375, 2.387)							
Ir–S	See CTDPIR (2.462)							
Au–S	See BITYIM (2.157, 2.161)							
9.1.1.3 Sulphur (μ_3–S)								
Cr–S		2.299	2.308	0.035	2.253	2.328	17	
Fe–S		2.281	2.282	0.035	2.261	2.306	237	99
Co–S		2.223	2.230	0.047	2.173	2.264	11	
Ni–S	All BIYCUH	2.201	2.203	0.007	2.195	2.207	6	
Cu–S	All CIHRIU	2.163	2.161	0.007	2.157	2.166	12	
Mo–S	Excluding BALJIH, CEFYAN	2.352	2.347	0.019	2.340	2.356	51	
Ru–S	See BUPVUD (2.354, 2.366, 2.350)							
Rh–S	All CEGCIA	2.351	2.352	0.006	2.347	2.356	12	
Os–S		2.428	2.428	0.037	2.406	2.451	60	
Pt–S	See CIXRUW (2.357, 2.369, 2.372)							
9.2.1.1 Alkanethiolates [terminal, SR, R = C (sp^3)]								
S–C		1.829	1.829	0.026	1.816	1.846	213	
Ti–S	See BIPFUB10 (2.404), CIRHUG (2.333)							
V–S	(5,6), (III,IV)	2.378	2.377	0.007	2.371	2.385	13	
Cr–S	See LDHPCR10 (2.332), MCENCR (2.337), SCYSCR (2.417)							
Mn–S	(4,5), (II,III): all	2.366	2.339	0.054	2.322	2.432	11	30
	(4), (II): all CEMSIW	2.433	2.434	0.008	2.425	2.440	4	
	(5), (III)	2.328	2.323	0.011	2.319	2.339	7	
Fe–S	(4—6,*), (−)	2.271	2.269	0.028	2.251	2.296	72	99
Co–S	(4,6,*), (II,III)	2.254	2.249	0.025	2.233	2.271	18	8
Ni–S	(4), (II)	2.187	2.186	0.007	2.181	2.192	8	
Zn–S	See AMETZN (2.295)							
Mo–S	(4—6,8,*), (II—VI)	2.401	2.408	0.050	2.366	2.424	66	
Tc–S	(5,6), (III,V)	2.302	2.302	0.015	2.286	2.314	8	
Cd–S	See ABPENC (2.444)							
Ir–S	See BEPZEB (2.512), COCKAG (2.411)							
Pt–S	(4), (II)	2.320	2.317	0.015	2.308	2.335	5	
Au–S	See AGLPAU (2.293)							
Hg–S	(2—4), (II)	2.402	2.403	0.065	2.339	2.464	4	
9.2.1.2 Alkanethiolates [μ-SR, R = C (sp^3)]								
S–C		1.840	1.837	0.028	1.822	1.858	194	
V–S	(6,7), (III): all	2.438	2.418	0.052	2.393	2.493	24	30
	: short < 2.44	2.401	2.401	0.019	2.386	2.418	15	
	: long > 2.48	2.500	2.493	0.016	2.489	2.513	9	
Cr–S	(6,*), (−)	2.342	2.349	0.022	2.332	2.356	23	
Mn–S	See BUFPUN01 (2.346, 2.631), MCETMN (2.242, 2.270)							
Fe–S	(4—6,*), (−): all	2.298	2.289	0.059	2.255	2.349	109	
	: excluding five > 2.41	2.291	2.280	0.049	2.251	2.325	104	
Co–S	(4,6,*), (−)	2.294	2.298	0.037	2.280	2.315	20	8
Ni–S	(4,*), (−)	2.201	2.199	0.024	2.183	2.227	16	
Cu–S	All CEDNOO	2.278	2.277	0.020	2.265	2.291	12	12
Zn–S	See MCECZN (2.284, 2.343)							
Nb–S	All BAGBUG	2.555	2.556	0.017	2.548	2.566	8	
Mo–S	(5—7), (−)	2.460	2.455	0.047	2.419	2.490	60	
Ru–S	(*), (−)	2.400	2.400	0.063	2.336	2.457	8	
Pd–S	(4,*), (−)	2.328	2.329	0.007	2.321	2.332	16	
Cd–S	See CAHGUN (2.528, 2.622)							
W–S	(6,7), (−): excluding asymmetrics	2.466	2.464	0.051	2.421	2.478	14	151
Os–S	(5,*), (−)	2.414	2.411	0.011	2.405	2.421	10	
Ir–S	(4,5,*), (−)	2.413	2.397	0.050	2.375	2.443	32	
Pt–S	(4), (II)	2.337	2.343	0.046	2.292	2.379	8	
Hg–S	(2—4,*), (−): excluding asymmetrics	2.494	2.454	0.115	2.407	2.598	8	151
9.2.1.3 Alkanethiolates (μ_3-SR)								
S–C(sp^3)	Secondary, tertiary	1.871	1.864	0.020	1.853	1.890	11	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
9.2.1.3 Alkanethiolates (μ_3-SR)—(*continued*)								
S–C(sp^2)		1.769	1.765	0.011	1.762	1.780	9	
Fe–S	(*), (−): all	2.177	2.148	0.051	2.137	2.224	29	30
	: short < 2.16	2.137	2.139	0.012	2.126	2.146	17	
	: long > 2.21	2.233	2.224	0.022	2.219	2.243	12	
Ru–S	See CHPRUS10 (2.272, 2.273, 2.275)							
Ag–S		2.641	2.625	0.118	2.572	2.688	24	
Ir–S	See BAMDOI10 (2.339, 2.342, 2.467)							
9.2.2.1 Arenethiolates (terminal, SR)								
S–C		1.761	1.762	0.020	1.748	1.773	127	
Mn–S	All CEMSES	2.376	2.377	0.006	2.370	2.382	4	
Fe–S	(4—6,*), (−)	2.302	2.298	0.027	2.283	2.318	45	
Co–S	(4—6), (−)	2.247	2.255	0.019	2.245	2.258	7	8
Ni–S	(4), (−)	2.215	2.217	0.017	2.195	2.230	6	
Cu–S	(3—5), (I,II)	2.292	2.271	0.111	2.184	2.425	6	12
	(3), (I): (2.170, 2.188)							
	(4), (II): (2.263, 2.278)							
	(5), (II): (2.425, 2.425)							
Zr–S	See OCBTZR (2.542)							
Mo–S	(5,6,*), (−): all	2.408	2.412	0.056	2.376	2.429	31	
	(5,6), (−): all	2.402	2.411	0.044	2.374	2.427	30	
Tc–S	See BUMCER (2.340, 2.353, 2.358)							
Ru–S	(4,5), (IV)	2.238	2.214	0.067	2.204	2.258	6	
	Excluding one of 2.373	2.210	2.211	0.010	2.202	2.219	5	
Cd–S	See MERQCD10 (2.425, 2.446)							
W–S	See BILRET (2.425)							
Os–S	See CAJCEV (2.507)							
Ir–S	(6), (III)	2.382	2.378	0.032	2.354	2.414	4	
Pt–S	See BATPER (2.365), CFTPVP (2.304), MTPAPT (2.308)							
Hg–S	(3,4), (II)	2.413	2.369	0.088	2.362	2.527	7	
	(3,4), (II): excluding two > 2.52	2.362	2.365	0.012	2.352	2.370	5	
9.2.2.2 Arenethiolates (μ-SR)								
S–C		1.782	1.783	0.018	1.775	1.791	66	
Mn–S	All CEMSES	2.462	2.459	0.016	2.448	2.478	10	
Fe–S	(4,5), (−)	2.318	2.331	0.052	2.263	2.370	26	151
Co–S	(4,6), (−)	2.312	2.318	0.029	2.310	2.329	14	8,151
Cu–S	All CBZTET10	2.288	2.285	0.026	2.264	2.304	12	
Zn–S	(4), (II)	2.351	2.352	0.021	2.338	2.364	16	
Mo–S	(7), (II,III)	2.513	2.534	0.044	2.456	2.548	12	
Rh–S	(4,5), (I,II)	2.352	2.361	0.038	2.307	2.382	12	
Pd–S	(4), (II)	2.294	2.296	0.084	2.200	2.379	6	151
Ag–S	(3,*), (I)	2.454	2.454	0.047	2.408	2.501	8	151
W–S	(6,*), (−)	2.484	2.479	0.048	2.447	2.494	14	
Ir–S	All HPSCIR	2.407	2.406	0.009	2.399	2.415	4	
9.3.1.1 *S*-Thiocyanates (terminal, SCN) (see also 4.5.2.1)								
S–C		1.660	1.660	0.024	1.646	1.676	36	
C–N		1.140	1.139	0.020	1.131	1.150	36	
Cu–S	See CIKJUB (2.733), STETCU (2.606)							
Rh–S	See ACOXRH (2.374, 2.385)							12
Pd–S	(4), (II)	2.351	2.362	0.029	2.329	2.374	9	
Ag–S	(4,5), (I)	2.564	2.546	0.043	2.531	2.613	6	
Pt–S	(4), (II)	2.322	2.322	0.007	2.314	2.328	4	
Au–S	See BACVOQ10 (2.791), BEHYUI (2.469)							
Hg–S	(3,4), (II)	2.493	2.472	0.043	2.461	2.513	11	26
9.3.1.2 *S*-Thiocyanates (μ-SCN)† (see also 4.5.2.2)								
Mn–S	See TCMNET10 (2.691)							
Ni–S	See TCYENI10 (2.570)							
Cu–S	(5), (II): excluding CEVLAQ (2.323), COHHIQ (2.412)	2.808	2.792	0.059	2.760	2.865	5	12
Ag–S	See CENSUJ (2.474), CENTAQ (2.496)							
Cd–S	(5,6), (II)	2.679	2.663	0.090	2.602	2.772	4	
Pt–S	See TPPTCP01 (2.408)							
Hg–S		2.550	2.536	0.053	2.508	2.592	8	26
9.4.1 Thioketones (terminal, $S=CR_2$)								
S–C	(1.657, 1.603)							
Mn–S	See BEHGAW (2.193)							
Os–S	See CAFJUO (2.349)							
9.4.2 Thiourea [terminal, $S=C(NH_2)_2$]								
S–C		1.725	1.721	0.019	1.714	1.732	40	
C–N		1.322	1.324	0.016	1.315	1.332	80	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
9.4.2 Thiourea [terminal, S=C(NH_2)$_2$]—(*continued*)								
Fe–S	All TDCURF	2.588	2.588	0.024	2.567	2.608	4	
Co–S	See BEXTON (2.300), BOVGAU (2.281, 2.300), CTHUCO10 (2.502, 2.553)							
Ni–S	See TIOUNB (2.494, 2.503, 2.520)							9
Cu–S	(3—6), (I,II): excluding one at 2.943	2.295	2.296	0.052	2.245	2.333	14	12
	(3,4), (I)	2.287	2.296	0.045	2.240	2.331	12	
Pd–S	All THUPDC	2.334	2.336	0.013	2.320	2.345	4	
Ag–S	(3,4), (I)	2.493	2.484	0.048	2.454	2.536	6	
Re–S	See OACTUR (2.340, 2.355), OATURE (2.311)							
9.5.1.1 Dithiocarboxylates (terminal, S_2CR)								
(None)								
9.5.1.2 Dithiocarboxylates (chelating, S_2CR, R = any C)								
S–C		1.685	1.684	0.015	1.674	1.696	44	
C–C		1.483	1.479	0.025	1.461	1.505	22	
Ti–S	All CSACTI	2.526	2.526	0.032	2.503	2.550	6	
Mn–S	See BESBIK10 (2.344, 2.376)							
Ni–S	See PTCDNI20 (2.213, 2.216)							
Cu–S	See PHTHCU01 (2.400, 2.422)							9
Mo–S	(5—8), (II,IV,V): all	2.505	2.493	0.071	2.464	2.529	24	
	: excluding two > 2.69	2.486	2.485	0.035	2.464	2.518	22	44
Pd–S	All PDTHBA10	2.328	2.325	0.009	2.322	2.335	6	
W–S	See CONKEV (2.471, 2.473)							
Re–S	See BESBOQ10 (2.488, 2.503)							
Pt–S	See CERDAE (2.321, 2.322)							
9.5.1.3 Dithiocarboxylates (μ-S_2CR, R = any C)								
S–C		1.678	1.678	0.016	1.667	1.686	38	
C–C		1.517	1.516	0.022	1.503	1.537	20	
Ni–S	All DTPANI10	2.214	2.210	0.010	2.208	2.225	4	9
Mo–S	(5), (II)	2.464	2.465	0.008	2.458	2.470	12	
Pd–S	(*), (II)	2.325	2.325	0.010	2.319	2.330	10	
Pt–S	(5,6), (II)	2.319	2.319	0.009	2.310	2.326	12	
9.5.2.1 Thiocarboxylates (chelating, SOCR) (see also 5.5.7.1)								
Ni–S	(6), (II)	2.453	2.452	0.016	2.444	2.456	9	
9.5.2.2 Thiocarboxylates (μ-SOCR) (see also 5.5.7.2)								
Ni–S	(4), (II)	2.178	2.176	0.010	2.172	2.181	8	
Cu–S	All BEFJIF10	2.274	2.271	0.010	2.268	2.284	4	
Rh–S	See TACDRH10 (2.256, 2.262)							
Ag–S	See CEFMIJ (2.513)							
9.6.1.1 Dithiocarbamates (terminal, S_2CNR_2, R = any C)								
(M)S–C		1.748	1.747	0.022	1.730	1.771	6	
C–S		1.674	1.676	0.013	1.661	1.684	6	
C–N		1.343	1.345	0.011	1.334	1.352	6	
N–C(R)		1.467	1.468	0.018	1.453	1.482	12	
Zn–S	See TMTCZN10 (2.299, 2.312)							
W–S	See CIXKAV (2.496)							
Pt–S	See IBTCPT (2.335)							24
Au–S	See AUDETC (2.333, 2.347)							
9.6.1.2 Dithiocarbamates (chelating, S_2CNR_2, R = any C)								
S–C		1.714	1.715	0.018	1.704	1.726	539	
C–N		1.324	1.322	0.021	1.313	1.334	269	
N–R		1.473	1.475	0.030	1.462	1.487	537	
V–S	All ETCOXV	2.402	2.405	0.010	2.391	2.409	4	
Cr–S	(6,7), (II,III)	2.416	2.407	0.026	2.396	2.441	24	
Mn–S	All MORTMN, MOTCMN	2.459	2.465	0.078	2.385	2.529	12	130
Fe–S	(5,6), (0,II,IV): mostly (III), all	2.354	2.336	0.060	2.307	2.422	112	30
	: <2.375 (mostly low spin)	2.319	2.313	0.026	2.299	2.340	78	
	: >2.390	2.436	2.434	0.020	2.428	2.449	34	
Co–S	(5,6), (III)	2.267	2.270	0.013	2.255	2.277	32	
Ni–S	(4,6), (II): excluding BDTCBR (2.261)	2.207	2.206	0.017	2.196	2.218	18	
Cu–S	(4,5), (II,III)	2.250	2.222	0.044	2.214	2.286	14	12,152
Zn–S	(4,5), (II)	2.436	2.452	0.056	2.406	2.466	16	
Zr–S	See BOVYUG (2.635, 2.724)							
Nb–S	All CAHJIE	2.602	2.586	0.054	2.565	2.632	6	
Mo–S	(5—7), (II—IV): all	2.513	2.507	0.059	2.478	2.530	164	
	: excluding asymmetry > 0.10	2.504	2.504	0.043	2.478	2.527	144	44,153
Tc–S	(5,7), (II,III,V)	2.457	2.476	0.043	2.405	2.490	14	
Ru–S	(6,7), (II—IV)	2.379	2.392	0.039	2.345	2.400	20	
Rh–S	All MOTCRH	2.370	2.374	0.014	2.353	2.382	6	
Pd–S	(4), (II)	2.323	2.319	0.031	2.315	2.323	18	
Cd–S	All BEGNUW	2.711	2.717	0.037	2.679	2.740	6	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
9.6.1.2 Dithiocarbamates (chelating, S_2CNR_2, R = any C)—(*continued*)								
Ta–S	All STAETC	2.577	2.559	0.056	2.538	2.613	6	
W–S	(6,7), (II,V)	2.526	2.531	0.031	2.496	2.550	6	24
Re–S	(5—7), (III—V)	2.442	2.441	0.040	2.410	2.474	20	
Os–S	(6,7), (III,IV)	2.410	2.417	0.021	2.405	2.424	20	
Ir–S	All EDTCIR	2.367	2.365	0.003	2.365	2.370	4	
Pt–S	See BOFJIP (2.347, 2.299)							
Au–S	(4,5), (III)	2.349	2.336	0.033	2.330	2.381	12	
Hg–S	See HGETCB10 (2.399, 2.965)							
9.6.2 Thiocarbamates (chelating, $SOCNR_2$) (see also 5.5.6)								
Ti–S	See EMTCTJ (2.477, 2.477, 2.489)							
Co–S	See TMTCPC (2.584)							
Zr–S	See BUWMAH (2.641), EMTCZR (2.669, 2.689)							
U–S		2.869	2.870	0.005	2.865	2.874	5	
9.7.1.1 Xanthates (terminal, S_2COR)								154
C–S(Ni)	(1.720)							
C=S(free)	(1.651)							
C–O(Me)	(1.334)							
Ni–S	See BIMMOZ (2.195)							
9.7.1.2 Xanthates (chelating, S_2COR)								154
S–C		1.676	1.677	0.018	1.664	1.688	32	
C–O		1.329	1.327	0.014	1.317	1.339	16	
V–S	All BIRYOO10	2.503	2.482	0.059	2.471	2.492	12	
Co–S	See CADHOE (2.254, 2.290)							
Ni–S	(4,6), (0,II)	2.407	2.418	0.056	2.346	2.455	8	
Zn–S	See EXAPYZ (2.294, 2.747)							
Mo–S	(5), (III)	2.517	2.516	0.009	2.508	2.525	4	
Pd–S	See TXPCPD (2.328, 2.332)							
Cd–S	See EXPNCD (2.647, 2.743)							
9.7.1.3 Xanthates (μ-S_2COR)								
C–S		1.690	1.689	0.006	1.686	1.697	4	
C–O	(1.330, 1.317)							
Cd–S		2.567	2.570	0.026	2.541	2.589	4	
9.7.2.1 Dithiocarbonates (chelating, S_2CO)								
S–C		1.728	1.722	0.033	1.711	1.737	9	
C–O		1.242	1.249	0.029	1.215	1.266	5	
Co–S	See BELTIV10 (2.259, 2.250)							
Rh–S	All MPTCRH	2.374	2.374	0.010	2.365	2.382	4	
Pd–S	See BEMLUA (2.318)							
Pt–S	See TCTPPU (2.340, 2.325)							
9.7.2.2 Dithiocarbonates (μ-S_2CO)								
S–C		1.684	1.683	0.006	1.678	1.690	4	
C–O	(1.336, 1.333)							
Mo–S	All EDTCMO	2.478	2.478	0.002	2.475	2.480	4	
9.8.1.1 Trithiocarbonate (terminal, CS_3)								
(None)								
9.8.1.2 Trithiocarbonate (chelating, CS_3)								
C–S(Fe)	(1.719, 1.720)							
C–S	(1.666)							
Fe–S	See BULZIR (2.325, 2.335)							
9.8.1.3 Trithiocarbonate (μ-CS_3)								
(None)								
9.8.2.1 Thioxanthates (σ-S_2CSR)								
(None)								
9.8.2.2 Thioxanthates (chelating, S_2CSR)								
(M)S–C		1.692	1.692	0.012	1.684	1.700	40	
C–SR		1.718	1.719	0.013	1.712	1.724	20	
Cr–S	All ETXACR10	2.400	2.398	0.008	2.395	2.408	12	
Fe–S	See ESEXFE10 (2.344, 2.333)							
Co–S	(6), (III)	2.272	2.271	0.007	2.264	2.277	14	
Ni–S	See BZTCDN (2.207, 2.211)							
Cu–S	See TPTHCC (2.451, 2.439)							
Mo–S	See IPTXMO (2.438, 2.454)							
Pd–S	All TETCPD	2.338	2.334	0.008	2.333	2.348	6	
9.8.2.3 Thioxanthates (μ-S_2CSR)								
(M)S–C		1.684	1.681	0.010	1.677	1.694	4	
C–SR	(1.749, 1.743)							
Fe–S	(6), (III)	2.281	2.285	0.011	2.269	2.288	4	
9.9.1 *o*-Dithioquinones (chelating, $C_6R_4S_2$)†								155
S–C^1		1.751	1.750	0.018	1.738	1.765	42	
C^1–$C^{1'}$		1.398	1.399	0.020	1.387	1.414	23	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
9.9.1 *o*-Dithioquinones (chelating, $C_6R_4S_2$)†—(*continued*)								155
C^1–C^2		1.403	1.401	0.017	1.391	1.412	42	
C^2–C^3		1.378	1.378	0.026	1.360	1.394	42	
C^3–$C^{3'}$		1.378	1.382	0.023	1.358	1.398	23	
Ti–S	See BTCPTI (2.411, 2.418)							
Fe–S	(4,5), (−)	2.223	2.227	0.012	2.211	2.232	8	
Co–S	(4,5), (−)	2.131	2.115	0.028	2.111	2.167	6	
Zr–S	See BZDTZR10 (2.537, 2.538, 2.554)							
Nb–S	All BZDTNB10	2.441	2.439	0.011	2.432	2.452	6	
Mo–S	(6,7), (−)	2.357	2.360	0.018	2.342	2.371	5	
Cd–S	All CADPEC	2.508	2.506	0.017	2.493	2.526	4	
Ta–S	All PABZTA	2.428	2.424	0.036	2.396	2.463	4	
Au–S	All BAMHUS	2.311	2.312	0.009	2.302	2.319	4	
9.9.2 α,β-Dithiones/dithiolates {chelating, $[S{=}C(R)]_2$}†								155
S–C_α		1.725	1.725	0.019	1.711	1.738	106	
C_α–$C_{\alpha'}$		1.352	1.356	0.024	1.337	1.367	55	
Ti–S	See CPMNTI (2.439, 2.455)							
Fe–S	(5), (−)	2.171	2.166	0.027	2.150	2.178	16	
Co–S	All PAPMCO10	2.229	2.230	0.020	2.211	2.248	4	8
Ni–S	(4), (−)	2.148	2.142	0.019	2.134	2.163	34	9
Cu–S	(4), (−)	2.258	2.258	0.013	2.250	2.264	10	
Mo–S	(6), (−)	2.387	2.391	0.011	2.377	2.397	9	
Ru–S	See TPRUET21 (2.282, 2.320)							
Rh–S	(5), (−)	2.308	2.318	0.027	2.280	2.327	4	
W–S	See ASCETU (2.364, 2.368, 2.382)							
Re–S	All REPETD10	2.324	2.328	0.011	2.318	2.332	6	
Pt–S	(4), (−)	2.258	2.257	0.010	2.249	2.269	14	
Au–S	(4), (−)	2.301	2.305	0.012	2.289	2.311	4	
9.9.3 α,α-Alkenedithiolates (chelating, $S_2C{=}CR_2$)†								155
S–C		1.734	1.736	0.023	1.715	1.749	11	
C=C		1.358	1.365	0.018	1.352	1.367	6	
Fe–S	See DEDTFE10 (2.288, 2.301, 2.305)							
Ni–S	See ANIDED10 (2.193, 2.196)							
Cu–S	See KCUDED10 (2.189, 2.199)							
9.10 Tertiary phosphine sulphides (σ-SPR_3)								
S–P		2.000	1.996	0.021	1.986	2.012	11	
P–C		1.805	1.806	0.017	1.799	1.817	33	
Mn–S	See BOFMOY (2.410)							
Ni–S	See BOPFOB (2.194)							
Cu–S	(3,4), (I,II)	2.280	2.302	0.044	2.236	2.313	5	
Mo–S	See OXCPSM10 (2.460)							
Pd–S	See COSWUC (2.334), EPPTPD (2.350)							
Au–S	See ZEGNOP (2.324)							
9.11.1.1 Dithiophosphinates (chelating, S_2PR_2)								
S–P		2.007	2.012	0.016	1.997	2.020	73	
P–C		1.828	1.832	0.025	1.809	1.848	73	
Ti–S	All ETPSTI	2.473	2.472	0.034	2.440	2.507	8	
Ni–S	All DMDTPN10	2.237	2.237	0.004	2.234	2.241	4	9
Zn–S	(4), (II)	2.422	2.446	0.052	2.369	2.452	4	
Mo–S	All BAVLAL11	2.535	2.538	0.033	2.504	2.565	4	
Ce–S	All BIYYOX	2.990	3.003	0.033	2.956	3.012	4	
Dy–S	All DCHPDY10	2.741	2.744	0.007	2.732	2.746	6	
Tm–S	All BIYYUD	2.870	2.851	0.084	2.794	2.948	8	
Lu–S	All DCHPLU10	2.692	2.695	0.007	2.684	2.697	6	
Th–S	(8), (IV)	2.908	2.911	0.017	2.900	2.921	12	
U–S	(7), (VI)	2.873	2.868	0.023	2.854	2.895	18	
9.11.1.2 Dithiophosphinates (μ-S_2PR_2)								
S–P		2.015	2.019	0.009	2.005	2.023	6	
P–C		1.810	1.810	0.007	1.803	1.818	6	
Zn–S	See BEDBUH (2.306, 2.321)							
Mo–S	All BUXMIQ	2.530	2.530	0.005	2.525	2.534	4	
9.12.1 Disulphide (η^2-S_2)								150,156
S–S		2.053	2.054	0.026	2.036	2.072	18	
V–S	See BONCIQ01 (2.393)							
Nb–S	(8), (V)	2.498	2.493	0.050	2.450	2.538	6	
Mo–S	(4,5,7), (IV—VI)	2.412	2.408	0.027	2.389	2.441	22	
Re–S	See CECGOG (2.410)							
Ir–S	See SPPEIR (2.389, 2.422)							
U–S	See BEFBIX (2.711)							
9.12.2 Polysulphur ligands (σ-SSZ, Z = any atom)								150,156
S–S		2.053	2.047	0.038	2.026	2.072	46	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
9.12.2 Polysulphur ligands (σ-SSZ, Z = any atom)—(*continued*)								150,156
Ti–S	(8), (IV)	2.432	2.434	0.017	2.416	2.448	4	
V–S	(6,8), (IV): all	2.348	2.316	0.086	2.277	2.453	6	
	(6), (IV): only μ-S_2	2.294	2.299	0.026	2.268	2.316	4	
Fe–S	(6), (II,III)	2.192	2.187	0.067	2.129	2.259	5	
Ni–S	(4,*), (−)	2.137	2.125	0.027	2.122	2.158	5	
Zn–S	See TPCUMZ (2.317)							
Mo–S	(5,7), (IV,VI)	2.415	2.397	0.060	2.372	2.472	10	
W–S	See CAFFEU (2.506), CPDYSW10 (2.419, 2.420)							
Re–S	All COJDOU	2.257	2.259	0.017	2.240	2.271	4	
Os–S	See PSTOSA (2.443)							
Pt–S	(4), (II)	2.316	2.336	0.053	2.260	2.351	4	
9.13.1.1 Dialkyl thioethers [terminal, SR_2, R = C (sp^3)]								158
S–C		1.817	1.817	0.019	1.807	1.827	570	
Cr–S	(6), (0)	2.397	2.418	0.043	2.348	2.428	8	
Mn–S	See PSMNPC10 (2.310)							
Fe–S	(5,6), (0,II): excluding CIJYOJ	2.301	2.304	0.028	2.278	2.328	8	
Co–S	(6), (II,III): all	2.316	2.263	0.106	2.243	2.456	40	8,30
	(6), (II)	2.483	2.479	0.030	2.461	2.508	11	
	(6), (III)	2.253	2.250	0.019	2.240	2.269	29	
Ni–S	(4—6), (I,II): excluding PTOCNI10	2.376	2.397	0.092	2.369	2.433	30	
	(6), (II)	2.416	2.399	0.037	2.391	2.440	22	
Cu–S	(3—6), (I,II): all	2.364	2.343	0.082	2.318	2.385	89	86
	(3,4), (I)	2.313	2.301	0.047	2.271	2.348	18	
	(4—6), (II): excluding three > 2.65	2.364	2.347	0.053	2.323	2.390	68	
Zn–S	See TAZTDG (2.601)							
Nb–S	(6), (III—V)	2.700	2.716	0.046	2.649	2.738	6	
Mo–S	(5—7), (0,II—IV): all	2.541	2.536	0.064	2.484	2.569	22	
	: excluding two > 2.700	2.525	2.533	0.039	2.484	2.560	20	
Ru–S	See BIGLAE (2.262, 2.333)							
Rh–S	(5,6,*), (0—II): all	2.430	2.415	0.064	2.406	2.481	7	
Pd–S	(4,5), (II)	2.283	2.275	0.030	2.262	2.307	21	
Ag–S	(3—6,*), (I): all	2.669	2.624	0.164	2.558	2.803	18	
Cd–S	See TDACCD10 (2.669)							
La–S	See APXLAP (3.032, 3.045)							
Ta–S	(6), (III)	2.657	2.634	0.067	2.619	2.706	5	
W–S	See CPHMOC (2.560), ESCTHW20 (2.570)							159
Ir–S	(6), (III)	2.353	2.361	0.032	2.325	2.376	5	
Pt–S	(4), (II)	2.244	2.242	0.012	2.233	2.256	4	
	(6), (IV)	2.470	2.473	0.009	2.461	2.478	4	
Au–S	See CIBLUU (2.275)							
Hg–S	(4,5), (II)	2.624	2.618	0.054	2.577	2.672	6	26
9.13.1.2 Dialkyl thioethers [μ-SR_2, R = C(sp^3)]								
S–C		1.830	1.826	0.032	1.810	1.850	24	
Fe–S	See OCHTPI (2.141, 2.206)							
Cu–S	See DTHCUC (2.314, 2.336)							
Mo–S	(6), (II,III)	2.376	2.390	0.039	2.335	2.404	4	
Ag–S	(3,5,6), (I)	2.534	2.537	0.031	2.504	2.561	6	
Ta–S	(6), (III)	2.390	2.390	0.007	2.384	2.396	5	
Ir–S	See CETSIR (2.327, 2.343)							
9.13.2 Thioethers [terminal, SR_2, $R_2 \neq C(sp^3)_2$]								
S–C (sp^2)		1.778	1.778	0.020	1.758	1.788	55	
S–C (sp^3)		1.826	1.823	0.020	1.811	1.837	39	
Cr–S	(6), (0)	2.384	2.384	0.014	2.370	2.391	11	
Mn–S	See BATZIF (2.389), CECCIW (2.434)							
Fe–S	(6), (II)	2.249	2.250	0.054	2.196	2.300	4	
Co–S	See BEMNIQ (2.468, 2.502)							
Ni–S	See BOSNEC (2.431, 2.473), BTZDNI (2.162, 2.165), DAPSMO (2.534)							
Cu–S	(4—6), (I,II)	2.418	2.438	0.069	2.347	2.470	4	
Mo–S	See FMBTMO (2.552)							
Rh–S	See CETMRH (2.312), HMTNRH (2.273)							
Pd–S	(4), (II)	2.295	2.292	0.008	2.290	2.302	5	
Cd–S	See CEZWEJ (2.738)							
Ta–S	See CIFMAF (2.706, 2.836)							
W–S	See MCTCEW (2.441), MEPOSW (2.555)							
Pt–S	(4), (II)	2.265	2.262	0.024	2.245	2.289	4	
Hg–S	See BAVKIS (3.124, 3.131)							
9.14.1.1 *S*-SO_2 (terminal) (see also 5.20)								104,160
S–O		1.421	1.428	0.041	1.389	1.454	16	
Fe–S	See BOGPIW (2.109)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
9.14.1.1 *S*-SO_2 (terminal) (see also 5.20)—(*continued*)								104,160
Ni–S	See SXPMNI01 (2.012)							9
Rh–S	See CPSXER (2.096), CSTPRH (2.450)							
Pt–S	(3,4), (0)	2.380	2.379	0.068	2.316	2.446	4	
9.14.1.2 *S*-SO_2 (μ)								160
S–O		1.458	1.457	0.021	1.438	1.476	19	
Fe–S	(6), (I)	2.253	2.258	0.032	2.222	2.280	4	
Rh–S	See CACFUH (2.249, 2.235), SOCPRH (2.252)							
Pt–S	(*), (0)	2.274	2.275	0.056	2.251	2.292	12	
9.14.2 *S*-SO_3 (σ)								104
S–O		1.477	1.479	0.012	1.471	1.485	33	
Co–S	(6), (III)	2.230	2.227	0.024	2.206	2.252	9	8
Au–S	See ENSPAU (2.301, 2.308)							
9.14.3 *S*-SO_3R (σ)								
S–O	(1.445, 1.448)							
S–O(R)	(1.619)							
Pt–S	See MSTPPT (2.305)							
9.15.1.1 Disulphides (σ-RSSR)								
S–S		2.050	2.040	0.025	2.032	2.079	7	
Co–S	See BINHUB (2.262), DSENCO (2.272)							
Ni–S	See BPESNI (2.455), PMISNI (2.470)							
Cu–S	See PYDSCU10 (2.396, 2.438)							
Ag–S	See CONSON (2.533)							
9.15.1.2 Disulphides (μ-σ:σ′-RSSR)								
S–S	(2.063, 2.065)							
Cu–S	See BIGLUY (2.332, 2.338)							
Ag–S	See CONSON (2.503, 2.638)							
9.16 *S*-Dialkyl sulphoxides [terminal, $S(O)R_2$] (see 5.17)								127
S–O		1.469	1.468	0.013	1.459	1.476	43	
S–C	Most R = primary alkyl	1.785	1.781	0.023	1.774	1.797	88	
Cr–S	See PCTXCR (2.331)							
Fe–S	See SPCNFE (2.307)							
Ru–S	(6), (II)	2.288	2.263	0.051	2.257	2.339	8	
Rh–S	(6), (II,III): all	2.315	2.290	0.067	2.284	2.329	7	
	(6), (III)	2.293	2.288	0.032	2.273	2.326	6	85
Pd–S	See PDDMSX10 (2.299)							
Pt–S	(4), (II)	2.223	2.219	0.033	2.199	2.232	26	
9.17 CS_2 (terminal, η^2) (see also 3.22.2)								
V–S	See CPCDSV (2.432, 2.444)							
Fe–S	See SPHFEC10 (2.333)							
Co–S	See TPHCOA (2.206)							
Ni–S	See COGWOK (2.195)							
Nb–S	See CPSNBA (2.503)							
10.1.1.1 Chlorine (terminal)								
Ti–Cl	(−), (−): all	2.305	2.311	0.058	2.262	2.352	98	
	(6), not (III)	2.281	2.294	0.048	2.247	2.316	60	
	(7), (−)	2.313	2.320	0.046	2.269	2.361	8	
	(8), not (III)	2.362	2.363	0.018	2.352	2.369	24	
V–Cl	(−), (−): all	2.294	2.297	0.074	2.223	2.333	31	
	(5), (−)	2.224	2.218	0.041	2.187	2.265	9	
	(6), not (II)	2.297	2.318	0.047	2.261	2.319	17	30
Cr–Cl	(6), (−): all	2.335	2.318	0.055	2.303	2.370	9	
	(6), (−)	2.309	2.316	0.018	2.299	2.319	7	147
Mn–Cl	(−), (−): all	2.445	2.465	0.087	2.361	2.518	33	
	(5), (−): excluding MEIMMN	2.346	2.351	0.014	2.337	2.358	7	
	(6), (II)	2.516	2.495	0.048	2.478	2.560	15	
Fe–Cl	(−), (−): all	2.262	2.246	0.070	2.205	2.311	119	
	(4), (II)	2.301	2.303	0.028	2.275	2.327	15	
	(4), (III)	2.195	2.192	0.016	2.184	2.207	39	
	(5), (III)	2.235	2.224	0.028	2.214	2.252	10	
	(6), (II)	2.384	2.363	0.053	2.342	2.435	9	
	(6), (III)	2.308	2.310	0.036	2.292	2.330	22	
Co–Cl	(−), (−): all	2.272	2.259	0.048	2.244	2.281	191	86
	(4), (−)	2.254	2.256	0.026	2.232	2.271	96	
	(6), (II)	2.414	2.417	0.057	2.348	2.468	11	
	(6), (III): excluding three > 2.36	2.260	2.256	0.019	2.248	2.274	70	
Ni–Cl	(−), (−): all	2.339	2.314	0.117	2.243	2.426	63	
	(4), (II)	2.217	2.206	0.044	2.183	2.252	18	
	(5), (II)	2.308	2.306	0.019	2.302	2.314	11	
	(6), (II)	2.441	2.428	0.053	2.406	2.467	26	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
10.1.1.1 Chlorine (terminal)—(*continued*)								
Cu–Cl	(−), (−): all	2.276	2.254	0.092	2.232	2.292	362	12
	(2), (I)	2.090	2.090	0.010	2.080	2.099	6	
	(3), (I)	2.179	2.156	0.044	2.140	2.220	15	
	(4), (I)	2.361	2.351	0.065	2.321	2.406	11	
	(4), (II)	2.248	2.246	0.032	2.233	2.263	153	
	(5), (II): all	2.323	2.276	0.123	2.240	2.362	145	86
	: short < 2.4	2.269	2.260	0.048	2.233	2.296	116	
	: long > 2.4	2.537	2.515	0.091	2.467	2.618	29	
	(6), (II): all	2.354	2.284	0.188	2.256	2.327	17	
	: short < 2.4	2.274	2.280	0.035	2.242	2.298	14	
Zn–Cl	(−), (−): all	2.255	2.256	0.035	2.231	2.276	183	
	(4), (−)	2.253	2.256	0.033	2.229	2.276	173	
	(5), (−)	2.257	2.255	0.033	2.232	2.286	8	
Zr–Cl	(−), (−): all	2.470	2.449	0.061	2.429	2.522	31	
	(6), (−)	2.426	2.425	0.027	2.410	2.453	8	
	(8), (−)	2.464	2.447	0.037	2.440	2.492	13	
	(9), (−)	2.561	2.559	0.008	2.555	2.570	6	
Nb–Cl	(−), (−): all	2.395	2.401	0.053	2.351	2.429	94	
	(6), (−)	2.374	2.382	0.041	2.339	2.405	65	
	(7), (−)	2.415	2.416	0.069	2.348	2.481	5	
	(8), (−)	2.457	2.463	0.036	2.429	2.483	19	
Mo–Cl	(−), (−): all	2.410	2.404	0.072	2.368	2.445	193	
	(5), (−)	2.409	2.414	0.043	2.394	2.444	28	
	(6), (−)	2.389	2.388	0.053	2.356	2.419	112	44,85
	(7), (−)	2.481	2.474	0.049	2.440	2.524	14	
Tc–Cl	(5,6), (−): all	2.359	2.328	0.077	2.318	2.359	29	86
	(−), not (III): *trans* to PR_3	2.323	2.325	0.018	2.317	2.333	23	44,85
Ru–Cl	(−), (−): all	2.416	2.416	0.049	2.386	2.441	115	
	(6), (−)	2.409	2.415	0.040	2.385	2.434	102	44,161
	(5), (−)	2.434	2.455	0.051	2.371	2.483	7	
Rh–Cl	(−), (−): all	2.377	2.364	0.052	2.342	2.391	139	86
	(4), (−)	2.369	2.370	0.026	2.353	2.387	40	
	(5), (−)	2.400	2.388	0.053	2.363	2.437	23	
	(6), (−)	2.374	2.354	0.060	2.335	2.393	76	86
Pd–Cl	(−), (−): all	2.331	2.312	0.067	2.298	2.356	248	
	(4), (−)	2.326	2.312	0.043	2.298	2.354	224	
	(5), (−): excluding two > 2.8	2.345	2.320	0.045	2.316	2.376	13	
Ag–Cl	See AGSURE10 (2.854), CMURAG (2.650), PMBPAG10 (2.502)							145
Cd–Cl	(−), (−): all	2.499	2.471	0.085	2.443	2.550	45	
	(4), (−)	2.448	2.451	0.023	2.436	2.458	18	
	(6), (−): all	2.556	2.550	0.085	2.495	2.591	22	
	(6), (−): excluding two > 2.7	2.536	2.546	0.055	2.494	2.581	20	
La–Cl	See CERKUF (2.751)							
Ce–Cl	See CLCAME01 (2.594, 2.605, 2.619)							
Pr–Cl	See TPYRPR (2.877)							
Nd–Cl	See BIDNEH (2.871), BOKPEW (2.666, 2.670)							
Er–Cl	See BOBWAQ (2.613, 2.620)							
Yb–Cl	See BAWLAM (2.593), BAWLEQ (2.594, 2.596)							
Hf–Cl	See BIHWUK (2.365), CTMSIC (2.436)							
Ta–Cl	(−), (−): all	2.399	2.388	0.068	2.355	2.440	119	
	(6), (−)	2.383	2.375	0.055	2.349	2.418	83	
	(7), (−)	2.428	2.404	0.067	2.380	2.445	•15	
	(7), (−): excluding two > 2.5	2.406	2.398	0.034	2.378	2.439	13	
	(8), (−)	2.463	2.497	0.088	2.383	2.541	17	30
	(8), (−): excluding four < 2.4 from COWSOW	2.505	2.510	0.046	2.462	2.544	13	
W–Cl	(−), (−): all	2.408	2.395	0.059	2.370	2.433	124	
	(5), (−)	2.390	2.393	0.030	2.374	2.409	19	
	(6), (−)	2.392	2.388	0.045	2.364	2.422	80	
	(7), (−)	2.472	2.453	0.056	2.428	2.529	12	
Re–Cl	(−), (−): all	2.389	2.380	0.062	2.355	2.411	116	86
	(5), (−)	2.368	2.378	0.026	2.355	2.387	14	
	(6), (−): excluding three long > 2.49	2.380	2.378	0.042	2.355	2.409	90	85,162
Os–Cl	(5,6), (−): all	2.368	2.361	0.077	2.307	2.411	54	
	(6), (−)	2.357	2.357	0.053	2.307	2.389	50	44,85
Ir–Cl	(−), (−): all	2.390	2.370	0.051	2.355	2.429	83	
	(4), (−)	2.389	2.381	0.055	2.355	2.418	11	
	(5), (−)	2.380	2.368	0.038	2.356	2.416	7	
	(6), (−): all	2.391	2.370	0.052	2.353	2.439	65	30
	: short < 2.4	2.361	2.359	0.020	2.349	2.372	46	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
10.1.1.1 Chlorine (terminal)—(*continued*)								
Ir–Cl	(6), (−): long > 2.4	2.463	2.465	0.028	2.440	2.470	19	
Pt–Cl	(−), (−): all	2.324	2.310	0.038	2.297	2.348	354	41,86
	(4), (−)	2.323	2.308	0.038	2.297	2.349	293	86
	(5), (−)	2.330	2.321	0.048	2.303	2.346	15	
	(6), (−)	2.326	2.316	0.036	2.306	2.327	42	
Au–Cl	(−), (−): all	2.301	2.276	0.094	2.271	2.287	54	86,144
	(4), not (I,II)	2.276	2.276	0.010	2.270	2.284	36	
Hg–Cl	(−), (−): all	2.423	2.391	0.120	2.328	2.480	101	26,86
	(2), (−)	2.330	2.332	0.018	2.317	2.350	11	
	(3), (−)	2.292	2.289	0.016	2.281	2.305	5	
	(4), (−): all	2.447	2.440	0.121	2.349	2.521	68	
	: excluding three > 2.76	2.430	2.437	0.091	2.348	2.480	65	
Th–Cl	(7,8), (−): all	2.728	2.752	0.039	2.690	2.756	8	
U–Cl	(−), (−): all	2.646	2.653	0.046	2.625	2.671	61	
	(6), (−): all	2.644	2.656	0.045	2.625	2.621	40	
	: excluding two < 2.254	2.653	2.656	0.023	2.630	2.671	38	
	(8), (−)	2.642	2.651	0.028	2.614	2.659	14	
10.1.1.2 Chlorine (μ-Cl)								134
Ti–Cl	(6—8), (III,IV): all	2.520	2.536	0.039	2.486	2.545	24	
	(6,7), (IV)	2.459	2.465	0.017	2.438	2.473	6	
	(7,8), (III)	2.541	2.540	0.014	2.532	2.548	18	
V–Cl	(6), (II): all CANZUM	2.476	2.474	0.006	2.472	2.482	6	
Cr–Cl	See CATSEV (2.372, 2.377)							
Mn–Cl	(5—6), (I,II): all	2.539	2.555	0.066	2.512	2.575	18	
	(6), (II)	2.559	2.559	0.046	2.532	2.583	14	
Fe–Cl	(5,*), (−)	2.306	2.289	0.027	2.288	2.341	6	
Co–Cl	(6), (II)	2.397	2.403	0.026	2.370	2.417	4	
Ni–Cl	(4—6), (II): all	2.372	2.404	0.093	2.242	2.426	36	9
	(5,6), (II)	2.426	2.410	0.051	2.384	2.459	20	86
	(5,6), (II)	2.402	2.402	0.025	2.382	2.422	14	151
	(4), (II)	2.238	2.236	0.005	2.235	2.239	10	
Cu–Cl	(3—6,*), (I,II): all	2.337	2.313	0.098	2.280	2.359	66	12
	(3), (I)	2.275	2.276	0.021	2.263	2.280	12	
	(4), (I)	2.364	2.360	0.065	2.307	2.411	10	
	(4), (II)	2.343	2.347	0.039	2.303	2.383	8	
	(5), (II): all	2.367	2.315	0.137	2.296	2.519	26	30
	: short < 2.34	2.284	2.306	0.058	2.276	2.315	18	
	: long > 2.50	2.554	2.554	0.041	2.519	2.574	8	
Zn–Cl	(4), (II)	2.364	2.359	0.019	2.351	2.372	6	
Y–Cl	(8,9), (III)	2.710	2.699	0.042	2.678	2.754	4	
Zr–Cl	(6,8), (III,IV)	2.588	2.576	0.053	2.541	2.638	6	
Nb–Cl	(6—8), (II—IV)	2.531	2.512	0.048	2.503	2.567	26	
Mo–Cl	(6,7), (II—V)	2.486	2.486	0.040	2.473	2.509	40	85
Tc–Cl	See OXPTCC (2.679)							
Ru–Cl	(6,*), (II—IV)	2.428	2.427	0.056	2.377	2.486	12	85
Rh–Cl	(4—6,*), (I—III): all	2.444	2.417	0.064	2.393	2.478	34	
	(4), (−)	2.408	2.406	0.025	2.391	2.414	18	
	(5), (I)	2.578	2.584	0.030	2.546	2.603	4	
	(6), (−)	2.470	2.476	0.042	2.457	2.500	16	
Pd–Cl	(4,5), (II): all	2.419	2.416	0.065	2.382	2.463	50	
	(4), (II): all	2.404	2.407	0.058	2.342	2.438	42	
	: Pd–Cl–Pd > 85°	2.432	2.425	0.063	2.389	2.472	14	
	: Pd–Cl–Pd < 85°	2.390	2.401	0.051	2.332	2.429	28	
Ag–Cl	See BEBGEU (2.618, 2.639)							
Cd–Cl	(6,*), (−)	2.629	2.628	0.043	2.602	2.653	52	
Pr–Cl	See BAMZUK (2.805, 2.821)							
Yb–Cl	See MCPYBC (2.627, 2.647)							
Ta–Cl	(6,8), (−): all	2.513	2.510	0.049	2.477	2.553	26	
	: Ta–Cl–Ta < 70°	2.501	2.500	0.040	2.475	2.543	22	
	: Ta–Cl–Ta > 90°	2.584	2.573	0.037	2.556	2.624	4	
W–Cl	(6), (II,III,V): all	2.514	2.549	0.097	2.393	2.598	6	
Re–Cl	(6,*), (I,III,IV): all	2.456	2.426	0.060	2.399	2.515	35	30,85
	(*), (−)	2.409	2.415	0.016	2.393	2.422	12	
	(6), (−): all	2.481	2.509	0.059	2.439	2.517	23	
	: Re–Cl–Re > 83°	2.514	2.515	0.012	2.502	2.525	17	
	: Re–Cl–Re > 70°	2.385	2.391	0.026	2.359	2.405	6	
Os–Cl	(6), (−): all	2.430	2.431	0.023	2.410	2.450	4	
Ir–Cl	(6), (III): all	2.442	2.428	0.060	2.392	2.455	12	
Pt–Cl	(4,6), (−): all	2.455	2.496	0.073	2.401	2.506	12	
	(4), (−)	2.363	2.359	0.050	2.320	2.410	4	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
10.1.1.2 Chlorine (μ-Cl)—(*continued*)								134
Pt–Cl	(6), (–)	2.501	2.501	0.010	2.495	2.506	8	
Hg–Cl	(4—6), (II): all	2.757	2.728	0.122	2.686	2.780	20	
	: excluding TAMHGC	2.723	2.719	0.062	2.681	2.762	18	
U–Cl	(8), (–): all PMCPUC10	2.900	2.905	0.014	2.882	2.912	6	
10.1.1.3 Chlorine (μ_3-Cl)								
Ti–Cl	See COTTIC10 (2.557, 2.609)							
Co–Cl	See EFASCO01 (2.479)							
Cu–Cl	(4,*), (I,II): all asymmetric	2.476	2.464	0.139	2.369	2.527	24	12
Nb–Cl	See BUVCAW10 (2.524, 2.945, 2.817)							
Mo–Cl	See CIKHOT (2.484, 2.490, 2.513)							
Pd–Cl	See CEHMOR (2.520, 2.520, 2.525)							
Ag–Cl	(4), (I)	2.653	2.642	0.073	2.600	2.724	12	
Cd–Cl	(6), (II)	2.740	2.738	0.057	2.700	2.783	9	
W–Cl	See TMPHWE (2.462, 2.465, 2.476)							
Hg–Cl	See CEGNAD (2.519, 2.937, 3.115), METHGD (2.715, 2.922, 3.065)							
11.1 Arsines (AsR_3, R = any C)								137
As–C		1.943	1.943	0.021	1.931	1.955	405	
Ti–As	See CIRHUG (2.692, 2.690), PASETI (2.677)							
Cr–As	(6), (0)	2.460	2.467	0.040	2.417	2.494	4	38
Mn–As	(6), (0,I)	2.400	2.405	0.013	2.387	2.410	6	
Fe–As	(5,6,*), (0,II)	2.352	2.339	0.043	2.328	2.362	8	
Co–As	(5,6,*), (–)	2.323	2.326	0.021	2.307	2.337	16	8
Ni–As	(4—6), (–): excluding CMASNI	2.333	2.340	0.035	2.309	2.356	11	9
Cu–As	(4,*), (I)	2.367	2.369	0.016	2.362	2.380	8	
Nb–As	(8), (IV,V)	2.741	2.739	0.008	2.735	2.750	5	
Mo–As	(6,7), (II)	2.582	2.583	0.036	2.546	2.618	8	
Tc–As	All DASTCA10	2.512	2.511	0.005	2.508	2.517	4	
Ru–As	(5,6,*), (–)	2.446	2.450	0.031	2.415	2.475	12	
Rh–As	(4—6), (I,III): all	2.416	2.400	0.039	2.394	2.427	12	
	(4—6), (I)	2.400	2.399	0.015	2.392	2.409	10	
Pd–As	(4,6), (II,IV)	2.386	2.387	0.052	2.339	2.441	12	
	(4), (II)	2.372	2.376	0.046	2.334	2.401	10	
Re–As	All PASMRE	2.575	2.573	0.006	2.570	2.582	4	
Pt–As	(3—5), (0,II)	2.366	2.387	0.058	2.318	2.402	11	
11.2 Arsenic ligands (all types except AsR_3)								
V–As	See BAJZER (2.536)							
Cr–As	(6), (–): μ_3-As, μ-AsR_2, μ-AsR, σ-As_2R_2, σ-As_2R_4	2.431	2.417	0.050	2.386	2.480	23	38
Mn–As	(6), (–): μ_3-As, μ-AsR_2, *etc.*	2.375	2.319	0.126	2.247	2.508	11	30
	: short < 2.32	2.269	2.250	0.039	2.240	2.319	6	
	: long > 2.46 (μ-AsR_2)	2.502	2.508	0.029	2.476	2.525	5	
Fe–As	(4—6,*), (–): σ-As_4O_5, μ_3-AsR, μ-AsR_2, *etc.*	2.349	2.326	0.057	2.315	2.377	38	
	: μ-AsR_2, μ_3-AsR only	2.341	2.327	0.041	2.315	2.376	31	
Co–As	(4—6,*): μ-AsR_2, $(OAsR_2)_2$, As_2, *etc.*	2.316	2.308	0.050	2.270	2.368	24	
Ni–As	See CADYAH (2.262), IATCNI (2.736)							
Mo–As	(6,7,*), (–): μ-AsR_2, μ_3-As, μ-As_2, μ-As_5	2.582	2.563	0.092	2.546	2.664	30	
Ru–As	(*), (–): μ-AsR_2	2.420	2.418	0.029	2.394	2.447	6	
Rh–As	See COSTEJ (2.470, 2.490)							
Pd–As	See COWGEA (2.447, 2.478)							
W–As	See BEBREF (2.549, 2.558), BIGHAA (2.351)							
Os–As	See BAHHOH (2.481, 2.483)							
12.1 Selenium ligands (all types)								158,163
Cr–Se	See BAMCOH (2.562), BELFUT (2.453)							
Mn–Se	See BUJBIR (2.356, 2.358, 2.486, 2.481)							
Fe–Se	(–), (–): μ- and μ_3-Se; μ-SeR	2.393	2.399	0.038	2.359	2.424	13	
Ni–Se	(4,6), (II,IV): chelating Se–R *etc.*, excluding TMENSN (2.678)	2.351	2.357	0.040	2.319	2.387	12	
Cu–Se	See APROCU (3.109)							
Zr–Se	See COMYUY (2.639, 2.670)							
Mo–Se	See TFMESM (2.491)							
Rh–Se	All CEGCOG	2.457	2.457	0.002	2.455	2.460	4	
Ag–Se	See CONSUT (2.581, 2.616, 2.711)							
W–Se	See COLFEO (2.635, 2.637), SNSCRB (2.735)							
Re–Se	See BIZZAL (2.572, 2.585)							
Os–Se	See SECPOS (2.541, 2.553)							
Ir–Se	See BOHDUX (2.529, 2.539)							
Pt–Se	See BESSAT (2.443, 2.461), BIHSAM (2.400, 2.376), BSEMEP (2.598, 2.590)							
Hg–Se	See BEGPUY (2.624, 2.615), CICLOP (2.637), DPSEHG01 (2.653, 2.918), MSEUHG (2.477)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
13.1.1.1 Bromine (terminal)								
Cr–Br	See TBCBFE (2.577)							
Mn–Br	(−), (−): all	2.588	2.548	0.094	2.534	2.685	8	
	(6), not (II)	2.541	2.539	0.010	2.534	2.551	4	
Fe–Br	See BAVHEL (2.494), BPEPFE (2.368), BTPPFE (2.348)							
Co–Br	(−), (−): all	2.416	2.390	0.086	2.383	2.401	14	
	(4), (−)	2.384	2.388	0.017	2.381	2.390	7	
	(6), not (II)	2.389	2.394	0.015	2.374	2.399	5	
Ni–Br	(−), (−): all	2.410	2.372	0.098	2.339	2.458	47	
	(4), not (I)	2.341	2.343	0.029	2.309	2.368	23	
	(5), (−): all	2.428	2.391	0.101	2.353	2.458	12	
	: short < 2.5	2.389	2.380	0.044	2.348	2.427	10	
	(6), (−)	2.554	2.548	0.028	2.536	2.572	9	
Cu–Br	(−), (−): all	2.412	2.400	0.109	2.357	2.428	60	12
	(3), (I)	2.298	2.284	0.028	2.280	2.325	6	
	(4), (−)	2.393	2.387	0.042	2.356	2.425	22	
	(5), (−): all	2.465	2.419	0.121	2.392	2.480	29	
	: short < 2.46	2.407	2.401	0.023	2.390	2.423	22	
	: long > 2.50	2.648	2.598	0.124	2.547	2.732	7	
Zn–Br	(−), (−): all	2.390	2.395	0.029	2.360	2.417	17	
	(4), (−)	2.386	2.393	0.028	2.357	2.399	15	
Mo–Br	(−), (−): all	2.616	2.595	0.071	2.568	2.654	32	
	(6), (−)	2.603	2.587	0.042	2.574	2.625	13	85
	(7), (−)	2.651	2.655	0.049	2.625	2.676	9	
Tc–Br	See CAKGIE (2.440)							
Ru–Br	(6), (II): all	2.521	2.538	0.035	2.477	2.547	6	
Rh–Br	(−), (−): all	2.530	2.526	0.039	2.500	2.564	13	
	(6), (−)	2.536	2.529	0.033	2.521	2.562	10	
Pd–Br	(4), (−): all	2.458	2.434	0.061	2.412	2.538	11	
	(4), not (I): all	2.450	2.433	0.057	2.410	2.469	10	
	: excluding two > 2.53	2.424	2.430	0.018	2.406	2.439	8	
Ag–Br	See BTCMAN (2.450)							
Cd–Br	(−), (−): all	2.611	2.582	0.064	2.569	2.659	6	
	(4), (−)	2.588	2.576	0.032	2.567	2.622	4	
Ta–Br	See BOBXOF (2.604)							
W–Br	(6,7), (−): all	2.619	2.611	0.042	2.590	2.644	8	
Re–Br	(5—7), (−): all	2.573	2.603	0.065	2.493	2.627	15	
	(6,7), (−)	2.606	2.613	0.039	2.563	2.629	11	
Os–Br	See BRFOSA10 (2.627), CIRJAO (2.558), COVVUE (2.545)							
Ir–Br	(5,6), (−): all	2.580	2.593	0.054	2.518	2.633	8	
Pt–Br	(−), (−): all	2.460	2.437	0.054	2.421	2.503	22	
	(4), (II): all	2.438	2.426	0.040	2.417	2.446	14	
	: excluding two > 2.5	2.424	2.423	0.018	2.414	2.434	12	
Au–Br	(−), (−): all	2.413	2.407	0.028	2.387	2.435	9	
	(3,4), (−)	2.417	2.411	0.028	2.390	2.438	8	
Hg–Br	(−), (−): all	2.539	2.519	0.089	2.499	2.549	14	
	(4), (−): all	2.555	2.529	0.089	2.508	2.560	11	
	: excluding two > 2.70	2.517	2.509	0.028	2.493	2.540	9	
U–Br	(6), (−): all	2.797	2.800	0.030	2.770	2.828	13	
13.1.1.2 Bromine (μ-Br)								134
Ti–Br	See BMCPTI (2.705, 2.722)							
Cr–Br	See BIWBEO (2.575, 2.607)							
Mn–Br	See TMAMNB01 (2.698, 2.711)							
Fe–Br	See BVINBF (2.443, 2.463)							
Ni–Br	(5), (II)	2.494	2.483	0.047	2.460	2.519	6	9
Cu–Br	(−), (−): all	2.494	2.471	0.061	2.451	2.548	20	12
	(3,4), (I)	2.483	2.469	0.057	2.451	2.487	12	
Mo–Br	(6), (−)	2.667	2.641	0.047	2.636	2.724	6	
Tc–Br	See CAWBAD (2.843)							
Ru–Br	(−), (−)	2.572	2.576	0.031	2.537	2.599	6	85
Rh–Br	(6), (III)	2.594	2.582	0.029	2.573	2.630	6	
Cd–Br	(−), (−)	2.776	2.753	0.055	2.730	2.843	6	
Re–Br	(−), (−)	2.651	2.659	0.027	2.635	2.670	20	
Ir–Br	(6), (III): all PMCBRI	2.570	2.570	0.006	2.565	2.576	4	
Pt–Br	(6), (IV): all BSEMEP	2.629	2.630	0.007	2.622	2.635	4	
Hg–Br	(4), (II): all $[Hg_2Br_6]^{2-}$	2.762	2.754	0.047	2.720	2.810	4	
13.1.1.3 Bromine (μ_3-Br)								
Cu–Br	(4,*), (I): all	2.543	2.544	0.066	2.491	2.599	13	12
Cd–Br	See CAHGOH (2.925, 2.971, 3.005)							

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
14.1 Tellurium (all ligand types)								158,163,164
Cr–Te	See COSSAE (2.801, 2.813)							
Mn–Te	(−), (−): μ- and μ_3-Te	2.486	2.474	0.027	2.464	2.515	5	
Fe–Te	(−), (−): μ-TeR, μ_3-Te	2.560	2.551	0.056	2.538	2.576	13	
Mo–Te	See HTEMOA (2.791)							
Pt–Te	See CEXNAU (2.575)							
Hg–Te	(−), (−): Ph_2Te, PhTe	2.732	2.717	0.055	2.687	2.786	5	
15.1.1.1 Iodine (terminal)								
V–I	See BIVGAO (2.653)							
Cr–I	See CPAINC (2.669), CPCBCR (2.781)							
Mn–I	See ICPNMN (2.645)							
Fe–I	(−), (−): all	2.593	2.599	0.050	2.548	2.632	10	
	(6), (II)	2.623	2.624	0.027	2.599	2.645	5	
Co–I	(−), (−): all	2.640	2.611	0.094	2.563	2.743	8	
	Not (6), (II)	2.593	2.575	0.042	2.559	2.644	6	
Ni–I	(−), (−): all	2.673	2.626	0.150	2.545	2.804	22	
	(4), (−)	2.514	2.516	0.026	2.489	2.538	5	
	(5), (II): all	2.706	2.658	0.151	2.605	2.834	11	30
	: short < 2.67	2.608	2.609	0.047	2.550	2.658	7	
	: long > 2.83	2.877	2.848	0.099	2.804	2.980	4	
	(6), (II)	2.810	2.821	0.087	2.724	2.885	4	
Cu–I	(−), (−): all	2.594	2.563	0.077	2.528	2.664	12	
	(3), (I): not CENFAC01	2.534	2.531	0.026	2.511	2.561	6	12
	(5), (II)	2.682	2.674	0.043	2.647	2.725	4	
Zn–I	(−), (−): all	2.574	2.561	0.036	2.549	2.599	12	
	(4), (−)	2.564	2.556	0.024	2.547	2.578	10	
Zr–I	See COPVIM (2.897), COPVOS (2.869)							
Mo–I	(−), (−): all	2.867	2.848	0.135	2.777	2.878	35	30
	(6), (−)	2.797	2.773	0.065	2.758	2.866	12	85
	(7), (−)	2.855	2.858	0.027	2.823	2.873	11	
	(8), (−)	2.841	2.848	0.039	2.809	2.870	5	
Ru–I	(6,7), (II,IV): all	2.744	2.743	0.028	2.719	2.770	6	
	(6), (II)	2.742	2.732	0.031	2.716	2.774	5	
Rh–I	(−), (−): all	2.715	2.701	0.071	2.663	2.766	12	
Pd–I	(−), (−): all	2.624	2.602	0.040	2.593	2.658	15	
	(4), not (I)	2.612	2.601	0.027	2.593	2.641	13	
Ag–I	See BEVMAQ (2.828)							
Cd–I	(−), (−): all	2.750	2.714	0.082	2.705	2.794	12	30
	(4), (−)	2.704	2.708	0.014	2.691	2.714	8	
Yb–I	See BAWKUF (3.027)							
W–I	(6,7), (−): all	2.840	2.869	0.063	2.802	2.878	7	
	(7), (II)	2.864	2.876	0.036	2.836	2.888	5	
Re–I	(4−6), (−): all	2.718	2.764	0.079	2.625	2.786	13	30
	(5), (−)	2.630	2.621	0.020	2.617	2.647	5	
	(6), (−)	2.784	2.772	0.021	2.765	2.806	7	
Os–I	(−), (−): all	2.774	2.760	0.055	2.733	2.817	6	
	(6), (II)	2.758	2.760	0.035	2.724	2.790	4	
Ir–I	(−), (−): all	2.729	2.691	0.089	2.681	2.752	10	86
	(6), (III)	2.685	2.687	0.008	2.679	2.691	5	
Pt–I	(−), (−): all	2.658	2.651	0.082	2.606	2.668	28	86
	(4), (II)	2.622	2.604	0.050	2.581	2.666	11	
	(6), (IV): excluding COTDOE (2.843)	2.652	2.654	0.020	2.647	2.667	15	
Au–I	See BESBEG (2.536, 2.551), CIYMIG (2.857), IFPPAU (2.599)							
Hg–I	(−), (−): all	2.702	2.691	0.059	2.669	2.743	20	
	(4), (−)	2.708	2.695	0.050	2.674	2.743	16	
15.1.1.2 Iodine (μ-I)								134
Mn–I	(6), (I): all COGSIA	2.719	2.725	0.014	2.705	2.726	4	
Fe–I	See PCRNIB (2.591, 2.605)							
Ni–I	See EAPZNI (2.755, 2.760)							
Cu–I	(−), (−): all	2.675	2.660	0.107	2.602	2.703	28	12
	(3,4), (−): all	2.647	2.660	0.051	2.591	2.688	25	
	(3), (−)	2.578	2.577	0.012	2.567	2.589	4	
	(4), (−)	2.661	2.660	0.044	2.642	2.692	21	
Mo–I		2.830	2.818	0.056	2.797	2.860	10	
Ru–I	See IPHPRU (2.685, 2.711)							
Rh–I	(6), (III)	2.730	2.734	0.014	2.715	2.741	4	
Pd–I	See CODJAG (2.665, 2.723)							
Ag–I	(4), (I)	2.907	2.914	0.019	2.887	2.918	4	
W–I	See BURFOJ (2.831, 2.862)							
Re–I	(−), (I)	2.817	2.816	0.015	2.804	2.830	6	

Table 3 (*continued*)

Bond	Substructure (Co-ordination number, oxidation state, comment)	*d*	*m*	σ	q_l	q_u	*n*	Note
15.1.1.2 Iodine (μ-I)—(*continued*)								134
Ir–I	(6), (III)	2.710	2.712	0.005	2.706	2.713	6	
Pt–I	(4), (II): all CODHIM	2.559	2.560	0.003	2.556	2.561	4	85
Hg–I	(4), (II)	2.927	2.931	0.039	2.891	2.957	6	
15.1.1.3 Iodine (μ_3-I)								
Cu–I	(−), (I): all	2.690	2.694	0.052	2.663	2.726	95	12
Ag–I	(−), (I): all	2.905	2.886	0.074	2.841	2.976	17	

Appendix 1: Footnotes and References to Tables 2 and 3

* Cluster complexes, no co-ordination number assigned.
† See Figure 3.

1 T. J. Marks and R. D. Ernst, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 3, pp. 173—270.
2 D. Cozak and M. Melník, *Coord. Chem. Rev.*, 1986, **74**, 53.
3 M. Melník and D. Cozak, *Rev. Inorg. Chem.*, 1986, **8**, 221.
4 C. E. Holloway and M. Melník, *Rev. Inorg. Chem.*, 1985, **7**, 75.
5 C. E. Holloway and M. Melník, *Rev. Inorg. Chem.*, 1986, **8**, 287.
6 C. E. Holloway and M. Melník, *J. Organomet. Chem.*, 1986, **304**, 41.
7 L. F. Larkworthy, K. B. Nolan, and P. O'Brien, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 3, pp. 699—969.
8 D. A. Buckingham and C. R. Clark, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 4, pp. 635—900.
9 L. Sacconi, F. Mani, and A. Bencini, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 5, pp. 1—347.
10 K. Nag and A. Chakravorty, *Coord. Chem. Rev.*, 1980, **33**, 87.
11 B. J. Hathaway, *Struct. Bonding (Berlin)*, 1984, **57**, 55.
12 B. J. Hathaway, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 5, pp. 553—774.
13 C. E. Holloway, I. M. Walker, and M. Melník, *Rev. Inorg. Chem.*, 1986, **8**, 170.
14 C. E. Holloway and M. Melník, *Rev. Inorg. Chem.*, 1985, **7**, 161.
15 R. Davis, L. A. P. Kane-Maguire, and S. W. Kirtley, 'Comprehensive Organometallic Chemistry, Pergamon, London, 1982, vol. 3, pp. 1079—1148.
16 M. Melník and P. Sharrock, *Coord. Chem. Rev.*, 1985, **65**, 49.
17 G. Bandolini, U. Mazzi, E. Roncari, and E. Deutsch, *Coord. Chem. Rev.*, 1982, **44**, 191.
18 M. Melník and J. E. Van Lier, *Coord. Chem. Rev.*, 1986, **77**, 275.
19 D. G. Tuck, *Rev. Inorg. Chem.*, 1979, **1**, 209.
20 F. A. Hart, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 3, pp. 1059—1127.
21 K. N. Raymonds and C. W. Eigenbrot, jun., *Acc. Chem. Res.*, 1980, **13**, 276.
22 J-C. G. Bünzli and D. Wessner, *Coord. Chem. Rev.*, 1984, **60**, 191.
23 C. E. Holloway and M. Melník, *Rev. Inorg. Chem.*, 1985, **7**, 1.
24 S. W. Kirtley, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 3, pp. 1255—1319.
25 M. Melník and R. V. Parrish, *Coord. Chem. Rev.*, 1986, **70**, 157.
26 K. Brodersen and H. U. Hummel, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 5, pp. 1047—1097.
27 R. G. Teller and R. Bau, *Struct. Bonding (Berlin)*, 1981, **44**, 1.
28 K. B. Gilbert, S. K. Boocock, and S. G. Shore, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 6, pp. 879—945.
29 R. N. Grimes, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 6, pp. 459—542.
30 Distribution is bimodal.
31 G. E. Herberich, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 1, pp. 381—410.
32 W. Siebert, *Adv. Organomet. Chem.*, 1980, **18**, 301.
33 G. E. Herberich and H. Ohst, *Adv. Organomet. Chem.*, 1985, **25**, 199.
34 J. S. Bradley, *Adv. Organomet. Chem.*, 1982, **22**, 1.
35 M. Tachikawa and E. L. Muetterties, *Prog. Inorg. Chem.*, 1981, **28**, 203.
36 M. A. Gallop and W. R. Roper, *Adv. Organomet. Chem.*, 1985, **25**, 121.
37 H. P. Kim and R. J. Angelici, *Adv. Organomet. Chem.*, 1987, **27**, 51.
38 S. W. Kirtley, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 3, pp. 783—951.
39 J. Holton, M. F. Lappert, R. Pearce, and P. I. W. Yarrow, *Chem. Rev.*, 1983, **83**, 135.
40 M. I. Bruce and A. G. Swincer, *Adv. Organomet. Chem.*, 1982, **22**, 59.
41 F. R. Hartley, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 6, pp. 471—762.
42 E. Sappa, A. Tiripicchio, and P. Braunstein, *Coord. Chem. Rev.*, 1985, **65**, 219.
43 Distances for M–C–N ⩾ 173° only.
44 Distances for ligands *trans* to oxo excluded.
45 Y. Yamamoto, *Coord. Chem. Rev.*, 1980, **32**, 193.
46 E. Singleton and H. E. Oosthuizen, *Adv. Organomet. Chem.*, 1982, **22**, 209.
47 P. M. Maitlis, P. Espinet, and M. J. H. Russell, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 6, pp. 279—349.
48 Distances for M–C–O ⩾ 173° only.
49 D. J. Sikova, D. W. Macomber, and M. D. Rausch, *Adv. Organomet. Chem.*, 1985, **25**, 317.
50 M. D. Johnson, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 4, pp. 331—376.
51 P. W. Jolly, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 6, pp. 15—36.
52 R. Colton and M. J. Mcormick, *Coord. Chem. Rev.*, 1980, **31**, 1.
53 W. A. Herrmann, *Adv. Orgamomet. Chem.*, 1982, **20**, 159.
54 J. A. Labinger, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 3, pp. 705—782.
55 U. Schubert, *Coord. Chem. Rev.*, 1984, **55**, 261.
56 P. W. Jolly, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 6, pp. 37—100.
57 G. K. Anderson, *Adv. Organomet. Chem.*, 1982, **20**, 39.
58 D. M. P. Mingos, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 3, pp. 1—88.
59 S. J. Bryan, P. G. Huggett, K. Wade, J. A. Daniels, and J. R. Jennings, *Coord. Chem. Rev.*, 1982, **44**, 149.
60 A. J. Deeming, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 4, pp. 377—512.
61 P. W. Jolly, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 6, pp. 101—143.
62 I. Omae, *Coord. Chem. Rev.*, 1983, **51**, 1.
63 Distribution is positively skewed.
64 E. Sappa, A. Tiripicchio, and P. Braunstein, *Chem. Rev.*, 1983, **83**, 203.
65 J. L. Templeton, P. B. Winston, and B. C. Ward, *J. Am. Chem. Soc.*, 1981, **103**, 7713—7721.
66 P. W. Jolly, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 6, pp. 147—182.
67 P. W. Jolly, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 6, pp. 183—187.
68 H. Yasuda, K. Tatsumi, and A. Nakamura, *Acc. Chem. Res.*, 1985, **18**, 120.

69 G. Erker, C. Krüger, and G. Müller, *Adv. Organomet. Chem.*, 1984, **24**, 1.
70 P. W. Jolly, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 6, pp. 189—228.
71 D. J. Cardin, M. F. Lappert, C. L. Raston, and P. I. Riley, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 3, pp. 559—633.
72 R. D. Ernst, *Struct. Bonding (Berlin)*, 1984, **57**, 1; *Acc. Chem. Res.*, 1985, **18**, 56.
73 P. Powell, *Adv. Organomet. Chem.*, 1986, **26**, 125.
74 E. L. Muetterties, J. R. Bleeke, E. J. Wucherer, and T. A. Albright, *Chem. Rev.*, 1982, **82**, 499.
75 P. W. Jolly, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 6, pp. 229—231.
76 D. J. Gulliver and W. Levason, *Coord. Chem. Rev.*, 1982, **46**, 1.
77 E. I. Steifel, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 3, pp. 1375—1420.
78 W. L. Gladfelter, *Adv. Organomet. Chem.*, 1984, **24**, 41.
79 W. A. Nugent and B. L. Haymore, *Coord. Chem. Rev.*, 1980, **31**, 123.
80 B. F. G. Johnson, B. L. Haymore, and J. R. Dilworth, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 2, pp. 99—159.
81 Distribution may be affected by unresolved *trans* influence effects.
82 Distances for ligands in the axial site in $M_2(\mu\text{-}O_2CR)_4$ adducts only.[83]
83 F. H. Jardine, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 4, pp. 901—1096.
84 K. Vrieze and G. Van Koten, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 2, pp. 189—244.
85 Distances for ligand in the axial site in $M_2(\mu\text{-}O_2CR)_4$ adducts excluded.[83]
86 Distribution is positively skewed.
87 Unresolved metal oxidation state effects present in this distribution.
88 P. Pelikan and R. Boča, *Coord. Chem. Rev.*, 1984, **55**, 55.
89 G. J. Leigh and R. L. Richards, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 3, pp. 1265—1299.
90 K. A. Connor and R. A. Walton, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 4, pp. 125—213.
91 Distribution is negatively skewed.
92 Distribution may be distorted by unresolved bond angle dependence within ligand.
93 H. W. Roesky and K. K. Pandey, *Adv. Inorg. Chem., Radiochem.*, 1983, **26**, 337.
94 M. H. Chisholm and I. P. Rothwell, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 2, pp. 170—176.
95 M. Calligaris and L. Randaccio, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 2, pp. 715—738.
96 Distribution may be distorted by unresolved metal spin state effects.
97 B. Chiswell, E. D. Mackenzie, and L. F. Lindoy, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 4, pp. 1—122.
98 T. Mashiko and D. Dolphin, 'Comprehensive Coordination Chemistry', Pergamon, London, 1987, vol. 2, pp. 813–898.
99 S. M. Nelson, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 4, pp. 217—276.
100 Distribution includes distances for ligands in axial site in $M_2(O_2CR)_4$ adducts.[83]
101 D. S. Moore and S. D. Robinson, *Adv. Inorg. Chem., Radiochem.*, 1986, **30**, 1.
102 R. W. Kemmit and D. R. Russell, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 5, pp. 1—276.
103 M. A. Hitchiman and G. L. Rowbottom, *Coord. Chem. Rev.*, 1982, **42**, 55.
104 B. J. Hathaway, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 2, pp. 413—434.
105 D. A. House, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 2, pp. 23—72.
106 F. Bottomley and L. Sutin, *Adv. Organomet. Chem.*, 1988, **28**, 339.
107 L. V. Boas and J. C. Pessoa, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 3, pp. 453—583.
108 C. D. Garner and J. M. Charnock, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 3, pp. 1329—1374.
109 Distribution may be affected by unresolved ligand substituent effects.
110 W. P. Griffith, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 4, pp. 519—633.
111 M. Melník, *Coord. Chem. Rev.*, 1982, **42**, 259.
112 T. Theophanides and P. D. Harvey, *Coord. Chem. Rev.*, 1987, **76**, 237.
113 G. B. Deacon and R. J. Phillips, *Coord. Chem. Rev.*, 1980, **33**, 227.
114 M. Melník, *Coord. Chem. Rev.*, 1981, **36**, 1.
115 E. Boyar and S. D. Robinson, *Coord. Chem. Rev.*, 1983, **50**, 109.
116 Distribution may be affected by unresolved metal co-ordination number effects.
117 C. G. Pierpont and R. M. Buchanan, *Coord. Chem. Rev.*, 1981, **38**, 45.
118 Distances for monoanionic ligand.
119 Distances for neutral ligand.
120 Distances for dianionic ligand.
121 D. A. Palmer and R. Van Eldik, *Chem. Rev.*, 1983, **83**, 651.
122 U. Casellato, P. A. Vigato, and M. Vidali, *Coord. Chem. Rev.*, 1981, **36**, 183.
123 R. Boca, *Coord. Chem. Rev.*, 1983, **50**, 1.
124 M. H. Gubelmann and A. F. Williams, *Struct. Bonding (Berlin)*, 1983, **55**, 1.
125 H. A. O. Hill and D. G. Tew, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 2, pp. 315—333.
126 C. A. McAuliffe and D. S. Barratt, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 3, 323—361.
127 J. A. Davies, *Adv. Inorg. Chem., Radiochem.*, 1981, **24**, 115.
128 N. M. N. Gowda, S. B. Naikar, and G. K. N. Reddy, *Adv. Inorg. Chem., Radiochem.*, 1984, **28**, 255.
129 Distances for ligands *trans* to oxo only.
130 B. Chiswell, E. D. Mackenzie, and L. F. Lindoy, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 4, pp. 1—112.
131 Distances for cluster complexes only.
132 J. B. Farmer, *Adv. Inorg. Chem., Radiochem.*, 1982, **25**, 187.
133 R. C. Fay, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 3, pp. 363—451.
134 A. J. Edwards, 'Comprehensive Coordination Chemistry,' Pergamon, London, vol. 2, pp. 675—688.
135 P. G. Harrison and T. Kikabbai, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 2, pp. 15—21; K. M. McKay and B. K. Nicholson, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1982, vol. 6, pp. 1043—1114; B. J. Aylett, *Adv. Inorg. Chem., Radiochem.*, 1982, **25**, 1.
136 G. Huttner and K. Evertz, *Acc. Chem. Res.*, 1986, **19**, 406.
137 C. A. McAuliffe, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 2, pp. 989—1066.
138 A. H. Cowley and N. C. Norman, *Prog. Inorg. Chem.*, 1986, **34**, 1.
139 Distances for structures in which the three P–C bond lengths vary by <0.1 Å only.
140 Distances excluded for ligands in the axial site of an octahedral complex containing a planar N_4 or N_2O_2 macrocyclic ligand (see 141).
141 P. D. Smith, B. R. James, and D. H. Dolphin, *Coord. Chem. Rev.*, 1981, **39**, 31.
142 D. M. Roundhill, 'Comprhensive Coordination Chemistry,' Pergamon, London, 1987, vol. 5, pp. 351—531.
143 As for footnote 139, but variation <0.07 Å only.
144 R. J. Puddephatt, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 5, pp. 861—923.
145 R. J. Lancashire, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 5, pp. 775—859.
146 As for footnote 139, but variation <0.15 Å only.
147 Distances for ligands *trans* to ≡CR excluded.
148 J. F. Nixon, *Adv. Inorg. Chem., Radiochem.*, 1985, **29**, 41.
149 As for footnote 139, but variation <0.1 Å in both P–O and O–C lengths.
150 A. Müller and E. Diemann, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 2, pp. 515—550.
151 Distances excluded for cases where the M–L lengths within a bridge differ by >0.1 Å.
152 W. Levason and M. D. Spicer, *Coord. Chem. Rev.*, 1987, **76**, 45.
153 Distances for ligands *trans* to =NR excluded.
154 G. Winter, *Rev. Inorg. Chem.*, 1980, **2**, 253.
155 R. Eisenberg, *Prog. Inorg. Chem.*, 1970, **12**, 295.
156 A. Müller, W. Jaegermann, and J. H. Enemark, *Coord. Chem. Rev.*, 1982, **46**, 245.
157 A. Müller and E. Diemann, *Adv. Inorg. Chem., Radiochem.*, 1987, **31**, 89.

158 S. G. Murray and F. R. Hartley, *Chem. Rev.*, 1981, **81**, 365.
159 Z. Dori, *Prog. Inorg. Chem.*, 1981, **28**, 239.
160 R. R. Ryan, G. J. Kubas, D. C. Moody, and P. G. Eller, *Struct. Bonding (Berlin)*, 1981, **46**, 47.
161 Distances for ligands *trans* to hydride excluded.
162 Distances for ligands *trans* to ≡N excluded.
163 F. J. Berry, 'Comprehensive Coordination Chemistry,' Pergamon, London, 1987, vol. 2, pp. 661—674.
164 H. J. Gysling, *Coord. Chem. Rev.*, 1982, **42**, 133.

Appendix 2: Short-form References to Individual CSD Entries Cited in Table 3

ABPENC *Inorg. Chem.*, 1977, **16**, 177.
ABTCMO *Inorg. Chem.*, 1978, **17**, 1981.
ABZAMN *Zh. Strukt. Khim.*, 1978, **19**, 1120.
ACACSC *Inorg. Chem.*, 1973, **12**, 927.
ACANRE *J. Organomet. Chem.*, 1977, **140**, 309.
ACAQGD *J. Chem. Soc., Dalton Trans.*, 1980, 454.
ACATEN *Finn. Chem. Lett.*, 1977, 246.
ACBZNM *Bull. Chem. Soc. Jpn.*, 1976, **49**, 595.
ACCDSC10 *Dokl. Akad. Nauk SSSR.*, 1980, **250**, 852.
ACETCR *Inorg. Chem.*, 1978, **17**, 2004.
ACHPHG *J. Chem. Res.*, 1979, **360**, 4101.
ACMPRU *J. Chem. Soc., Dalton Trans.*, 1976, 2184.
ACMRHD *J. Chem. Soc., Dalton Trans.*, 1979, 409.
ACNCOB20 *J. Am. Chem. Soc.*, 1983, **105**, 4662.
ACNCVO *Acta Crystallogr., Sect. B*, 1975, **31**, 1833.
ACNTCC *J. Am. Chem. Soc.*, 1978, **100**, 5756.
ACOXRH *Latv. PSR Zinat. Akad. Vestis, Kim. Ser.*, 1980, 48.
ACPCRB *Inorg. Chem.*, 1980, **19**, 328.
ACPMNA *J. Organomet. Chem.*, 1981, **204**, 79.
ACSNRU *J. Chem. Soc., Dalton Trans.*, 1978, 76.
ACTFIR *J. Chem. Soc., Dalton Trans.*, 1975, 2556.
ACTHTA *Inorg. Chem.*, 1980, **19**, 2354.
ACTPEN *J. Am. Chem. Soc.*, 1974, **96**, 4820.
ACTPRE *J. Organomet. Chem.*, 1976, **112**, 297.
ACURLB *Dokl. Akad. Nauk SSSR*, 1979, **248**, 1337.
ACYPCI *Inorg. Chem.*, 1977, **16**, 1593.
ADAGPC *Inorg. Chem.*, 1977, **16**, 2469.
ADASMO *Inorg. Chem.*, 1980, **19**, 777.
ADBPPD *Inorg. Chem.*, 1979, **18**, 176.
ADMEHH *Can. J. Chem.*, 1981, **59**, 1311.
ADOOSA *J. Am. Chem. Soc.*, 1979, **101**, 7265.
ADOOSB *J. Am. Chem. Soc.*, 1979, **101**, 7265.
AENCUS *Cryst. Struct. Commun.*, 1978, **7**, 565.
AFMZRH *J. Chem. Soc., Dalton Trans.*, 1979, 371.
AFNICD *Koord. Khim.*, 1981, **7**, 461.
AFXPCM *J. Chem. Soc., Dalton Trans.*, 1977, 1966.
AGENPC10 *Acta Chem. Scand., Ser. A*, 1978, **32**, 555.
AGIMHN01 *Acta Chem. Scand.*, 1971, **25**, 1758.
AGLPAU *Cryst. Struct. Commun.*, 1980, **9**, 679.
AGSURE10 *Inorg. Chem.*, 1968, **7**, 1351.
ALANIC *J. Am. Chem. Soc.*, 1972, **94**, 1858.
ALBCIW *Cryst. Struct. Commun.*, 1977, **6**, 253.
ALCPPV *J. Organomet. Chem.*, 1976, **121**, 189.
ALETPD *J. Organomet. Chem.*, 1974, **65**, 427.
AMAQDY *Koord. Khim.*, 1981, **7**, 445.
AMETZN *Acta Crystallogr., Sect. B*, 1978, **34**, 2859.
AMMPMN *Acta Crystallogr., Sect. B*, 1977, **33**, 2648.
AMPMNC *Acta Crystallogr., Sect. B*, 1977, **33**, 2763.
AMXPPD *Acta Crystallogr., Sect. B*, 1979, **35**, 2411.
ANIDED10 *Inorg. Chem.*, 1976, **15**, 1853.
APDPZC *Acta Crystallogr., Sect. B*, 1974, **30**, 1370.
APIMCO *Koord. Khim.*, 1979, **5**, 762.
APIMNI *Koord. Khim.*, 1979, **5**, 762.
APROCU *Finn. Chem. Lett.*, 1978, 71.
APRPIR *Cryst. Struct. Commun.*, 1974, **3**, 721.
APXLAP *J. Chem. Soc., Dalton Trans.*, 1980, 376.
AQACAL *Inorg. Chem.*, 1968, **7**, 2295.
AQNCZN *Koord. Khim.*, 1979, **5**, 1889.
AQOURI *Inorg. Chem.*, 1980, **19**, 1067.
AQOXCU *Acta Crystallogr., Sect. B*, 1980, **36**, 1650.
AQSUMN *Acta Crystallogr., Sect. B*, 1981, **37**, 1214.
ASCETU *Inorg. Chem.*, 1973, **12**, 2140.
ASMETE *Inorg. Chem.*, 1981, **20**, 1617.
ATCTPR *Z. Anorg. Allg. Chem.*, 1979, **456**, 163.
AUDETC *Cryst. Struct. Commun.*, 1973, **2**, 81.
AXEXAC *Inorg. Chem.*, 1979, **18**, 3015.
AZBCTI10 *Gazz. Chim. Ital.*, 1980, **110**, 423.
AZBRHA10 *J. Chem. Soc., Dalton Trans.*, 1972, 2138.
AZCPTI *Acta Crystallogr., Sect. B*, 1977, **33**, 578.
AZENPD10 *J. Chem. Soc., Dalton Trans.*, 1976, 725.
AZMLMN *Chem. Ber.*, 1981, **114**, 276.
AZNPYD *Acta Crystallogr., Sect. B*, 1974, **30**, 628.
AZPPBW10 *J. Chem. Soc., Dalton Trans.*, 1980, 1150.
AZTLAW *Gazz. Chim. Ital.*, 1978, **108**, 627.
BABFOZ *Acta Crystallogr., Sect. B*, 1981, **37**, 1656.
BABNAT *Zh. Strukt. Khim.*, 1981, **22**, 113—3.
BABTUT *Inorg. Chem.*, 1981, **20**, 1545.
BABWAC *Inorg. Chem.*, 1981, **20**, 2023.
BACREC10 *Acta Crystallogr., Sect. B*, 1982, **38**, 1738.
BACVOQ10 *Acta Crystallogr., Sect. B*, 1982, **38**, 2047.
BAGBUG *J. Organomet. Chem.*, 1981, **206**, C33.
BAGWAH *J. Chem. Soc., Dalton Trans.*, 1981, 1798.
BAHHOH *J. Chem. Soc., Dalton Trans.*, 1981, 1879.
BAHPEF *Nouv. J. Chim.*, 1981, **5**, 423.
BAHVAH *J. Chem. Soc., Dalton Trans.*, 1981, 1997.
BAJZAN *J. Organomet. Chem.*, 1981, **220**, 125.
BAJZER *J. Organomet. Chem.*, 1981, **220**, 45.
BAKDOG *J. Am. Chem. Soc.*, 1981, **103**, 5747.
BAKDUM *J. Am. Chem. Soc.*, 1981, **103**, 5747.
BAKPUY *Proc. Natl. Sci. Counc. B, ROC*, 1981. **5**, 139.
BALJIH *J. Am. Chem. Soc.*, 1981, **103**, 1927.
BALWUG *Chem. Ber.*, 1981, **114**, 2754.
BALZUJ *Acta Crystallogr., Sect. B*, 1981, **37**, 2062.
BAMCIB10 *J. Am. Chem. Soc.*, 1984, **106**, 2328.
BAMCOH *Chem. Ber.*, 1981, **114**, 3220.
BAMDOI10 *Nouv. J. Chim.*, 1983, **7**, 545.
BAMHUS *Inorg. Chem.*, 1981, **20**, 2872.
BAMTAK10 *Inorg. Chem.*, 1984, **23**, 2303.
BAMVUG *Inorg. Chem.*, 1981, **20**, 2869.
BAMZUK *J. Chem. Soc., Chem. Commun.*, 1981, 1190.
BANDAV *Zh. Neorg. Khim.*, 1981, **26**, 718.
BANGIG10 *Inorg. Chem.*, 1982, **21**, 3741.
BANVUH10 *J. Am. Chem. Soc.*, 1984, **106**, 2041.
BAPHAB *Inorg. Chem.*, 1981, **20**, 2390.
BAPKEI *Inorg. Chem.*, 1981, **20**, 2372.
BAPPIR *Inorg. Chem.*, 1981, **20**, 2386.
BASLIQ10 *Inorg. Chem.*, 1984, **23**, 2823.
BASMOX *J. Am. Chem. Soc.*, 1981, **103**, 4255.
BASSAP *Z. Anorg. Allg. Chem.*, 1981, **479**, 113.
BATLPT10 *J. Chem. Soc. A*, 1970, 1873.
BATNIT *J. Chem. Soc., Dalton Trans.*, 1981, 2321.
BATPER *J. Chem. Soc., Dalton Trans.*, 1981, 2471.
BATZIF *Can. J. Chem.*, 1981,**59**, 2391.
BAVHEL *Cryst. Struct. Commun.*, 1981, **10**, 1523.
BAVJOX10 *J. Am. Chem. Soc.*, 1983, **105**, 4671.
BAVKAK *Cryst. Struct. Commun.*, 1981, **10**, 1259.
BAVKIS *Inorg. Chem.*, 1981, **20**, 3819.
BAVLAL11 *Z. Naturforsch., Teil B*, 1982, **37**, 1437.
BAVMUG *Acta Crystallogr., Sect. B*, 1981, **37**, 2223.
BAVSIA *Inorg. Chem.*, 1981, **20**, 3598.
BAWBUW01 *Inorg. Chem.*, 1981, **20**, 3571.
BAWDIM10 *Chem. Lett.*, 1981, 1501.
BAWKUF *Inorg. Chem.*, 1981, **20**, 3271.
BAWLAM *Inorg. Chem.*, 1981, **20**, 3271.
BAWLEQ *Inorg. Chem.*, 1981, **20**, 3271.
BAWRIA *Acta Crystallogr., Sect. B*, 1982, **38**, 105.
BAWTOI *J. Chem. Soc., Chem. Commun.*, 1982, 27.
BAWZUU *Cryst. Struct. Commun.*, 1981, **10**, 1227.
BAXFEL *J. Chem. Soc., Chem. Commun.*, 1982, 75.
BAXFOV *Z. Anorg. Allg. Chem.*, 1981, **482**, 113.
BAXHEN *Inorg. Chem.*, 1981, **20**, 3890.
BAXJOZ *Acta Crystallogr., Sect. B*, 1982, **38**, 96.
BAXLER *J. Organomet. Chem.*, 1981, **218**, C39.
BAYCOS *J. Chem. Soc., Chem. Commun.*, 1979, 750.
BAYDIO *Acta Crystallogr., Sect. B*, 1982, **38**, 262.

BAYJAM *Sci. Sin.*, 1981, **24**, 1111.
BCATMO *Inorg. Chem.*, 1979, **18**, 1616.
BCAZWB *J. Chem. Soc., Chem. Commun.*, 1980, 879.
BCBXMO *J. Am. Chem. Soc.*, 1978, **100**, 1727.
BCETPN *J. Am. Chem. Soc.*, 1977, **99**, 8102.
BDMFRU *J. Organomet. Chem.*, 1976, **117**, 171.
BDODFE *J. Am. Chem. Soc.*, 1975, **97**, 5739.
BDTCBR *J. Am. Chem. Soc.*, 1973, **95**, 774.
BEAMRH *Inorg. Chem.*, 1979, **18**, 129.
BEBGEU *J. Chem. Soc., Dalton Trans.*, 1982, 207.
BEBREF *Z. Naturforsch., Teil B*, 1981, **36**, 1580.
BEBTUX *J. Chem. Soc., Chem. Commun.*, 1982, 215.
BECTIM *J. Chem. Soc., Dalton Trans.*, 1982, 129.
BECVOU *J. Chem. Soc., Dalton Trans.*, 1982, 319.
BECXIQ *J. Organomet. Chem.*, 1981, **222**, 343.
BEDBUH *J. Am. Chem. Soc.*, 1981, **103**, 7398.
BEDDAP *J. Chem. Soc., Dalton Trans.*, 1982, 187.
BEDGAS *J. Organomet. Chem.*, 1982, **226**, C1.
BEDZAL *Zh. Strukt. Khim.*, 1981, **22**, 120—5.
BEFBIX *Inorg. Chem.*, 1982, **21**, 237.
BEFJIF10 *J. Am. Chem. Soc.*, 1984, **106**, 3727.
BEGBIY01 *Inorg. Chem.*, 1982, **21**, 192.
BEGFEY *Inorg. Chem.*, 1982, **21**, 431.
BEGKAZ *Inorg. Chem.*, 1981, **20**, 4361.
BEGNAC *Acta Crystallogr., Sect. B*, 1982, **38**, 942.
BEGNUW *J. Chem. Soc., Dalton Trans.*, 1982, 493.
BEGPUY *J. Chem. Soc., Dalton Trans.*, 1982, 607.
BEGYAN *J. Chem. Soc., Chem. Commun.*, 1982, 287.
BEHGAW *J. Organomet. Chem.*, 1981, **221**, 183.
BEHHIF *Inorg. Chem.*, 1982, **21**, 223.
BEHLOP *Chem. Ber.*, 1982, **115**, 738.
BEHMOQ *J. Chem. Soc., Dalton Trans.*, 1982, 407.
BEHYUI *Acta Crystallogr., Sect. B*, 1982, **38**, 1318.
BEJBEX *J. Am. Chem. Soc.*, 1982, **104**, 922.
BEJGAY *Inorg. Chem.*, 1982, **21**, 218.
BEJGIG *Inorg. Chem.*, 1981, **20**, 4293.
BEJHUT *Inorg. Chim. Acta*, 1982, **57**, 29.
BEJJAB *Inorg. Chim. Acta*, 1982, **57**, 29.
BEJNIN *Acta Crystallogr., Sect. B*, 1982, **38**, 1165.
BEJTIT *Acta Crystallogr., Sect. B*, 1982, **38**, 1288.
BEKPUC *Aust. J. Chem.*, 1981, **34**, 2061.
BELFUT *Z. Naturforsch., Teil B*, 1982, **37**, 13.
BELGOO10 *Khim. Fiz.*, 1983, 1459.
BELJEH *J. Chem. Soc., Dalton Trans.*, 1982, 713.
BELLEJ *Zh. Strukt. Khim.*, 1981, **22**, 124—6.
BELTIV10 *Inorg. Chem.*, 1982, **21**, 4166.
BELTUH *Organometallics*, 1982, **1**, 302.
BEMLAG10 *Chem. Ber.*, 1982, **115**, 3830.
BEMLUA *Chem. Ber.*, 1982, **115**, 1004.
BEMNIQ *Z. Naturforsch., Teil B*, 1982, **37**, 341.
BEMPOY10 *Koord. Khim.*, 1981, **7**, 1880.
BENDAZ *J. Am. Chem. Soc.*, 1982, **104**, 994.
BENDED *Inorg. Chem.*, 1982, **21**, 1014.
BENFEF *J. Chem. Soc., Chem. Commun.*, 1982, 493.
BENIIB *J. Organomet. Chem.*, 1979, **169**, 219.
BENLOV *Inorg. Chem.*, 1982, **21**, 987.
BENNOX *J. Organomet. Chem.*, 1981, **221**, 375.
BENRAN *J. Organomet. Chem.*, 1982, **228**, 153.
BEPDEF *Inorg. Chem.*, 1982, **21**, 1208.
BEPJIP *Koord. Khim.*, 1982, **8**, 111.
BEPZEB *Cryst. Struct. Commun.*, 1982, **11**, 175.
BEPZIF *Cryst. Struct. Commun.*, 1982, **11**, 169.
BERTAT *Cryst. Struct. Commun.*, 1982, **11**, 305.
BESBEG *Z. Anorg. Allg. Chem.*, 1982, **485**, 81.
BESBIK10 *Z. Naturforsch., Teil B*, 1983, **38**, 747.
BESBOQ10 *Z. Naturforsch., Teil B*, 1983, **38**, 747.
BESFOU *J. Am. Chem. Soc.*, 1982, **104**, 1272.
BESHAI *J. Am. Chem. Soc.*, 1982, **104**, 1756.
BESJOY *Inorg. Chem.*, 1982, **21**, 917.
BESPIY *J. Am. Chem. Soc.*, 1982, **104**, 1710.
BESSAT *J. Am. Chem. Soc.*, 1982, **104**, 1290.
BESSEX *J. Am. Chem. Soc.*, 1982, **104**, 1426.
BESXRU *Inorg. Chem.*, 1976, **15**, 2270.
BETCUY10 *J. Am. Chem. Soc.*, 1983, **105**, 4662.
BEVMAQ *Acta Crystallogr., Sect. B*, 1982, **38**, 1603.
BEVYIK *Chem. Ber.*, 1982, **115**, 2271.
BEWMAR *J. Chem. Soc., Dalton Trans.*, 1982, 1013.
BEWVEE *Can. J. Chem.*, 1981, **59**, 3123.
BEXJUJ *J. Chem. Soc., Dalton Trans.*, 1982, 899.
BEXLEV *Polyhedron*, 1982, **1**, 89.
BEXTON *Bull. Soc. Chim. Belg.*, 1982, **91**, 171.
BEYFEQ *J. Organomet. Chem.*, 1982, **232**, 229.
BEYGAN *J. Organomet. Chem.*, 1982, **232**, 41.
BHZEPT *J. Chem. Soc., Dalton Trans.*, 1976, 2386.
BIBFUN *J. Am. Chem. Soc.*, 1982, **104**, 2147.
BIBJAX *Polyhedron*, 1982, **1**, 37.
BIBJEB *Polyhedron*, 1982, **1**, 37.
BIBSAG *Cryst. Struct. Commun.*, 1982, **11**, 733.
BICPDB *J. Chem. Soc., Dalton Trans.*, 1975, 2263.
BIDCAS *J. Am. Chem. Soc.*, 1982, **104**, 2329.
BIDNEH *Koord. Khim.*, 1982, **8**, 402.
BIFYUK *Acta Crystallogr., Sect. B*, 1982, **38**, 2155.
BIFZEV *Acta Crystallogr., Sect. B*, 1982, **38**, 2155.
BIGFAY01 *J. Am. Chem. Soc.*, 1982, **104**, 2165.
BIGHAA *Chem. Ber.*, 1982, **115**, 2035.
BIGLAE *J. Chem. Soc., Dalton Trans.*, 1982, 1465.
BIGLUY *J. Chem. Soc., Dalton Trans.*, 1982, 1401.
BIGPOW *Inorg. Chem.*, 1982, **21**, 2444.
BIGVAO *Inorg. Chim. Acta*, 1981, **52**, 169.
BIHCUQ *Inorg. Chem.*, 1982, **21**, 2350.
BIHFAZ *Inorg. Chem.*, 1982, **21**, 2257.
BIHGOO *J. Chem. Soc., Chem. Commun.*, 1982, 932.
BIHJOR10 *Koord. Khim.*, 1984, **10**, 844.
BIHLOT01 *Inorg. Chem.*, 1982, **21**, 3284.
BIHSAM *Inorg. Chem.*, 1982, **21**, 2624.
BIHWUK *J. Chem. Soc., Chem. Commun.*, 1982, 805.
BIHYEW *Am. Cryst. Assoc., Ser. 2*, 1982, **10**, 16.
BIJJAF *J. Chem. Soc., Chem. Commun.*, 1982, 1006.
BIJJUZ10 *J. Am. Chem. Soc.*, 1983, **105**, 7295.
BIJKOU *J. Am. Chem. Soc.*, 1982, **104**, 3722.
BIJPAL *Inorg. Chem.*, 1982, **21**, 3090.
BIJWEW *Inorg. Chem.*, 1982, **21**, 3173.
BIKTIY *Inorg. Chem.*, 1982, **21**, 2647.
BILDIJ *Organometallics*, 1982, **1**, 38.
BILMUE *Inorg. Chem.*, 1982, **21**, 2578.
BILRET *J. Chem. Soc., Chem. Commun.*, 1982, 1025.
BILSIY *Inorg. Chem.*, 1982, **21**, 2867.
BILWIC *J. Am. Chem. Soc.*, 1981, **103**, 7358.
BIMAOU10 *Acta Crystallogr., Sect. B*, 1974, **30**, 2659.
BIMMOZ *Bull. Chem. Soc. Jpn.*, 1982, **55**, 2083.
BIMTCU *Inorg. Chem.*, 1979, **18**, 141.
BIMTEW *J. Organomet. Chem.*, 1982, **235**, 105.
BINFUZ *J. Am. Chem. Soc.*, 1982, **104**, 4278.
BINHUB *Inorg. Chem.*, 1982, **21**, 3186.
BINJEN *Inorg. Chem.*, 1982, **21**, 2889.
BINRAR *Acta Crystallogr., Sect. B*, 1982, **38**, 2468.
BIPFUB10 *Acta Crystallogr., Sect. C*, 1983, **39**, 42.
BIPHHG *Cryst. Struct. Commun.*, 1981, **10**, 613.
BIPTAV *Inorg. Chim. Acta*, 1981, **52**, 205.
BIPYHG *Cryst. Struct. Commun.*, 1978, **7**, 165.
BIRJUH *Kristallografiya*, 1982, **27**, 489.
BIRLIX *Chem. Ber.*, 1982, **115**, 3049.
BIRXIJ *Cryst. Struct. Commun.*, 1982, **11**, 847.
BIRYOO10 *Z. Anorg. Allg. Chem.*, 1983, **498**, 85.
BISCEL *Inorg. Chim. Acta*, 1982, **59**, 225.
BISHUG *Cryst. Struct. Commun.*, 1982, **11**, 1163.
BISIPT *J. Chem. Soc., Dalton Trans.*, 1979, 1294.
BISJOC *Cryst. Struct. Commun.*, 1982, **11**, 1049.
BISKOD *Acta Crystallogr., Sect. B*, 1982, **38**, 2674.
BISNEW *Chem. Ber.*, 1982, **115**, 3224.
BISPAU *Acta Chem. Scand., Ser. A*, 1981, **35**, 739.
BISZIM *Cryst. Struct. Commun.*, 1982, **11**, 861.
BITKIY *Chem. Ber.*, 1982, **115**, 3152.
BITRAX *J. Chem. Soc., Chem. Commun.*, 1982, 1081.
BITSAY *Z. Kristallogr.*, 1982, **159**, 173.
BITYIM *Z. Naturforsch., Teil B*, 1982, **37**, 944.
BIVGAO *J. Chem. Soc., Chem. Commun.*, 1982, 1039.
BIVWIM *Acta Chem. Scand., Ser. A*, 1982, **36**, 767.
BIWBEO *J. Organomet. Chem.*, 1982, **229**, 169.
BIWLAU *Inorg. Chim. Acta*, 1982, **60**, 141.

BIWVEI *Inorg. Chim. Acta*, 1982, **61**, 195.
BIXBUF10 *J. Organomet. Chem.*, 1984, **269**, 91.
BIYCUH *Angew. Chem., Int. Ed. Engl.*, 1982, **21**, 705.
BIYHOG *Inorg. Chem.*, 1982, **21**, 3270.
BIYJIC *J. Am. Chem. Soc.*, 1982, **104**, 3773.
BIYPAA *Acta Crystallogr., Sect. B*, 1982, **38**, 2886.
BIYVIO *J. Organomet. Chem.*, 1981, **220**, 251.
BIYWUB *Inorg. Chim. Acta*, 1982, **61**, 255.
BIYXAI *Inorg. Chem.*, 1982, **21**, 3295.
BIYYOX *J. Chem. Soc., Dalton Trans.*, 1982, 1809.
BIYYUD *J. Chem. Soc., Dalton Trans.*, 1982, 1809.
BIZJEZ *J. Organomet. Chem.*, 1982, **238**, 223.
BIZZAL *J. Chem. Soc., Dalton Trans.*, 1982, 2065.
BMCPTI *Inorg. Chem.*, 1977, **16**, 1645.
BMTCFE *J. Chem. Soc., Chem. Commun.*, 1978, 506.
BNTLFE *Acta Crystallogr., Sect. B*, 1980, **36**, 1950.
BNZCTC *J. Organomet. Chem.*, 1974, **73**, 103.
BOBSUG *J. Am. Chem. Soc.*, 1982, **104**, 5250.
BOBTOB *Organometallics*, 1982, **1**, 1013.
BOBWAQ *Organometallics*, 1982, **1**, 998.
BOBXOF *J. Am. Chem. Soc.*, 1982, **104**, 4879.
BOBXUL *J. Am. Chem. Soc.*, 1982, **104**, 4879.
BOBYAS *J. Am. Chem. Soc.*, 1982, **104**, 4865.
BOBZUN *J. Chem. Soc., Chem. Commun.*, 1982, 1421.
BOCCOC *Inorg. Chem.*, 1978, **17**, 1995.
BOCLOU *Acta Crystallogr., Sect. B*, 1982, **38**, 3081.
BOCWAR *Organometallics*, 1982, **1**, 1085
BOCWEV *Organometallics*, 1982, **1**, 1066.
BODGUW10 *J. Am. Chem. Soc.*, 1984, **106**, 5926.
BODYEY *J. Am. Chem. Soc.*, 1982, **104**, 5515.
BODZEZ *Bull. Chem. Soc. Jpn.*, 1982, **55** 2840.
BOFCEE *J. Chem. Soc., Dalton Trans.*, 1982, 1795.
BOFJIP *J. Chem. Soc., Dalton Trans.*, 1982, 2343.
BOFMOY *Z. Naturforsch., Teil B*, 1982, **37**, 1289.
BOGFOS *J. Chem. Soc., Chem. Commun.*, 1983, 5.
BOGPIW *Z. Naturforsch., Teil B*, 1982, **37**, 1234.
BOHBIJ *Inorg. Chem.*, 1982, **21**, 3811.
BOHDUX *Inorg. Chem.*, 1982, **21**, 3666.
BOHGAG *Acta Crystallogr., Sect. C*, 1983, **39**, 49.
BOHPUJ *J. Chem. Soc., Dalton Trans.*, 1983, 1.
BOHYEC *Ko Hsueh Tung Pao*, 1982, **27**, 728.
BOJJUF *J. Chem. Soc., Dalton Trans.*, 1982, 2203.
BOJSUO *Z. Anorg. Allg. Chem.*, 1982, **491**, 73.
BOKPEW *J. Chem. Soc., Chem. Commun.*, 1983, 69.
BOKXEE *Chem. Ber.*, 1982, **115**, 3830.
BOLCIO10 *J. Am. Chem. Soc.*, 1984, **106**, 3214.
BOLJAN *Inorg. Chem.*, 1982, **21**, 4096.
BOLRID *Acta Crystallogr., Sect. C*, 1983, **39**, 188.
BOMMEV *Cryst. Struct. Commun.*, 1982, **11**, 1655.
BONCIQ01 *Organometallics*, 1983, **2**, 350.
BONSUS *Z. Naturforsch., Teil B*, 1983, **38**, 67.
BOPFOB *Chem. Ber.*, 1983, **116**, 46.
BOPPAX10 *J. Am. Chem. Soc.*, 1983, **105**, 4826.
BOPPIF10 *Acta Crystallogr., Sect. C*, 1984, **40**, 1322.
BOPSII *J. Am. Chem. Soc.*, 1982, **104**, 6360.
BOPTEF *Acta Crystallogr., Sect. C*, 1983, **39**, 181.
BOPWAE *Inorg. Chem.*, 1982, **21**, 4301.
BOPWEI *Inorg. Chem.*, 1982, 3903.
BORVIN *Inorg. Chem.*, 1982, **21**, 4050.
BOSKUP *J. Am. Chem. Soc.*, 1982, **104**, 6961.
BOSNEC *Inorg. Chem.*, 1982, **21**, 3923.
BOSRUW *J. Am. Chem. Soc.*, 1982, **104**, 6161.
BOTFOF *Koord. Khim.*, 1982, **8**, 1700.
BOTGAS *J. Am. Chem. Soc.*, 1982, **104**, 7378.
BOTPCU *J. Chem. Soc., Dalton Trans.*, 1977, 37.
BOTTAF *J. Am. Chem. Soc.*, 1982, **104**, 7325.
BOTVIP10 *Inorg. Chim. Acta*, 1984, **87**, 129.
BOTWUC *Zh. Strukt. Khim.*, 1982, **23**, 135—3.
BOVCAQ *J. Chem. Soc., Chem. Commun.*, 1983, 206.
BOVGAU *Koord. Khim.*, 1982, **8**, 1527.
BOVLED *J. Chem. Soc., Chem. Commun.*, 1983, 267.
BOVLUT *J. Chem. Soc., Chem. Commun.*, 1983, 222.
BOVYUG *Inorg. Chem.*, 1983, **22**, 759.
BOWCAR10 *J. Chem. Soc., Dalton Trans.*, 1983, 1557.
BOWLII *Polyhedron*, 1982, **1**, 840.
BOWLUU *Polyhedron*, 1982, **1**, 561.
BOWYOB *J. Chem. Soc., Dalton Trans.*, 1983, 205.
BOXHUR *Polyhedron*, 1982, **1**, 617.
BOXNEH *Inorg. Chem.*, 1983, **22**, 45.
BOYLUW *J. Struct. Chem.*, 1982, **1**, 73—1.
BOYTOY *Organometallics*, 1982, **1**, 1074.
BOYZOE *J. Chem. Soc., Chem. Commun.*, 1983, 356.
BOZBOH *J. Chem. Soc., Dalton Trans.*, 1983, 253.
BOZDID *Koord. Khim.*, 1982, **8**, 1561.
BOZMIM *J. Am. Chem. Soc.*, 1983, **105**, 416.
BOZNEJ *Inorg. Chem.*, 1983, **22**, 171.
BOZRAJ *Inorg. Chem.*, 1983, **22**, 395.
BOZYIY *Inorg. Chem.*, 1983, **22**, 884.
BPBRNI10 *Cryst. Struct. Commun.*, 1982, **11**, 1713.
BPEPFE *Inorg. Chem.*, 1978, **17**, 810.
BPESNI *Inorg. Chem.*, 1975, **14**, 1773.
BPHPRH10 *Acta Crystallogr., Sect. B*, 1974, **30**, 738.
BPNICU *Acta Crystallogr., Sect. B*, 1977, **33**, 1669.
BPYAGN *Cryst. Struct. Commun.*, 1973, **2**, 279.
BPYCPT *J. Chem. Soc., Dalton Trans.*, 1974, 1002.
BPYMNA *Inorg. Chim. Acta*, 1981, **53**, L197.
BQAPPD *J. Chem. Soc., Dalton Trans.*, 1978, 1490.
BRFOSA10 *J. Organomet. Chem.*, 1983, **249**, 149.
BRNOCR *Inorg. Chem.*, 1980, **19**, 3626.
BRNPIR *Inorg. Chem.*, 1980, **19**, 1803.
BSEMEP *J. Chem. Soc., Chem. Commun.*, 1979, 713.
BTCMAN *J. Cryst. Mol. Struct.*, 1971, **1**, 155.
BTCPTI *Z. Anorg. Allg. Chem.*, 1972, **390**, 195.
BTPCRE10 *J. Chem. Soc., Dalton Trans.*, 1978, 1189.
BTPPFE *Aust. J. Chem.*, 1977, **30**, 2655.
BTZDNI *J. Chem. Soc., Dalton Trans.*, 1976, 2382.
BUBBAB *Inorg. Chem.*, 1983, **22**, 371.
BUBKUE *J. Chem. Soc., Chem. Commun.*, 1983, 420.
BUCBEG *Inorg. Chem.*, 1983, **22**, 628.
BUCBUW *J. Am. Chem. Soc.*, 1983, **105**, 976.
BUCLUG *Inorg. Chem.*, 1983, **22**, 868.
BUCTOI *Inorg. Chem.*, 1983, **22**, 560.
BUCZOO *Chem. Ber.*, 1983, **116**, 951.
BUDBEH *Z. Naturforsch., Teil B*, 1983, **38**, 417.
BUDTEZ *Z. Naturforsch., Teil B*, 1983, **38**, 454.
BUDZEF *J. Organomet. Chem.*, 1983, **247**, 39.
BUFFUD *Acta Crystallogr., Sect. C*, 1983, **39**, 573.
BUFLET *Chem. Ber.*, 1983, **116**, 1070.
BUFNOF *J. Am. Chem. Soc.*, 1983, **105**, 1401.
BUFPUN01 *Inorg. Chem.*, 1983, **22**, 4091.
BUGFUE *J. Chem. Soc., Dalton Trans.*, 1983, 799.
BUGGAL *J. Chem. Soc., Dalton Trans.*, 1983, 799.
BUGRIE *J. Chem. Soc., Chem. Commun.*, 1983, 634.
BUHIPI *Gazz. Chim. Ital.*, 1975, **105**, 529.
BUHTON *Bull. Chem. Soc. Jpn.*, 1983, **56**, 657.
BUHVOP *Acta Crystallogr., Sect. C*, 1983, **39**, 540.
BUIMWA *J. Am. Chem. Soc.*, 1981, **103**, 357.
BUIMWB *J. Am. Chem. Soc.*, 1981, **103**, 357.
BUJBIR *Angew. Chem., Int. Ed. Engl.*, 1983, **22**, 314.
BUJFIV *J. Chem. Soc., Chem. Commun.*, 1983, 673.
BUJFUH *J. Chem. Soc., Chem. Commun.*, 1983, 648.
BUJNOJ *Phosphorus Sulfur*, 1983, **14**, 161.
BUJXAF *J. Chem. Soc., Dalton Trans.*, 1983, 809.
BUJYIO *Organometallics*, 1982, **1**, 1709.
BUKGET *Organometallics*, 1982, **1**, 1567.
BUKMID *Polyhedron*, 1982, **1**, 441.
BULLFE *Chem. Ber.*, 1972, **105**, 3936.
BULPED *J. Chem. Soc., Dalton Trans.*, 1983, 1131.
BULTEH *J. Chem. Soc., Dalton Trans.*, 1983, 911.
BULYOW *Inorg. Chim. Acta*, 1983, **71**, 141.
BULZIR *Inorg. Chim. Acta*, 1983, **70**, 29
BUMCER *Aust. J. Chem.*, 1982, **35**, 2413.
BUMEMO *J. Am. Chem. Soc.*, 1980, **102**, 1759.
BUNKAW *Organometallics*, 1982, **1**, 1538.
BUNKEA *J. Am. Chem. Soc.*, 1983, **105**, 2927.
BUNKIE *J. Am. Chem. Soc.*, 1983, **105**, 2927.
BUNMEC *J. Chem. Soc., Dalton Trans.*, 1983, 1479.
BUNZOZ *Inorg. Chem.*, 1983, **22**, 1221.
BUPCEU *Inorg. Chem.*, 1983, **22**, 1168.
BUPCIY *Inorg. Chem.*, 1983, **22**, 1168.

BUPCRH *Chem. Ber.*, 1977, **110**, 1020.
BUPJAX *J. Am. Chem. Soc.*, 1983, **105**, 2085.
BUPLAZ10 *Organometallics*, 1984, **3**, 599.
BUPMOO *Acta Crystallogr., Sect. C*, 1983, **39**, 838.
BUPPUX *Acta Crystallogr., Sect. C*, 1983, **39**, 858.
BUPSUA *Inorg. Chim. Acta*, 1983, **69**, 29.
BUPTEL *J. Organomet. Chem.*, 1983, **250**, 517.
BUPVUD *J. Organomet. Chem.*, 1983, **249**, 273.
BUPWOY10 *J. Chem. Soc., Dalton Trans.*, 1984, 1555.
BUPYOA *J. Organomet. Chem.*, 1983, **248**, 171.
BUPYUG *J. Organomet. Chem.*, 1983, **248**, 171.
BUPZIV *Z. Anorg. Allg. Chem.*, 1982, **495**, 127.
BURFOJ *J. Organomet. Chem.*, 1983, **249**, 127.
BURPEJ *Inorg. Chim. Acta*, 1983, **69**, 77.
BUSHEC *Z. Naturforsch., Teil B*, 1983, **38**, 733.
BUSLEG *J. Organomet. Chem.*, 1983, **250**, 183.
BUSRIQ *J. Chem. Soc., Dalton Trans.*, 1983, 1305.
BUSYIX *J. Chem. Soc., Dalton Trans.*, 1983, 1003.
BUTKUW *Inorg. Chem.*, 1983, **22**, 1409.
BUTTOZ *Organometallics*, 1983, **2**, 515.
BUVCAW10 *Z. Anorg. Allg. Chem.*, 1984, **514**, 25.
BUVGII *Inorg. Chem.*, 1983, **22**, 1865.
BUVLEJ *Organometallics*, 1983, **2**, 506.
BUVNIP *J. Cryst. Spectrosc.*, 1983, **13**, 303.
BUVNUB *J. Am. Chem. Soc.*, 1983, **105**, 2680.
BUVROZ *J. Chem. Soc., Chem. Commun.*, 1983, 951.
BUVSOA *Organometallics*, 1982, **1**, 1204.
BUWBAW *Zh. Strukt. Khim.*, 1983, **24**, 66—2.
BUWJUY *J. Organomet. Chem.*, 1983, **250**, 537.
BUWMAH *Organometallics*, 1983, **2**, 44.
BUWWOF01 *J. Chem. Soc., Dalton Trans.*, 1983, 2333.
BUWYIB *Bull. Chem. Soc. Jpn.*, 1983, **56**, 1982.
BUXGAC *Inorg. Chem.*, 1983, **22**, 1603.
BUXLEL *J. Am. Chem. Soc.*, 1983, **105**, 3353.
BUXMIQ *Inorg. Chem.*, 1983, **22**, 1306.
BUXTAP *Inorg. Chem.*, 1983, **22**, 1825.
BUYBUS *Polyhedron*, 1983, **2**, 185.
BUYKIP *J. Am. Chem. Soc.*, 1983, **105**, 4487.
BUYMAJ *J. Am. Chem. Soc.*, 1983, **105**, 4104.
BUYNEO *J. Am. Chem. Soc.*, 1983, **105**, 4092.
BUZMUE *J. Orgamomet. Chem.*, 1983, **251**, 413.
BUZPIV *Chem. Ber.*, 1983, **116**, 2994.
BUZRAP *Chem. Ber.*, 1983, **116**, 2765.
BUZYAW *J. Organomet. Chem.*, 1983, **252**, 71.
BUZZAX *J. Organomet. Chem.*, 1983, **252**, 231.
BVINBF *Isr. J. Chem.*, 1972, **10**, 201.
BXCAPD *J. Am. Chem. Soc.*, 1980, **102**, 1047.
BXZPCO *Inorg. Chem.*, 1977, **16**, 1665.
BZBCUA *Zh. Strukt. Khim.*, 1979, **20**, 89.
BZCPRU *Cryst. Struct. Commun.*, 1978, **7**, 583.
BZDTNB10 *Inorg. Chem.*, 1976, **15**, 1589.
BZDTZR10 *Inorg. Chem.*, 1976, **15**, 1595.
BZHREC *Chem. Ber.*, 1978, **111**, 3740.
BZHXDB *Inorg. Chem.*, 1981, **20**, 890.
BZTCDN *J. Am. Chem. Soc.*, 1973, **95**, 8566.
BZTCOV *Acta Crystallogr., Sect. B*, 1980, **36**, 304.
CABHIW *J. Struct. Chem.*, 1983, **2**, 29.
CABYIN *J. Chem. Soc., Dalton Trans.*, 1983, 1571.
CABYUZ *J. Chem. Soc., Dalton Trans.*, 1983, 2025.
CABZAG *J. Chem. Soc., Dalton Trans.*, 1983, 2025.
CACFUH *J. Chem. Soc., Chem. Commun.*, 1981, 963.
CACLUN *J. Chem. Soc., Dalton Trans.*, 1983, 2091.
CACMIC *J. Chem. Soc., Dalton Trans.*, 1983, 2011.
CACPIF *J. Chem. Soc., Dalton Trans.*, 1983, 1679
CACRIH *Polyhedron*, 1983, **2**, 843.
CACWOS *Organometallics*, 1983, **2**, 535
CADHOE *Acta Crystallogr., Sect. C*, 1983, **39**, 997.
CADMAV *Z. Anorg. Allg. Chem.*, 1983, **502**, 35.
CADPEC *Can. J. Chem.*, 1983, **61**, 1146.
CADYAH *Angew. Chem., Int. Ed. Engl.*, 1983, **22**, 503.
CAFCUH *Organometallics*, 1983, **2**, 935.
CAFFEU *Organometallics*, 1983, **2**, 938.
CAFFIY *Organometallics*, 1983, **2**, 938.
CAFJUO *Acta Crystallogr., Sect. C*, 1983, **39**, 1197.
CAFLAW *J. Organomet. Chem.*, 1983, **253**, 53.
CAFLEA *J. Organomet. Chem.*, 1983, **253**, 53.
CAFNOM *Acta Crystallogr., Sect. C*, 1983, **39**, 1041.
CAFSOR *Acta Crystallogr., Sect. C*, 1983, **39**, 1210.
CAFZUE *J. Organomet. Chem.*, 1983, **248**, C26.
CAGKEA *Organometallics*, 1983, **2**, 558.
CAGSAE *Acta Crystallogr., Sect. C*, 1983, **39**, 1367.
CAGSIM *J. Chem. Soc., Dalton Trans.*, 1983, 1873.
CAHGOH *Inorg. Chem.*, 1983, **22**, 1897.
CAHGUN *Inorg. Chem.*, 1983, **22**, 1794.
CAHHAU *Inorg. Chem.*, 1983, **22**, 1791.
CAHJIE *Inorg. Chem.*, 1983, **22**, 1744.
CAHRUY *J. Chem. Soc., Dalton Trans.*, 1983, 2117.
CAHZAM *J. Am. Chem. Soc.*, 1983, **105**, 5834.
CAHZUG *J. Am. Chem. Soc.*, 1983, **105**, 5804.
CAIMCO *J. Chem. Soc. A*, 1970, 2558.
CAJCEV *Transition Met. Chem.*, 1983, **8**, 127.
CAJFAU *Inorg. Chem.*, 1983, **22**, 1887.
CAJGEZ *J. Am. Chem. Soc.*, 1983, **105**, 5137.
CAJHOK *J. Chem. Soc., Chem. Commun.*, 1983, 1163.
CAKCIA *Inorg. Chem.*, 1983, **22**, 1739.
CAKGAW *J. Chem. Soc., Dalton Trans.*, 1983, 1789.
CAKGIE *Inorg. Chem.*, 1983, **22**, 1695.
CAKNEH01 *Inorg. Chem.*, 1984, **23**, 122.
CAKNIL10 *Inorg. Chim. Acta*, 1983, **75**, 199.
CAKSOW *Organometallics*, 1983, **2**, 1049.
CAKTUD *J. Am. Chem. Soc.*, 1983, **105**, 4955.
CALCEX *J. Am. Chem. Soc.*, 1981, **103**, 6507.
CALGAX *Inorg. Chem.*, 1981, **20**, 3904.
CALHIG *J. Chem. Soc., Chem. Commun.*, 1983, 1177.
CALNUY *J. Chem. Soc., Chem. Commun.*, 1983, 1283.
CAMCUO *Inorg. Chim. Acta*, 1983, **75**, 103.
CAMKIK *Organometallics*, 1983, **2**, 1172.
CAMLAD *Organometallics*, 1983, **2**, 1167.
CAMROX *Inorg. Chem.*, 1983, **22**, 2356.
CAMSOB *Rev. Chim. Miner.*, 1979, **16**, 555.
CAMTEP *J. Am. Chem. Soc.*, 1983, **105**, 5939.
CAMVER *J. Am. Chem. Soc.*, 1983, **105**, 5954.
CAMWOC *Angew. Chem., Int. Ed. Engl.*, 1983, **22**, 498.
CAMXOD *Nouv. J. Chim.*, 1983, **7**, 467.
CANBRU *J. Organomet. Chem.*, 1974, **72**, 247.
CANFAY *Inorg. Chem.*, 1983, **22**, 2351.
CANHAA *J. Organomet. Chem.*, 1984, **255**, 231.
CANZUM *J. Chem. Soc., Chem. Commun.*, 1983, 1377.
CAPFOO *J. Am. Chem. Soc.*, 1983, **105**, 6163.
CAPSOB *Inorg. Chim. Acta*, 1983, **75**, 173.
CARJOU *Organometallics*, 1983, **2**, 1369.
CARKIP *Organometallics*, 1983, **2**, 1437.
CARWAT *J. Chem. Soc., Chem. Commun.*, 1983, 1358.
CASDIJ *Z. Naturforsch., Teil B*, 1983, **38**, 1454.
CASPIV *Z. Anorg. Allg. Chem.*, 1983, **504**, 7.
CASVIB *J. Organomet. Chem.*, 1983, **256**, 349.
CASYEA *J. Chem. Soc., Chem. Commun.*, 1983, 1366.
CATETH *J. Am. Chem. Soc.*, 1978, **100**, 7882.
CATGEJ *J. Organomet. Chem.*, 1983, **111**, 256.
CATKOX *J. Chem. Soc., Chem. Commun.*, 1983, 1351.
CATKUD *J. Chem. Soc., Chem. Commun.*, 1983, 1351.
CATMIT *Inorg. Chem.*, 1983, **22**, 2736.
CATSEV *Z. Naturforsch., Teil B*, 1983, **38**, 1406.
CATSUL *Z. Naturforsch., Teil B*, 1983, **38**, 1488.
CAVMOB *J. Chem. Soc., Chem. Commun.*, 1983, 1490.
CAVREW *J. Am. Chem. Soc.*, 1983, **105**, 6162.
CAVVEA *J. Chem. Soc., Dalton Trans.*, 1983, 2375.
CAVYON *Koord. Khim.*, 1983, **9**, 986.
CAWBAD *Koord. Khim.*, 1983, **9**, 1114.
CAWGAI *Inorg. Chem.*, 1983, **22**, 2903.
CAWJAL *Inorg. Chem.*, 1983, **22**, 2892.
CAWLIV *Angew. Chem., Int. Ed. Engl.*, 1983, **22**, 774.
CAWSUO *Inorg. Chem.*, 1983, **22**, 3361.
CAWTAV *Inorg. Chem.*, 1983, **22**, 3355.
CAXMIX *Acta Crystallogr., Sect. C*, 1983, **39**, 1643.
CAXPUM *Acta Crystallogr., Sect. C*, 1983, **39**, 1620.
CAXYOP *Inorg. Chim. Acta*, 1983, **80**, 57.
CAYFAJ *J. Am. Chem. Soc.*, 1983, **105**, 7460.
CAYGAK *J. Organomet. Chem.*, 1983, **258**, 357.
CAYGOY *J. Am. Chem. Soc.*, 1983, **105**, 7280.

CAYJAN *Can. J. Chem.*, 1983, **61**, 2141.
CAYLAP *Angew. Chem., Int. Ed. Engl.*, 1983, **22**, 790.
CAYMAQ *Angew. Chem., Int. Ed. Engl.*, 1983, **22**, 414.
CAYXAB *Inorg. Chim. Acta*, 1983, **73**, 261.
CAZCIP *J. Sci. Hiroshima Univ., Ser. A*, 1983, **47**, 1.
CAZGUF *Jilin Daxue Ziran Kexue. Xuebao*, 1983, 103—2.
CAZHAM *Jilin Daxue Ziran Kexue. Xuebao*, 1983, 103—2.
CAZJAO10 *Z. Naturforsch., Teil B*, 1984, **39**, 880.
CAZJES10 *Z. Naturforsch., Teil B*, 1984, **39**, 880.
CAZZAE *Inorg. Chem.*, 1983, **22**, 3090.
CBACRC *J. Chem. Soc., Dalton Trans.*, 1980, 52.
CBFPPT10 *Inorg. Chem.*, 1973, **12**, 1663.
CBUTIR *Cryst. Struct. Commun.*, 1973, **2**, 527.
CBZTET10 *Polyhedron*, 1983, **2**, 1031.
CBZYTA *J. Am. Chem. Soc.*, 1978, **100**, 3793.
CCHXPC *Inorg. Chem.*, 1979, **18**, 166.
CCPZRA *Inorg. Chem.*, 1980, **19**, 3812.
CDACET *J. Chem. Soc., Dalton Trans.*, 1972, 956.
CDCYAC *J. Chem. Soc., Dalton Trans.*, 1974, 285.
CDMALD *J. Chem. Soc., Dalton Trans.*, 1974, 674.
CDMSOR *J. Chem. Soc., Dalton Trans.*, 1975, 2480.
CEBDIW *Acta Chem. Scand., Ser. A*, 1983, **37**, 697.
CEBREG *Finn. Chem. Lett.*, 1983, 120.
CECATI *Inorg. Chem.*, 1979, **18**, 1611.
CECCIW *Angew. Chem., Int. Ed. Engl.*, 1983, **22**, 996.
CECGOG *Angew. Chem., Int. Ed. Engl.*, 1983, **22**, 1000.
CECGUM *Angew. Chem., Int. Ed. Engl.*, 1983, **22**, 984.
CECKOK *Organometallics*, 1983, **2**, 1458.
CECLEB10 *Koord. Khim.*, 1984, **10**, 123.
CECLIF10 *Koord. Khim.*, 1984, **10**, 1128.
CECROR *Organometallics*, 1983, **2**, 1505.
CECWEM *Z. Kristallogr.*, 1983, **164**, 237.
CEDHUO *J. Chem. Soc., Chem. Commun.*, 1984, 175.
CEDMON *Organometallics*, 1983, **2**, 1595.
CEDNOO *Polyhedron*, 1983, **2**, 1031.
CEDXEO *Inorg. Chem.*, 1983, **22**, 3424.
CEFCUL *Inorg. Chem.*, 1983, **22**, 3480.
CEFHEA *Organometallics*, 1983, **2**, 1763.
CEFHOK *Kristallografiya*, 1983, **28**, 886.
CEFMAB *Polyhedron*, 1983, **2**, 1317.
CEFMIJ *Polyhedron*, 1983, **2**, 1201.
CEFNOQ *S. Afr. J. Chem.*, 1983, **36**, 97.
CEFPEI *Organometallics*, 1983, **2**, 1889.
CEFSIP *Angew Chem., Int. Ed. Engl.*, 1984, **23**, 68.
CEFVIS *J. Chem. Soc., Chem. Commun.*, 1984, 282.
CEFVOY *J. Am. Chem. Soc.*, 1984, **106**, 329.
CEFVUE *J. Am. Chem. Soc.*, 1983, **105**, 7789.
CEFYAN *Inorg. Chem.*, 1983, **22**, 3671.
CEGCIA *J. Chem. Soc., Dalton Trans.*, 1984, 55.
CEGCOG *J. Chem. Soc., Dalton Trans.*, 1984, 55.
CEGGUQ *Inorg. Chem.*, 1983, **22**, 3654.
CEGHAX *J. Am. Chem. Soc.*, 1983, **105**, 7750.
CEGHEB *J. Am. Chem. Soc.*, 1983, **105**, 7750.
CEGNAD *Z. Kristallogr.*, 1983, **164**, 259.
CEHFEA *J. Chem. Soc., Chem. Commun.*, 1984, 240.
CEHMOR *J. Am. Chem. Soc.*, 1984, **106**, 410.
CEHTUE *J. Am. Chem. Soc.*, 1983, **105**, 6763.
CEHXAO *Inorg. Chem.*, 1983, **22**, 3489.
CEJDEA *J. Am. Chem. Soc.*, 1984, **106**, 451
CEJPEM *Acta Crystallogr., Sect. C*, 1984, **40**, 82.
CEKGEE *Organometallics*, 1984, **3**, 293.
CEKGII *Organometallics*, 1984, **3**, 293.
CEKGOO *Acta Crystallogr., Sect. C*, 1984, **40**, 409.
CELJEI *Acta Crystallogr., Sect. C*, 1984, **40**, 354.
CELLAG *Acta Crystallogr., Sect. C*, 1984, **40**, 359.
CEMCUS *Inorg. Chim. Acta*, 1983, **72**, 141.
CEMMIQ *Inorg. Chem.*, 1983, **22**, 3706.
CEMSES *Inorg. Chem.*, 1983, **22**, 4091.
CEMSIW *Inorg. Chem.*, 1983, **22**, 4091.
CEMSUI *Inorg. Chem.*, 1984, **23**, 88.
CEMTIX *Inorg. Chem.*, 1984, **23**, 99.
CEMWEW *Inorg. Chem.*, 1983, **22**, 3911.
CEMXIB *J. Am. Chem. Soc.*, 1983, **105**, 7751.
CENFAC01 *J. Chem. Soc., Dalton Trans.*, 1983, 1917.
CENRES *Inorg. Chem.*, 1983, **22**, 3776.
CENSUJ *J. Chem. Soc., Dalton Trans.*, 1984, 229.
CENTAQ *J. Chem. Soc., Dalton Trans.*, 1984, 229.
CEPBII *J. Chem. Soc., Chem. Commun.*, 1984, 434.
CEPFPP *J. Chem. Soc., Dalton Trans.*, 1977, 2043.
CEPGUZ *J. Inorg. Biochem.*, 1983, **19**, 237.
CEPHOU *Inorg. Chem.*, 1984, **23**, 227.
CEPHUA *Inorg. Chem.*, 1984, **23**, 227.
CEPLUE *J. Chem. Soc., Chem. Commun.*, 1984, 485.
CEPMAL *Aust. J. Chem.*, 1983, **36**, 1107.
CEPMOZ *J. Am. Chem. Soc.*, 1974, **96**, 5427.
CEPYIF *J. Organomet. Chem.*, 1984, **262**, 123.
CERCUX *Acta Crystallogr., Sect. C*, 1984, **40**, 616.
CERDAE *Acta Crystallogr., Sect. C*, 1984, **40**, 619.
CERFAG *Acta Crystallogr., Sect. C*, 1984, **40**, 635.
CERFEK *Acta Crystallogr., Sect. C*, 1984, **40**, 635.
CERJIS *J. Organomet. Chem.*, 1984, **264**, 327.
CERKUF *J. Chem. Soc., Chem. Commun.*, 1984, 425.
CESGAI10 *Organometallics*, 1984, **3**, 1003.
CESJOZ *J. Cryst. Spectrosc.*, 1984, **14**, 21.
CESKIU *J. Cryst. Spectrosc.*, 1984, **14**, 143.
CESNAP *J. Chem. Soc., Dalton Trans.*, 1984, 735.
CESNET *J. Chem. Soc., Dalton Trans.*, 1984, 719.
CESTOJ *J. Am. Chem. Soc.*, 1984, **106**, 1699.
CESVUR *J. Am. Chem. Soc.*, 1984, **106**, 1853.
CESXUT *J. Chem. Soc., Chem. Commun.*, 1984, 501.
CESYAA *J. Chem. Soc., Chem. Commun.*, 1984, 501.
CESYII *Inorg. Chem.*, 1983, **22**, 3251.
CESZOP *Can. J. Chem.*, 1984, **62**, 332.
CESZUV *Can. J. Chem.*, 1984, **62**, 332.
CETGEN *Inorg. Chim. Acta*, 1983, **70**, 159.
CETGIR *Inorg. Chim. Acta*, 1983, **70**, 159.
CETKUH *J. Chem. Soc., Dalton Trans.*, 1984, 833.
CETMRH *Inorg. Chem.*, 1979, **18**, 2438.
CETPIR *J. Organomet. Chem.*, 1975, **90**, 101.
CETSIR *Acta Crystallogr., Sect. B*, 1980, **36**, 1206.
CEVFUE10 *J. Am. Chem. Soc.*, 1984, **106**, 5934.
CEVHOA *J. Am. Chem. Soc.*, 1984, **106**, 1323.
CEVLAQ *J. Chem. Soc., Dalton Trans.*, 1984, 785.
CEWZIN10 *Acta Crystallogr., Sect. C*, 1984, **40**, 1544.
CEXHUI *Inorg. Chem.*, 1984, **23**, 349.
CEXKAR *Inorg. Chem.*, 1984, **23**, 363.
CEXKUL *Inorg. Chem.*, 1984, **23**, 359.
CEXLUM *Inorg. Chem.*, 1984, **23**, 354.
CEXNAU *Organometallics*, 1984, **3**, 596.
CEXSAZ *Inorg. Chem.*, 1984, **23**, 511.
CEXTII *Organometallics*, 1984, **3**, 599.
CEXZIO *Inorg. Chem.*, 1984, **23**, 343.
CEXZOU *Inorg. Chem.*, 1984, **23**, 343.
CEYBEN *Inorg. Chem.*, 1984, **23**, 338.
CEYBIR *Inorg. Chem.*, 1984, **23**, 409.
CEYCOY *J. Chem. Soc., Dalton Trans.*, 1984, 399.
CEYCUE *J. Chem. Soc., Dalton Trans.*, 1984, 399.
CEYPEB *J. Organomet. Chem.*, 1984, **266**, 45.
CEYRON *Acta Crystallogr., Sect. C*, 1984, **40**, 795.
CEZKEX *Acta Crystallogr., Sect. C*, 1984, **40**, 751.
CEZMUP *Acta Crystallogr., Sect. C*, 1984, **40**, 746.
CEZNIE *Inorg. Chim. Acta*, 1984, **85**, L19.
CEZWEJ *Inorg. Chim. Acta*, 1984, **84**, 57.
CEZWOT *Inorg. Chim. Acta*, 1984, **84**, 179.
CEZXAG *Inorg. Chim. Acta*, 1984, **84**, 179.
CEZYUB *Inorg. Chim. Acta*, 1984, **84**, 187.
CFBYRH *Acta Crystallogr., Sect. B*, 1979, **35**, 2321.
CFTPVP *J. Organomet. Chem.*, 1978, **150**, 157.
CHBPTC *J. Am. Chem. Soc.*, 1979, **101**, 4581.
CHDQOS *J. Chem. Soc., Chem. Commun.*, 1978, 853.
CHGACA *Acta Crystallogr., Sect. B*, 1979, **35**, 1239.
CHGALD *J. Chem. Soc., Dalton Trans.*, 1978, 1573.
CHPCUP *Can. J. Chem.*, 1975, **53**, 1949.
CHPECI *J. Organomet. Chem.*, 1978, **149**, 345.
CHPMOC *Acta Crystallogr., Sect. B*, 1978, **34**, 2439.
CHPRUS10 *J. Chem. Soc., Dalton Trans.*, 1981, 2220.
CHVINO *Acta Crystallogr., Sect. B*, 1978, **34**, 2466.
CHXPCO *Aust. J. Chem.*, 1978, **31**, 47.
CIBGEZ *J. Chem. Soc., Chem. Commun.*, 1984, 799.
CIBHAW *Inorg. Chim. Acta*, 1984, **81**, 47.

CIBKED *Z. Naturforsch., Teil B*, 1984, **39**, 590.
CIBLUU *Z. Naturforsch., Teil B*, 1984, **39**, 538.
CIBYOB *Inorg. Chim. Acta*, 1984, **82**, 167.
CIBZAO *Inorg. Chim. Acta*, 1984, **82**, 167.
CICBOF *Inorg. Chim. Acta*, 1984, **82**, 161.
CICBUL *Inorg. Chim. Acta*, 1984, **82**, 161.
CICFID *Inorg. Chim. Acta*, 1984, **81**, 147.
CICLOP *Z. Naturforsch., Teil B*, 1984, **39**, 582.
CICYAO *Acta Crystallogr., Sect. C*, 1984, **40**, 935.
CIDBAS *Inorg. Chem.*, 1984, **23**, 936.
CIDBEW *Inorg. Chem.*, 1984, **23**, 945.
CIDBOG *Chem. Ber.*, 1984, **117**, 1052.
CIDHEC *J. Am. Chem. Soc.*, 1984, **106**, 2990.
CIDJEE *J. Am. Chem. Soc.*, 1984, **106**, 2965.
CIFCAV *J. Chem. Soc., Chem. Commun.*, 1984, 710.
CIFGON *Inorg. Chem.*, 1984, **23**, 914.
CIFMAF *J. Chem. Soc., Dalton Trans.*, 1984, 845.
CIFNIO *Inorg. Chem.*, 1984, **23**, 938.
CIFXOE *J. Chem. Soc., Chem. Commun.*, 1984, 841.
CIGCOK *Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 377.
CIGRAL *Inorg. Chim. Acta*, 1984, **92**, 151.
CIGVET *Inorg. Chem.*, 1984, **23**, 1009.
CIHLIO *Acta Crystallogr., Sect. C*, 1984, **40**, 1186.
CIHNEM *Acta Crystallogr., Sect. C*, 1984, **40**, 1161.
CIHRIU *Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 311.
CIHXIA *J. Organomet. Chem.*, 1984, **263**, C33.
CIHYOH *J. Am. Chem. Soc.*, 1984, **106**, 3054.
CIJDAA *J. Struct. Chem.*, 1984, **3**, 57.
CIJLUC *J. Organomet. Chem.*, 1984, **265**, 249.
CIJWIB *Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 376.
CIJYOJ *Acta Crystallogr., Sect. C*, 1984, **40**, 1172.
CIKHOT *J. Struct. Chem.*, 1984, **3**, 13.
CIKJUB *J. Am. Chem. Soc.*, 1984, **106**, 2579.
CIKKAI *J. Am. Chem. Soc.*, 1984, **106**, 2583.
CIKPUH *Angew. Chem., Int. Ed. Engl.*, 1983, **22**, 977.
CIKTOF *Inorg. Chim. Acta*, 1984, **84**, 221.
CILCUV *Organometallics*, 1984, **3**, 939.
CILYAX *Acta Crystallogr., Sect. C*, 1984, **40**, 1320.
CIMGEK *Acta Crystallogr., Sect. C*, 1984, **40**, 1357.
CIMINU10 *J. Am. Chem. Soc.*, 1975, **97**, 4519.
CIMVID *J. Chem. Soc., Chem. Commun.*, 1984, 1141.
CINKAL *J. Chem. Soc., Chem. Commun.*, 1984, 1000.
CINKUF *Inorg. Chem.*, 1984, **23**, 1387.
CINLAM *J. Orgamomet. Chem.*, 1984, **265**, C19.
CINREW *Koord. Khim.*, 1984, **10**, 850.
CIPDIO *J. Am. Chem. Soc.*, 1984, **106**, 3356.
CIPGAJ *Acta Crystallogr., Sect. C*, 1984, **40**, 1552.
CIPNEU *J. Am. Chem. Soc.*, 1984, **106**, 3527.
CIPTAW *Inorg. Chim. Acta*, 1984, **83**, 75.
CIPTMN *J. Chem. Soc., Dalton Trans.*, 1980, 1625.
CIRDAI *Polyhedron*, 1984, **3**, 651.
CIRHUG *Polyhedron*, 1984, **3**, 505.
CIRJAO *Polyhedron*, 1984, **3**, 385.
CIRMAR *Acta Crystallogr., Sect. C*, 1984, **40**, 1533.
CIRNOG *J. Chem. Soc., Dalton Trans.*, 1984, 2039.
CIRNUM *J. Chem. Soc., Dalton Trans.*, 1984, 2039.
CIRSAX *Inorg. Chem.*, 1984, **23**, 1739.
CIRSEB *Inorg. Chem.*, 1984, **23**, 1739.
CIRVOO *Acta Crystallogr., Sect. C*, 1984, **40**, 1562.
CISZOT *J. Chem. Soc., Chem. Commun.*, 1984, 1082.
CITCIR *J. Am. Chem. Soc.*, 1984, **106**, 3371.
CITDEO *Polyhedron*, 1984, **3**, 303.
CITKIZ *Aust. J. Chem.*, 1983, **36**, 2175.
CIXHEW *Inorg. Chem.*, 1984, **23**, 2271.
CIXJIC *J. Chem. Soc., Dalton Trans.*, 1984, 1675.
CIXKAV *Inorg. Chem.*, 1984, **23**, 2286.
CIXLIE *J. Am. Chem. Soc.*, 1984, **106**, 4460.
CIXRUW *Can. J. Chem.*, 1984, **62**, 696.
CIXTUY *Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 522.
CIXYAJ *Teor. Eksp. Khim.*, 1983, **19**, 685.
CIYBAN *Inorg. Chem.*, 1984, **23**, 2303.
CIYKAW *Organometallics*, 1984, **3**, 1223.
CIYMEC *Organometallics*, 1984, **3**, 1312.
CIYMIG *Organometallics*, 1984, **3**, 1310.
CIYTUZ01 *Organometallics*, 1984, **3**, 1158.
CIZBES *J. Chem. Soc., Chem. Commun.*, 1984, 1317.
CIZBOC *J. Chem. Soc., Dalton Trans.*, 1984, 1731.
CIZGIB02 *Kristallografiya*, 1984, **29**, 455.
CIZNUU *J. Chem. Soc., Dalton Trans.*, 1984, 1059.
CIZTEK *J. Organomet. Chem.*, 1984, **270**, C49.
CLBCNV *Inorg. Chem.*, 1980, **19**, 3379.
CLCAME01 *Zh. Neorg. Khim.*, 1983, **28**, 597.
CLFORE10 *Koord. Khim.*, 1980, **6**, 963.
CLOSMO *Transition Met. Chem.*, 1980, **5**, 172.
CLPDZN *Bull. Chem. Soc. Jpn.*, 1980, **53**, 1101.
CLPHTI *Inorg. Chem.*, 1966, **5**, 1782.
CLPOZN *Acta Crystallogr., Sect. B*, 1980, **36**, 2409.
CLPRCV *Acta Crystallogr., Sect. B*, 1981, **37**, 945.
CLPZIR *J. Inorg. Nucl. Chem.*, 1973, **35**, 4103.
CLTIMN *Inorg. Chem.*, 1978, **17**, 1848.
CLTPOC01 Unpublished work.
CLZRAL *J. Organomet. Chem.*, 1981, **208**, 327.
CMASNI *Inorg. Chim. Acta*, 1980, **40**, 171.
CMNCBR *J. Am. Chem. Soc.*, 1975, **97**, 3053.
CMPORZ *J. Am. Chem. Soc.*, 1978, **100**, 3025.
CMURAG *J. Cryst. Mol. Struct.*, 1972, **2**, 125.
CMZTFE *J. Am. Chem. Soc.*, 1974, **96**, 7826.
CNBPAC *J. Organomet. Chem.*, 1979, **165**, 39.
CNBRUB *J. Chem. Soc., Chem. Commun.*, 1981, 271.
CNCOPP10 *Inorg. Chem.*, 1973, **12**, 1304.
CNMPRE *Inorg. Chem.*, 1971, **10**, 578.
CNOFEA *Koord. Khim.*, 1981, **7**, 949.
CNOFEB *Koord. Khim.*, 1981, **7**, 949.
CNOPIR *Inorg. Chem.*, 1968, **7**, 2345.
CNPLPT *J. Chem. Soc., Dalton Trans.*, 1980, 973.
CNPRCV *J. Cryst. Mol. Struct.*, 1980, **10**, 61.
CNTPCP *J. Chem. Soc., Dalton Trans.*, 1980, 1932.
COBDUS *J. Chem. Soc., Dalton Trans.*, 1984, 1069.
COBGIJ *J. Chem. Soc., Dalton Trans.*, 1984, 1659.
COBHGA *Inorg. Chem.*, 1981, **20**, 863.
COBLIO *J. Am. Chem. Soc.*, 1984, **106**, 4749.
COBSOB *J. Organomet. Chem.*, 1984, **272**, C17.
COBXOG *J. Chem. Soc., Chem. Commun.*, 1984, 1400.
COCKAG *Inorg. Chem.*, 1984, **23**, 2207.
COCKOU *J. Chem. Soc., Chem. Commun.*, 1984, 1362.
COCLEL *J. Chem. Soc., Chem. Commun.*, 1984, 1351.
COCNAJ *Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 77.
COCPOZ *Acta Crystallogr., Sect. C*, 1984, **40**, 1699.
COCTCE *Inorg. Chem.*, 1972, **11**, 171.
COCTFT10 *Inorg. Chem.*, 1980, **19**, 2560.
COCXOH *J. Organomet. Chem.*, 1984, **272**, C62.
COCZEZ *Inorg. Chim. Acta*, 1984, **86**, 101.
CODCON *J. Chem. Soc., Chem. Commun.*, 1984, 1402.
CODHIM *J. Cryst. Spectrosc.*, 1984, **14**, 383.
CODJAG *Organometallics*, 1984, **3**, 1414.
CODJIO *Organometallics*, 1984, **3**, 1444.
CODPIR10 *Inorg. Chem.*, 1973, **12**, 260.
COFVIC *Z. Naturforsch., Teil B*, 1984, **39**, 1076.
COFZEC *Inorg. Chim. Acta*, 1984, **86**, L65.
COGHEL *J. Chem. Soc., Dalton Trans.*, 1984, 2081.
COGSIA *Gazz. Chim. Ital.*, 1983, **113**, 761.
COGWOK *Inorg. Chem.*, 1984, **23**, 2838.
COGXOL *Inorg. Chem.*, 1984, **23**, 2732.
COGXRU *Inorg. Chem.*, 1980, **19**, 3343.
COGXUR *Inorg. Chem.*, 1984, **23**, 2732.
COHCUX *Aust. J. Chem.*, 1984, **37**, 1395.
COHHIQ *Inorg. Chem.*, 1984, **23**, 2803.
COHNUI *Inorg. Chim. Acta*, 1984, **87**, 115.
COHTOI *J. Chem. Soc., Chem. Commun.*, 1984, 1425.
COJBOS *J. Chem. Soc., Chem. Commun.*, 1984, 1508.
COJDOU *Z. Naturforsch., Teil B*, 1984, **39**, 1199.
COJDUA *Z. Naturforsch., Teil B*, 1984, **39**, 1199.
COJYEF *Koord. Khim.*, 1984, **10**, 1116.
COKCIO *Acta Crystallogr., Sect. C*, 1984, **40**, 1820.
COKDUB *Acta Crystallogr., Sect. C*, 1984, **40**, 1836.
COKPIB *Inorg. Chim. Acta*, 1984, **95**, 147.
COKTIF *J. Chem. Soc., Chem. Commun.*, 1984, 1398.
COKZAD *Inorg. Chim. Acta*, 1984, **95**, 217.
COLDIQ *Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 721.
COLDOW *Inorg. Chem.*, 1984, **23**, 2459.

COLDUC *Inorg. Chem.*, 1984, **23**, 2459.
COLFEO *Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 726.
COLNAS *J. Am. Chem. Soc.*, 1984, **106**, 2033.
COLNEW *J. Am. Chem. Soc.*, 1984, **106**, 2033.
COLPIC *J. Am. Chem. Soc.*, 1984, **106**, 5561.
COLPOI *J. Am. Chem. Soc.*, 1984, **106**, 5561.
COLSEB *Inorg. Chem.*, 1984, **23**, 2519.
COLVII *Inorg. Chem.*, 1984, **23**, 2575.
COLWAB *Aust. J. Chem.*, 1984, **37**, 35.
COLZEI *Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 735.
COMMAS *J. Organomet. Chem.*, 1984, **276**, 287.
COMPEZ *Koord. Khim.*, 1984, **10**, 1266.
COMPRH *Z. Naturforsch., Teil B*, 1980, **35**, 1104.
COMSUS *J. Chem. Soc., Chem. Commun.*, 1984, 1689.
COMTBH *Inorg. Chem.*, 1979, **18**, 3037.
COMYUY *Organometallics*, 1984, **3**, 1495.
CONBIQ *J. Organomet. Chem.*, 1984, **276**, 99.
CONFEQ01 *J. Am. Chem. Soc.*, 1984, **106**, 5458.
CONKEV *J. Chem. Soc., Dalton Trans.*, 1984, 1343.
CONSON *J. Chem. Soc., Dalton Trans.*, 1984, 1781.
CONSUT *J. Chem. Soc., Dalton Trans.*, 1984, 1781.
CONTEE *J. Chem. Soc., Chem. Commun.*, 1984, 1283.
COPFOC *Acta Crystallogr., Sect. C*, 1984, **40**, 2030.
COPGAP *Acta Crystallogr., Sect. C*, 1984, **40**, 2035.
COPHAV *Acta Crystallogr., Sect. B*, 1980, **36**, 304.
COPKEX *J. Chem. Soc., Chem. Commun.*, 1985, 16.
COPLEY *J. Am. Chem. Soc.*, 1984, **106**, 5729.
COPMEZ *J. Organomet. Chem.*, 1984, **273**, C29.
COPMID *J. Organomet. Chem.*, 1984, **273**, C39.
COPNIR *J. Organomet. Chem.*, 1980, **197**, 95.
COPVIM *J. Am. Chem. Soc.*, 1984, **106**, 5178.
COPVOS *J. Am. Chem. Soc.*, 1984, **106**, 5178.
COPXIO *J. Am. Chem. Soc.*, 1984, **106**, 6305.
CORHOG *J. Am. Chem. Soc.*, 1984, **106**, 4478.
COSLAX *Bull. Chem. Soc. Jpn.*, 1984, **57**, 1809.
COSLEB *Bull. Chem. Soc. Jpn.*, 1984, **57**, 1809.
COSLIF *Bull. Chem. Soc. Jpn.*, 1984, **57**, 1809.
COSMOM *J. Chem. Soc., Chem. Commun.*, 1984, 1710.
COSROR *J. Organomet. Chem.*, 1984, **275**, 63.
COSSAE *J. Organomet. Chem.*, 1984, **273**, 221.
COSSOS *Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 640.
COSTEJ *Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 626.
COSTIN *J. Organomet. Chem.*, 1984, **276**, 79.
COSWUC *Acta Crystallogr., Sect. C*, 1985, **41**, 27.
COSZOZ *J. Am. Chem. Soc.*, 1984, **106**, 6841.
COTDOE *J. Organomet. Chem.*, 1984, **270**, 365.
COTFAS *J. Organomet. Chem.*, 1984, **273**, 333.
COTFEW *J. Organomet. Chem.*, 1984, **273**, 111.
COTFPT *J. Chem. Soc., Dalton Trans.*, 1980, 2095.
COTGEX *Inorg. Chem.*, 1984, **23**, 2867.
COTPOQ01 *Acta Crystallogr., Sect. B*, 1984, **40**, 606.
COTROP *J. Chem. Soc., Dalton Trans.*, 1975, 1898.
COTROQ *Aust. J. Chem.*, 1979, **32**, 1219.
COTSEJ *Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 160.
COTTIC10 *J. Organomet. Chem.*, 1975, **92**, 329.
COTZRF *J. Organomet. Chem.*, 1972, **42**, 129.
COTZRH10 *Inorg. Chem.*, 1975, **14**, 3053.
COVBIY *Inorg. Chem.*, 1984, **23**, 2853.
COVROU *J. Chem. Soc., Chem. Commun.*, 1984, 1585.
COVVUE *J. Organomet. Chem.*, 1984, **273**, 361.
COVYIV *J. Chem. Soc., Chem. Commun.*, 1985, 178.
COWGEA *Angew. Chem., Int. Ed. Engl.*, 1984, **23**, 740.
COWSOW *Acta Crystallogr., Sect. C*, 1985, **41**, 55.
CPAINC *J. Chem. Soc., Dalton Trans.*, 1979, 83.
CPASRU *Inorg. Chem.*, 1979, **18**, 2658.
CPBORN *Z. Naturforsch., Teil B*, 1978, **33**, 1410.
CPBUMO *J. Chem. Soc., Dalton Trans.*, 1973, 2629.
CPBZTB *J. Am. Chem. Soc.*, 1980, **102**, 6744.
CPCBCR *Chem. Ber.*, 1979, **112**, 1320.
CPCDSV *J. Chem. Soc., Dalton Trans.*, 1979, 1612.
CPCFEA10 *Inorg. Chem.*, 1982, **21**, 1321.
CPCLBT *Zh. Strukt. Khim.*, 1976, **17**, 1073.
CPCMZW *Inorg. Chem.*, 1979, **18**, 2423.
CPCOPT *J. Am. Chem. Soc.*, 1973, **95**, 2175.
CPDYSW10 *J. Cryst. Mol. Struct.*, 1972, **2**, 135.
CPETNB *J. Am. Chem. Soc.*, 1974, **96**, 5420.
CPFMPI10 *J. Chem. Soc., Dalton Trans.*, 1975, 291.
CPFPEY *J. Chem. Soc., Dalton Trans.*, 1974, 2025.
CPFPTI10 *J. Am. Chem. Soc.*, 1983, **105**, 416.
CPFVLV *J. Organomet. Chem.*, 1980, **197**, 217.
CPFYBA10 *Inorg. Chem.*, 1980, **19**, 2999.
CPHMOC *J. Organomet. Chem.*, 1981, **212**, 77.
CPHSTH *Acta Crystallogr., Sect. B*, 1980, **36**, 292.
CPHSVB *Inorg. Chem.*, 1980, **19**, 2755.
CPITTI *Acta Crystallogr., Sect. B*, 1976, **32**, 909.
CPMNTI *Acta Crystallogr., Sect. B*, 1976, **32**, 909.
CPMPTA *J. Chem. Soc., Dalton Trans.*, 1981, 793.
CPNOCC10 *J. Chem. Soc. A*, 1970, 605.
CPOMOA *J. Am. Chem. Soc.*, 1981, **103**, 1269.
CPPHZR *J. Organomet. Chem.*, 1981, **204**, 67.
CPPYMO10 *Acta Crystallogr., Sect. B*, 1977, **33**, 2608.
CPPYYB01 *Inorg. Chem.*, 1977, **16**, 2710.
CPSENI *Inorg. Chim. Acta*, 1980, **39**, 111.
CPSNBA *Acta Crystallogr., Sect. B*, 1980, **36**, 2986.
CPSNBB *Acta Crystallogr., Sect. B*, 1980, **36**, 2986.
CPSXER *Inorg. Chem.*, 1976, **15**, 797.
CPTCFF *J. Organomet. Chem.*, 1979, **179**, 187.
CPTHGD10 *J. Organomet. Chem.*, 1980, **192**, 65.
CPTICN10 *J. Chem. Soc., Dalton Trans.*, 1979, 152.
CPTIOO *J. Am. Chem. Soc.*, 1977, **99**, 5829.
CPTOMN *J. Chem. Soc., Chem. Commun.*, 1977, 404.
CPTPHF *J. Am. Chem. Soc.*, 1976, **98**, 2454.
CPYBHF *J. Chem. Soc., Chem. Commun.*, 1980, 810.
CPYRTI10 *Inorg. Chem.*, 1980, **19**, 2368.
CPZHZN *J. Chem. Soc., Dalton Trans.*, 1976, 447.
CPZRHF10 *Inorg. Chem.*, 1975, **14**, 352.
CRMTBH *Inorg. Chem.*, 1979, **18**, 3037.
CROPPH10 *Inorg. Chem.*, 1982, **21**, 657.
CSACTI *Cryst. Struct. Commun.*, 1980, **9**, 469.
CSCREC *Inorg. Chem.*, 1966, **5**, 1189.
CSTPRH *Inorg. Chem.*, 1969, **8**, 1921.
CTAZPD10 *Inorg. Chem.*, 1976, **15**, 2428.
CTDPIR *Inorg. Chem.*, 1980, **19**, 2733.
CTENCO20 *Acta Crystallogr., Sect. B*, 1975, **31**, 85.
CTERUC *J. Am. Chem. Soc.*, 1968, **90**, 5412.
CTHUCO10 *Inorg. Chem.*, 1969, **8**, 2367.
CTMPTC *J. Chem. Soc., Dalton Trans.*, 1976, 125.
CTMSIC *J. Chem. Soc., Dalton Trans.*, 1980, 2010.
CTNSCR10 *Inorg. Chem.*, 1979, **18**, 3548.
CTPIRB *J. Chem. Soc., Dalton Trans.*, 1979, 117.
CTZPRU *Inorg. Chem.*, 1973, **12**, 1676.
CUCOES *Bull. Chem. Soc. Jpn.*, 1978, **51**, 2920.
CUDPTZ10 *Aust. J. Chem.*, 1975, **28**, 2377.
CUMPCO *J. Organomet. Chem.*, 1976, **113**, 57.
CUSGAY *Inorg. Chem.*, 1984, **23**, 4758.
CUTROP01 *Acta Crystallogr., Sect. B*, 1978, **34**, 3071.
CVMOMP10 *Inorg. Chem.*, 1974, **13**, 1667.
CXFMPR *J. Chem. Soc., Dalton Trans.*, 1976, 390.
CXINPR10 *J. Organomet. Chem.*, 1976, **120**, 361.
CXPHOW *Acta Crystallogr., Sect. B*, 1978, **34**, 762.
CXPORH *J. Organomet. Chem.*, 1974, **71**, 125.
CYCRTF *J. Organomet. Chem.*, 1977, **131**, 65.
CYPRMO *Inorg. Chem.*, 1975, **14**, 98.
CYPRZR10 *Inorg. Chem.*, 1980, **19**, 2368.
CYSFAC10 *Inorg. Chem.*, 1968, **7**, 1770.
CYZNIC10 *Koord. Khim.*, 1979, **5**, 585.
DAESCO *Acta Chem. Scand., Ser. A*, 1978, **32**, 501.
DAPRCX *Finn. Chem. Lett.*, 1978, 58.
DAPSCR10 *Inorg. Chem.*, 1976, **15**, 1814.
DAPSMO *Aust. J. Chem.*, 1979, **32**, 1199.
DASTCA10 *Acta Crystallogr., Sect. B*, 1980, **36**, 1662.
DAZHCF *J. Am. Chem. Soc.*, 1977, **99**, 3293.
DAZRUC10 *J. Am. Chem. Soc.*, 1977, **99**, 6588.
DBEZHG *Acta Crystallogr., Sect. B*, 1979, **35**, 746.
DCAZPD *Inorg. Chem.*, 1975, **14**, 2475.
DCHPDY10 *J. Chem. Soc., Dalton Trans.*, 1980, 1300.
DCHPLU10 *J. Chem. Soc., Dalton Trans.*, 1980, 1300.
DCMCPD *Inorg. Chem.*, 1977, **16**, 2403.
DEDTFE10 *Inorg. Chem.*, 1977, **16**, 2691.
DETSOK *J. Am. Chem. Soc.*, 1985, **107**, 7212.

DFBENV *Inorg. Chem.*, 1976, **15**, 2976.
DIPNIP *Z. Naturforsch., Teil B*, 1979, **34**, 1289.
DMDECO01 *Acta Crystallogr., Sect. B*, 1979, **35**, 2547.
DMDTPN10 *Acta Crystallogr., Sect. B*, 1969, **25**, 1939.
DMHERU01 *J. Chem. Soc., Dalton Trans.*, 1978, 1040.
DMPCOV *Chem. Ber.*, 1978, **111**, 3472.
DMPMPW10 *Inorg. Chem.*, 1979, **18**, 2454.
DMPZCO *Can. J. Chem.*, 1979, **57**, 3119.
DMPZFE *Can. J. Chem.*, 1979, **57**, 3119.
DMSOHG *Acta Chem. Scand., Ser. A*, 1978, **32**, 95.
DMXPMO10 *Inorg. Chem.*, 1978, **17**, 2087.
DPCBWC *J. Am. Chem. Soc.*, 1977, **99**, 2127.
DPCLRE10 *Koord. Khim.*, 1977, **3**, 1060.
DPEPOW *J. Organomet. Chem.*, 1972, **34**, 353.
DPINRE *Chem. Ber.*, 1978, **111**, 2067.
DPKEVB *Inorg. Chem.*, 1981, **20**, 1173.
DPPTCC *Acta Crystallogr., Sect. B*, 1980, **36**, 159.
DPSCMN *J. Am. Chem. Soc.*, 1973, **95**, 783.
DPSEHG01 *Z. Naturforsch., Teil B*, 1978, **33**, 1227.
DSENCO *Inorg. Chem.*, 1980, **19**, 2545.
DTCPPD10 *J. Chem. Soc., Dalton Trans.*, 1976, 572.
DTHCUC *J. Chem. Soc., Dalton Trans.*, 1978, 416.
DTPANI10 *J. Chem. Soc., Dalton Trans.*, 1977, 2315.
EAPZNI *Can. J. Chem.*, 1979, **57**, 3099.
ECYFTI *J. Coord. Chem.*, 1974, **4**, 71.
EDTCIR *J. Chem. Soc., Dalton Trans.*, 1976, 32.
EDTCMO *Inorg. Chem.*, 1973, **12**, 2179.
EFASCO01 *Acta Crystallogr., Sect. B*, 1982, **38**, 2541.
EFMCPV *Inorg. Chem.*, 1979, **18**, 2282.
EFUMNI *J. Organomet. Chem.*, 1976, **110**, 129.
EINICI *Inorg. Chem.*, 1979, **18**, 1109.
EMABOB *J. Organomet. Chem.*, 1980, **191**, 15.
EMASOU10 *J. Inorg. Nucl. Chem.*, 1974, **36**, 1999.
EMTCTJ *J. Am. Chem. Soc.*, 1979, **101**, 5268.
EMTCZR *Inorg. Chem.*, 1978, **17**, 2120.
ENAZPU10 *Inorg. Chem.*, 1970, **9**, 2768.
ENGUPD *Can. J. Chem.*, 1980, **58**, 381.
ENSPAU *Acta Crystallogr., Sect. B*, 1975, **31**, 370.
EOBCPT10 *J. Chem. Soc., Dalton Trans.*, 1979, 684.
EPAILA *J. Chem. Soc., Chem. Commun.*, 1979, 774.
EPMSPN11 *Acta Crystallogr., Sect. B*, 1982, **38**, 748.
EPPTPD *Acta Crystallogr., Sect. B*, 1975, **31**, 2691.
ESALTJ *J. Chem. Soc., Dalton Trans.*, 1978, 545.
ESCTHW20 *J. Chem. Soc., Dalton Trans.*, 1981, 506.
ESEXFE10 *Inorg. Chem.*, 1970, **9**, 2775.
ESICRE *Inorg. Chem.*, 1977, **16**, 2321.
ESITCO *J. Am. Chem. Soc.*, 1971, **93**, 7156.
ETACHG *Aust. J. Chem.*, 1979, **32**, 311.
ETCOXV *J. Chem. Soc., Dalton Trans.*, 1976, 26.
ETDYRE *Chem. Ber.*, 1981, **114**, 867.
ETNTCD *Koord. Khim.*, 1980, **6**, 1606.
ETPSCO10 *Chem. Ber.*, 1983, **116**, 1441.
ETPSTI *Z. Anorg. Allg. Chem.*, 1981, **472**, 133.
ETXACR10 *Acta Crystallogr., Sect. B*, 1974, **30**, 2788.
EXAPYZ *Aust. J. Chem.*, 1976, **29**, 731.
EXPHCO *J. Organomet. Chem.*, 1978, **150**, 279.
EXPNCD *Aust. J. Chem.*, 1976, **29**, 739.
EYCCMN *Inorg. Chem.*, 1979, **18**, 3483.
EYPCOS *Inorg. Chem.*, 1979, **18**, 156.
EYPIPD *J. Organomet. Chem.*, 1977, **129**, 273.
FACCRE *Inorg. Chem.*, 1978, **17**, 176.
FACMNB *Inorg. Chem.*, 1981, **20**, 1287.
FACTNI *Acta Crystallogr., Sect. B*, 1981, **37**, 240.
FAHGME *J. Chem. Soc., Chem. Commun.*, 1974, 646.
FAHGME10 *Cryst. Struct. Commun.*, 1982, **11**, 565.
FAMPMO *J. Am. Chem. Soc.*, 1980, **102**, 1558.
FAPZTH10 *Inorg. Chem.*, 1976, **15**, 1827.
FATBOS10 *J. Organomet. Chem.*, 1983, **259**, 215.
FBSIMO *Inorg. Chem.*, 1981, **20**, 199.
FDMSON *J. Chem. Soc., Dalton Trans.*, 1975, 2171.
FEBUTS10 *Inorg. Chem.*, 1970, **9**, 2430.
FEFRMT *Acta Crystallogr., Sect. B*, 1980, **36**, 3107.
FEHPYO *Aust. J. Chem.*, 1978, **31**, 713.
FEPICA *Inorg. Chem.*, 1980, **19**, 658.
FLCPNI *J. Fluorine Chem.*, 1980, **16**, 339.
FLDXCO10 *J. Chem. Soc., Dalton Trans.*, 1982, 337.
FLMECE *Inorg. Chem.*, 1980, **19**, 3553.
FMBCNI *J. Chem. Soc., Dalton Trans.*, 1975, 2466.
FMBTMO *J. Chem. Soc., Chem. Commun.*, 1979, 410.
FMEACA10 *J. Organomet. Chem.*, 1981, **220**, 239.
FMPENR *Acta Crystallogr., Sect. B*, 1977, **33**, 319.
FMPHNI *Inorg. Chem.*, 1978, **17**, 3478.
FMPZCO *Cryst. Struct. Commun.*, 1976, **5**, 441.
FMSEPD *Inorg. Chem.*, 1979, **18**, 1129.
FMTPHG *Acta Crystallogr., Sect. B*, 1979, **35**, 1770.
FPCYTP10 *Koord. Khim.*, 1976, **2**, 278.
FPOTIP *Helv. Chim. Acta*, 1972, **55**, 2990.
FSCUCO *Inorg. Chem.*, 1980, **19**, 2945.
FSMICO *J. Am. Chem. Soc.*, 1976, **98**, 5153.
FTLAMN *Inorg. Chem.*, 1980, **19**, 2740.
GEIAYB10 *Koord. Khim.*, 1983, **9**, 1131.
HAPZPT10 *J. Am. Chem. Soc.*, 1977, **99**, 5277.
HBHOSM *J. Chem. Soc., Dalton Trans.*, 1979, 1983.
HBMPMO *J. Chem. Soc., Dalton Trans.*, 1980, 467.
HBTHFY *Inorg. Chem.*, 1978, **17**, 844.
HBUPRH *J. Chem. Soc., Chem. Commun.*, 1979, 498.
HCYPMO02 *Inorg. Chem.*, 1977, **16**, 3303.
HDYCMN *J. Chem. Soc., Dalton Trans.*, 1979, 1630.
HENAEB *Zh. Neorg. Khim.*, 1980, **25**, 1999.
HEPPTB *Can. J. Chem.*, 1978, **56**, 1773.
HETALA11 *Koord. Khim.*, 1982, **8**, 1688.
HETCRB10 *J. Am. Chem. Soc.*, 1981, **103**, 6073.
HETPOS *J. Chem. Soc., Chem. Commun.*, 1981, 801.
HETSRE *Inorg. Chem.*, 1977, **16**, 2325.
HETXCU *Inorg. Chem.*, 1978, **17**, 3034.
HFCATH *Inorg. Chem.*, 1979, **18**, 1611.
HFURMN *J. Organomet. Chem.*, 1980, **197**, 357.
HGETCB10 *Acta Crystallogr., Sect. B*, 1973, **29**, 2115.
HGTXZO *Acta Crystallogr., Sect. B*, 1979, **35**, 1702.
HGXIMC *J. Chem. Soc., Dalton Trans.*, 1976, 96.
HIMPDA *J. Chem. Soc., Dalton Trans.*, 1980, 1992.
HISTPD *Acta Crystallogr., Sect. B*, 1976, **32**, 2472.
HMPCIC01 *J. Am. Chem. Soc.*, 1978, **100**, 3071.
HMPEZR *J. Am. Chem. Soc.*, 1980, **102**, 4941.
HMTCRC10 *Acta Crystallogr., Sect. B*, 1975, **31**, 423.
HMTNRH *Cryst. Struct. Commun.*, 1979, **8**, 1011.
HMTZCR *Inorg. Chem.*, 1977, **16**, 1055.
HMYCFE01 *J. Am. Chem. Soc.*, 1981, **103**, 1485.
HNBPRH10 *Inorg. Chem.*, 1976, **15**, 2462.
HOSTBC10 *Inorg. Chem.*, 1979, **18**, 1909.
HPCXNI *Inorg. Chem.*, 1977, **16**, 1127.
HPETOS *J. Chem. Soc., Dalton Trans.*, 1981, 788.
HPHOMO10 *Acta Crystallogr., Sect. B*, 1972, **28**, 1278.
HPMCRH11 *Inorg. Chem.*, 1984, **23**, 1828.
HPMXCW10 *Z. Anorg. Allg. Chem.*, 1979, **455**, 43.
HPNONI *Acta Crystallogr., Sect. B*, 1980, **36**, 1944.
HPSCIR *Acta Crystallogr., Sect. B*, 1976, **32**, 1513.
HPZPOS *Inorg. Chem.*, 1975, **14**, 2617.
HTEMOA *Z. Anorg. Allg. Chem.*, 1981, **473**, 91.
HTSIXI10 *J. Organomet. Chem.*, 1979, **164**, 371.
HXETOW10 *J. Am. Chem. Soc.*, 1981, **103**, 6093.
HYBIOS *Inorg. Chem.*, 1979, **18**, 2255.
HZBTFE *Z. Naturforsch., Teil B*, 1978, **33**, 1341.
IATCNI *Rec. J. R. Neth. Chem. Soc.*, 1980, **99**, 65.
IBTCPT *Inorg. Chem.*, 1978, **17**, 394.
ICNPCU10 *Acta Crystallogr., Sect. B*, 1982, **38**, 2145.
ICNPIR *Inorg. Chem.*, 1969, **8**, 1282.
ICPNMN *Acta Crystallogr., Sect. B*, 1980, **36**, 1933.
IFPPAU *J. Chem. Soc., Dalton Trans.*, 1972, 1481.
IMDZAG *J. Chem. Soc., Dalton Trans.*, 1980, 1682.
IMIDZA *Z. Anorg. Allg. Chem.*, 1980, **464**, 187.
IMNPTA10 *Inorg. Chem.*, 1981, **20**, 2899.
IMZCUN *J. Chem. Soc., Dalton Trans.*, 1975, 263.
IMZZNN *J. Am. Chem. Soc.*, 1978, **100**, 6063.
INDCEP *Acta Crystallogr., Sect. B*, 1979, **35**, 457.
INDMTI *Inorg. Chem.*, 1975, **14**, 1757.
INDRHA *J. Chem. Soc., Dalton Trans.*, 1981, 400.
INDRHB *J. Chem. Soc., Dalton Trans.*, 1981, 400.
IPHPRU *J. Chem. Soc., Dalton Trans.*, 1977, 366.
IPPHWH01 *Inorg. Chem.*, 1984, **23**, 4103.

IPRNIP *Tetrahedron Lett.*, 1972, 1457.
IPTXMO *Inorg. Chem.*, 1978, **17**, 414.
IPVRUB *J. Chem. Soc., Chem. Commun.*, 1981, 476.
IRCNIR *Inorg. Chem.*, 1980, **19**, 3168.
IRTCPP10 *J. Am. Chem. Soc.*, 1971, **93**, 2391.
ISNHSM *Inorg. Chem.*, 1979, **18**, 2045.
ITDASC *Inorg. Chem.*, 1975, **14**, 624.
KCPTCR01 *Inorg. Chem.*, 1981, **20**, 158.
KCUDED10 *Inorg. Chem.*, 1976, **15**, 1853.
KOXHFP10 *Acta Crystallogr., Sect. B*, 1977, **33**, 3126.
KXOXRE *Acta Crystallogr., Sect. B*, 1975, **31**, 1594.
LDHPCR10 *J. Chem. Soc., Dalton Trans.*, 1977, 1604.
LIBCRC *J. Chem. Soc., Dalton Trans.*, 1980, 1863.
MABUMO10 *J. Organomet. Chem.*, 1977, **129**, 91.
MADCZB10 *Acta Crystallogr., Sect. B*, 1976, **32**, 1687.
MAEMAZ11 *Acta Crystallogr., Sect. B*, 1980, **36**, 2950.
MALCDB *Koord. Khim.*, 1980, **6**, 793.
MALLPT *J. Organomet. Chem.*, 1975, **90**, 111.
MAMPZN *Acta Crystallogr., Sect. B*, 1977, **33**, 1310.
MAQUNI10 *J. Chem. Soc., Dalton Trans.*, 1975, 2494.
MARHAA10 *J. Chem. Soc. A*, 1971, 817.
MASBCM *J. Chem. Soc., Dalton Trans.*, 1974, 783.
MAUFMS *Inorg. Chem.*, 1977, **16**, 2138.
MAZCOC *J. Am. Chem. Soc.*, 1981, **103**, 1431.
MBZACR *Inorg. Chem.*, 1979, **18**, 3566.
MBZCRC *J. Organomet. Chem.*, 1975, **94**, 409.
MBZCRP *J. Organomet. Chem.*, 1975, **101**, 209.
MCBCMN *J. Organomet. Chem.*, 1977, **139**, C68.
MCECZN *J. Am. Chem. Soc.*, 1973, **95**, 1170.
MCENCR *Inorg. Chem.*, 1973, **12**, 2690.
MCETMN *J. Chem. Soc., Dalton Trans.*, 1977, 1077.
MCHFHB10 *J. Am. Chem. Soc.*, 1978, **100**, 2709.
MCPEIR *Inorg. Chem.*, 1976, **15**, 58.
MCPNZR *J. Am. Chem. Soc.*, 1976, **98**, 8351.
MCPYBC *Inorg. Chem.*, 1975, **14**, 1376.
MCTCEW *J. Chem. Soc., Chem. Commun.*, 1979, 30.
MCYTAG10 *Inorg. Chem.*, 1979, **18**, 240.
MDNCAZ10 *Inorg. Chem.*, 1978, **17**, 444.
MEAZAU *Inorg. Chem.*, 1981, **20**, 853.
MEDOFE10 *J. Org. Chem.*, 1981, **46**, 3630.
MEGUHG *J. Chem. Soc., Dalton Trans.*, 1980, 1693.
MEIMMN *Acta Crystallogr., Sect. B*, 1976, **32**, 687.
MEKTMO *Acta Crystallogr., Sect. B*, 1975, **31**, 297.
MENTFE *J. Am. Chem. Soc.*, 1974, **96**, 6519.
MEOBFE *J. Organomet. Chem.*, 1981, **208**, 353.
MEORHC *J. Chem. Soc., Dalton Trans.*, 1980, 2467.
MEPEFE10 *Organometallics*, 1983, **2**, 1220.
MEPGFE *Can. J. Chem.*, 1979, **57**, 3113.
MEPOSW *J. Am. Chem. Soc.*, 1981, **103**, 817.
MEPRUA *J. Chem. Soc., Dalton Trans.*, 1980, 1771.
MEPZFE *Inorg. Chem.*, 1980, **19**, 3655.
MERQCD10 *Latv. PSR Zinat. Akad. Vestis, Kim. Ser.*, 1979, 259.
MESACV *Acta Crystallogr., Sect. B*, 1978, **34**, 1842.
MESOCO *Inorg. Chem.*, 1976, **15**, 2758.
MESTCR *J. Organomet. Chem.*, 1981, **210**, 211.
METHGD *Aust. J. Chem.*, 1979, **32**, 1165.
MICPIR10 *J. Chem. Soc., Dalton Trans.*, 1978, 1119.
MINCNI *J. Coord. Chem.*, 1971, **1**, 275.
MNACAZ30 *Inorg. Chem.*, 1975, **14**, 722.
MNAZHG *Transition Met. Chem.*, 1981, **6**, 86.
MNMTBH *Inorg. Chem.*, 1979, **18**, 3037.
MNPHCY03 *Acta Crystallogr., Sect. B*, 1980, **36**, 2963.
MNPROP *Acta Crystallogr., Sect. B*, 1977, **33**, 2964.
MNTPPI10 *J. Am. Chem. Soc.*, 1977, **99**, 2557.
MNXCMN *J. Organomet. Chem.*, 1978, **146**, 39.
MOBOCO10 *J. Chem. Soc., Dalton Trans.*, 1974, 1876.
MODIPT *Inorg. Chem.*, 1981, **20**, 633.
MOPAZW *Inorg. Chem.*, 1980, **19**, 1450.
MORTMN *J. Am. Chem. Soc.*, 1976, **98**, 5159.
MOSHIS10 *J. Chem. Soc., Dalton Trans.*, 1975, 1077.
MOTCMN *J Chem. Soc., Dalton Trans.*, 1975, 2517.
MOTCRH *J. Chem. Soc., Dalton Trans.*, 1975, 2517.
MPASCO *Can. J. Chem.*, 1977, **55**, 438.
MPAUSN *Acta Crystallogr., Sect. B*, 1978, **34**, 278.
MPBMOE10 *J. Chem. Soc., Dalton Trans.*, 1982, 429.
MPCRCO *Chem. Ber.*, 1978, **111**, 3472.
MPEYCR10 *J. Chem. Soc., Dalton Trans.*, 1983, 671.
MPFPNI *J. Chem. Soc., Dalton Trans.*, 1972, 670.
MPMYRU *J. Am. Chem. Soc.*, 1979, **101**, 4128.
MPNDAG *Inorg. Chem.*, 1975, **14**, 632.
MPORFE10 *Inorg. Chem.*, 1983, **22**, 2982.
MPPCDC *Inorg. Chim. Acta*, 1980, **38**, 191.
MPPDBN *J. Chem. Soc., Chem. Commun.*, 1978, 322.
MPRUAC *S. Afr. J. Chem.*, 1978, **31**, 155.
MPTBRH *J. Chem. Soc., Dalton Trans.*, 1980, 804.
MPTCRH *J. Chem. Soc., Dalton Trans.*, 1976, 1713.
MPYOER10 *Cryst. Struct. Commun.*, 1981, **10**, 703.
MPZHZN *J. Chem. Soc., Dalton Trans.*, 1976, 447.
MSEUHG *J. Organomet. Chem.*, 1979, **172**, 201.
MSIPEP *J. Chem. Soc., Dalton Trans.*, 1979, 1749.
MSISMN *J. Organomet. Chem.*, 1973, **47**, 403.
MSORHB *Inorg. Chem.*, 1980, **19**, 2347.
MSTPPT *Transition Met. Chem.*, 1979, **4**, 147.
MTPAPT *Acta Crystallogr., Sect. B*, 1971, **27**, 73.
MTXPVE *J. Am. Chem. Soc.*, 1973, **95**, 6046.
MXOXRE10 *J. Chem. Soc., Dalton Trans.*, 1980, 2467.
MYCCMN10 *Inorg. Chem.*, 1982, **21**, 645.
NBCZNB10 *Koord. Khim.*, 1979, **5**, 1103.
NBPCCO *Acta Crystallogr., Sect. B*, 1978, **34**, 1978.
NBPMOX *Inorg. Chem.*, 1976, **15**, 1196.
NCPRHB *J. Organomet. Chem.*, 1980, **192**, 235.
NEPPRE *Inorg. Chem.*, 1967, **6**, 197.
NETNIP02 *Inorg. Chem.*, 1982, **21**, 1729.
NETPRE *Inorg. Chem.*, 1967, **6**, 204.
NIAQAC03 *Kristallografiya*, 1980, **25**, 287.
NIPHTI *J. Am. Chem. Soc.*, 1980, **102**, 6702.
NMEDNI10 *Aust. J. Chem.*, 1981, **34**, 2047.
NMSPEM *Acta Crystallogr., Sect. B*, 1974, **30**, 2778.
NOMPRE *J. Am. Chem. Soc.*, 1980, **102**, 6154.
NPHZIR *Inorg. Chem.*, 1977, **16**, 2462.
NPMCMN *Chem. Ber.*, 1972, **105**, 1230.
NPMCTI *J. Am. Chem. Soc.*, 1976, **98**, 8358.
NPNTAB *J. Am. Chem. Soc.*, 1981, **103**, 169.
NRBIRB *Inorg. Chem.*, 1980, **19**, 3755.
NREDTC10 *J. Chem. Soc., Dalton Trans.*, 1972, 1079.
NSDPRH10 *Inorg. Chem.*, 1977, **16**, 2473.
NSMEDT02 *Acta Crystallogr., Sect. C*, 1984, **40**, 1687.
NSOSPP10 *J. Chem. Soc., Dalton Trans.*, 1975, 463.
NTPAAG *Z. Kristallogr.*, 1980, **152**, 253.
NTPHCU *J. Chem. Soc., Dalton Trans.*, 1975, 1993.
NTPOCE *Inorg. Chem.*, 1971, **10**, 115.
NTPYCR *Inorg. Chim. Acta*, 1977, **22**, 81.
OACPMN *J. Chem. Soc., Chem. Commun.*, 1978, 62.
OACTUR *Acta Crystallogr., Sect. B*, 1976, **32**, 2707.
OAMSCO *Inorg. Chem.*, 1979, **18**, 125.
OATURE *Acta Crystallogr., Sect. B*, 1977, **33**, 944.
OAZPMN10 *Acta Crystallogr., Sect. B*, 1974, **30**, 1635.
OCBTZR *J. Organomet. Chem.*, 1979, **166**, 179.
OCHTPI *J. Am. Chem. Soc.*, 1974, **96**, 5070.
OCPPRE *Inorg. Chem.*, 1968, **7**, 1784.
OCTCMO10 *J. Chem. Soc., Dalton Trans.*, 1982, 187.
ODACND *Acta Chem. Scand.*, 1970, **24**, 3527.
ODMNBR *Inorg. Chem.*, 1980, **19**, 1801.
OHCPLU *J. Chem. Soc., Chem. Commun.*, 1981, 706.
ONBCBU *Koord. Khim.*, 1977, **3**, 1600.
OPENBO10 *Acta Crystallogr., Sect. B*, 1971, **27**, 1582.
OTPCHG *Can. J. Chem.*, 1979, **57**, 2217.
OTPHMO *Inorg. Chem.*, 1980, **19**, 2061.
OXBUDC10 *Inorg. Chem.*, 1978, **17**, 1976.
OXCFOR *Transition Met. Chem.*, 1976, **1**, 151.
OXCOCP10 *Chem. Ber.*, 1979, **112**, 1731.
OXCPSM10 *J. Chem. Soc., Dalton Trans.*, 1978, 1350.
OXMCHF *Inorg. Chem.*, 1976, **15**, 2284.
OXMCUA *Inorg. Chem.*, 1981, **20**, 537.
OXPTCC *J. Am. Chem. Soc.*, 1980, **102**, 1570.
PABZTA *Inorg. Chem.*, 1975, **14**, 1358.
PACPRH10 *Inorg. Chem.*, 1976, **15**, 97.
PAIDMO *Inorg. Chem.*, 1979, **18**, 1634.
PAPMCO10 *Inorg. Chem.*, 1970, **9**, 2211.
PASACR *Acta Crystallogr., Sect. B*, 1979, **35**, 951.

PASETI *Inorg. Chim. Acta*, 1981, **50**, 125.
PASMRE *Aust. J. Chem.*, 1975, **28**, 1201.
PAUELI10 *Inorg. Chem.*, 1977, **16**, 1090.
PAZHGN *Z. Anorg. Allg. Chem.*, 1974, **409**, 1.
PAZMPI *J. Am. Chem. Soc.*, 1976, **98**, 7608.
PAZPPT10 *Inorg. Chem.*, 1976, **15**, 2794.
PBARTC *Inorg. Chem.*, 1975, **14**, 2027.
PBUDRI10 *Inorg. Chem.*, 1980, **19**, 3590.
PCBASC *J. Organomet. Chem.*, 1977, **142**, 195.
PCFMRU10 *J. Cryst. Mol. Struct.*, 1975, **5**, 163.
PCHIRH10 *Inorg. Chem.*, 1982, **21**, 1307.
PCLPIR *Inorg. Chem.*, 1980, **19**, 1231.
PCLTCA10 *Inorg. Chem.*, 1982, **21**, 1941.
PCOPIM10 *J. Organomet. Chem.*, 1979, **172**, 251.
PCPCOS *Inorg. Chem.*, 1980, **19**, 134.
PCPHYB *Inorg. Chem.*, 1976, **15**, 2226.
PCRNIB *Z. Anorg. Allg. Chem.*, 1981, **475**, 109.
PCTATL10 *Inorg. Chem.*, 1980, **19**, 2352.
PCTXCR *Cryst. Struct. Commun.*, 1977, **6**, 835.
PDDMSX10 *Acta Crystallogr.*, 1967, **23**, 788.
PDPMNC *Z. Naturforsch., Teil B*, 1976, **31**, 1166.
PDPMZR10 *J. Am. Chem. Soc.*, 1977, **99**, 6645.
PDTHBA10 *J. Chem. Soc., Dalton Trans.*, 1975, 2250.
PEAMNI *Inorg. Chem.*, 1977, **16**, 1669.
PEYEPP *J. Organomet. Chem.*, 1976, **117**, 91.
PEYHGP *Acta Crystallogr., Sect. B*, 1978, **34**, 3382.
PFPBTI *Inorg. Chem.*, 1978, **17**, 3257.
PGECBC *J. Organomet. Chem.*, 1979, **179**, 215.
PHACCS *Koord. Khim.*, 1980, **6**, 1407.
PHCORE *J. Organomet. Chem.*, 1980, **188**, 367.
PHGMQU *Aust. J. Chem.*, 1978, **31**, 537.
PHGTFA *Izv. Jug. Cent. Krist., Ser. A*, 1976, **11**, 32.
PHHGAC01 *Croat. Chem. Acta*, 1984, **57**, 145.
PHIMDW *J. Chem. Soc., Chem. Commun.*, 1981, 103.
PHPCIR10 *S. Afr. J. Chem.*, 1983, **36**, 85.
PHPECU01 *J. Organomet. Chem.*, 1978, **159**, 441.
PHPNCD *J. Chem. Soc., Chem. Commun.*, 1980, 492.
PHQUMO *Inorg. Chem.*, 1977, **16**, 2970.
PHRLCU *Acta Crystallogr., Sect. B*, 1980, **36**, 2407.
PHSNFE *J. Organomet. Chem.*, 1981, **205**, 193.
PHTHCU01 *Cryst. Struct. Commun.*, 1982, **11**, 1495.
PHTPRE *J. Chem. Soc., Chem. Commun.*, 1978, 825.
PHYZMN *Koord. Khim.*, 1979, **5**, 909.
PIVMNB10 *J. Am. Chem. Soc.*, 1975, **97**, 2712.
PMBPAG10 *Inorg. Chem.*, 1983, **22**, 2356.
PMCBRI *Inorg. Chem.*, 1979, **18**, 1215.
PMCMNB *Inorg. Chem.*, 1973, **12**, 2262.
PMCPUC10 *Organometallics*, 1982, **1**, 170.
PMCZNE *Inorg. Chem.*, 1978, **17**, 388.
PMDTTI10 *Inorg. Chem.*, 1979, **18**, 3069.
PMECAC *Inorg. Chem.*, 1977, **16**, 2367.
PMENIB20 *Inorg. Chem.*, 1978, **17**, 632.
PMISNI *Inorg. Chem.*, 1974, **13**, 2529.
PMPDCU *Acta Crystallogr., Sect. B*, 1979, **35**, 3058.
PMPZAG10 *Acta Crystallogr., Sect. B*, 1979, **35**, 177.
PMYPCW *Inorg. Chem.*, 1973, **12**, 2923.
PNENCO10 *Inorg. Chem.*, 1976, **15**, 2989.
PNMNCP *J. Am. Chem. Soc.*, 1978, **100**, 6766.
PNOLTI *J. Am. Chem. Soc.*, 1980, **102**, 5969.
PNPMOA *J. Am. Chem. Soc.*, 1981, **103**, 398.
POIRID *Transition Met. Chem.*, 1980, **5**, 222.
POSHRH10 *J. Chem. Soc., Dalton Trans.*, 1981, 515.
POTCDR *Inorg. Chem.*, 1972, **11**, 161.
PPCOCO01 *J. Organomet. Chem.*, 1980, **193**, 247.
PPEAUC *Chem. Ber.*, 1977, **110**, 2751.
PPHCHN10 *Inorg. Chem.*, 1969, **8**, 2719.
PPMEIR *Inorg. Chim. Acta*, 1979, **37**, L543.
PPMERH *Inorg. Chim. Acta*, 1979, **37**, L543.
PPZBNI *Inorg. Chim. Acta*, 1976, **17**, 121.
PRNRHC *Inorg. Chem.*, 1981, **20**, 600.
PRNRHD *Inorg. Chem.*, 1981, **20**, 600.
PRXHQV *Inorg. Chem.*, 1973, **12**, 1758.
PRZBAG *J. Chem. Soc., Dalton Trans.*, 1981, 956.
PSIBTI *Inorg. Chem.*, 1978, **17**, 3257.
PSMNPC10 *Inorg. Chem.*, 1975, **14**, 1138.
PSNIMO *Acta Crystallogr., Sect. B*, 1981, **37**, 439.
PSTOSA *J. Am. Chem. Soc.*, 1980, **102**, 6346.
PTCDNI20 *J. Am. Chem. Soc.*, 1972, **94**, 7323.
PTHCZN *J. Am. Chem. Soc.*, 1977, **99**, 1101.
PTHFFE *J. Am. Chem. Soc.*, 1980, **102**, 2302.
PTOCNI10 *J. Chem. Soc., Dalton Trans.*, 1984, 575.
PXBURE *Can. J. Chem.*, 1973, **51**, 1116.
PXTCMO10 *J. Chem. Soc., Dalton Trans.*, 1977, 356.
PYAZCU10 *Acta Crystallogr., Sect. B*, 1972, **28**, 1052.
PYBPIR *J. Chem. Soc., Chem. Commun.*, 1977, 589.
PYDSCU10 *J. Am. Chem. Soc.*, 1976, **98**, 7569.
PYHGAN10 *Cryst. Struct. Commun.*, 1976, **5**, 149.
PYMCXC *Z. Anorg. Allg. Chem.*, 1977, **432**, 203.
PYMOPH *Inorg. Chem.*, 1979, **18**, 3562.
PYRCUD *J. Chem. Soc., Chem. Commun.*, 1980, 906.
PYRMNC *J. Am. Chem. Soc.*, 1976, **98**, 1166.
PYRZNI *Koord. Khim.*, 1980, **6**, 1891.
PYSLCU *Inorg. Chem.*, 1977, **16**, 310.
PYXCDC *J. Inorg. Nucl. Chem.*, 1978, **40**, 1259.
PYZBNI *Cryst. Struct. Commun.*, 1979, **8**, 965.
PYZCUA01 *Acta Crystallogr., Sect. B*, 1975, **31**, 762.
PYZRUA *Inorg. Chem.*, 1981, **20**, 1522.
PYZTCI *J. Am. Chem. Soc.*, 1974, **96**, 3438.
PZALPD10 *J. Cryst. Mol. Struct.*, 1977, **7**, 137.
PZBZRU10 *Inorg. Chem.*, 1975, **14**, 3046.
PZCPTI *Inorg. Chem.*, 1978, **17**, 2074.
RACCAF *J. Chem. Soc., Chem. Commun.*, 1980, 186.
REPETD10 *Inorg. Chem.*, 1966, **5**, 411.
RUCABO *J. Am. Chem. Soc.*, 1980, **102**, 5782.
RUNCPP10 *Helv. Chim. Acta*, 1979, **62**, 2159.
SALASM10 *Inorg. Chem.*, 1977, **16**, 289.
SALEZN *Chem. Pharm. Bull.*, 1979, **27**, 424.
SAZPZR *Inorg. Chem.*, 1979, **18**, 2908.
SCATUR *J. Am. Chem. Soc.*, 1978, **100**, 7882.
SCLIRA10 *Inorg. Chem.*, 1981, **20**, 2691.
SCPDCC *Inorg. Chem.*, 1979, **18**, 3542.
SCQUCO *J. Chem. Soc., Dalton Trans.*, 1981, 1504.
SCYSCR *Inorg. Chem.*, 1977, **16**, 1494.
SDAPOU20 *Acta Crystallogr., Sect. B*, 1979, **35**, 3091.
SECPOS *J. Am. Chem. Soc.*, 1979, **101**, 6577.
SFSTPD *Koord. Khim.*, 1980, **6**, 1115.
SIBONI *J. Organomet. Chem.*, 1980, **191**, 27.
SMHXAZ10 *Inorg. Chem.*, 1979, **18**, 3044.
SMNICD *J. Am. Chem. Soc.*, 1972, **94**, 1858.
SNCOCR *Cryst. Struct. Commun.*, 1980, **9**, 383.
SNSCRB *J. Organomet. Chem.*, 1981, **216**, 245.
SNTLHF *J. Chem. Soc., Chem. Commun.*, 1981, 117.
SOCPRH *Chem. Ber.*, 1981, **114**, 716.
SPCNFE *J. Chem. Soc., Dalton Trans.*, 1980, 1965.
SPHFEC10 *Inorg. Chem.*, 1978, **17**, 2568.
SPPEIR *J. Am. Chem. Soc.*, 1972, **94**, 3413.
STAETC *Inorg. Chem.*, 1978, **17**, 1410.
STETCU *Inorg. Chem.*, 1969, **8**, 2763.
SULPDC10 *Acta Crystallogr., Sect. B*, 1976, **32**, 669.
SULPMS *Inorg. Chem.*, 1976, **15**, 1807.
SXPMNI01 *Inorg. Chem.*, 1976, **15**, 2768.
TABYCP10 *Inorg. Chem.*, 1979, **18**, 171.
TACDRH10 *Zh. Neorg. Khim.*, 1978, **23**, 1044.
TACNIH10 *Acta Chem. Scand., Ser. A*, 1977, **31**, 501.
TACPTH *J. Am. Chem. Soc.*, 1977, **99**, 1775.
TACTHB *Acta Crystallogr., Sect. B*, 1978, **34**, 3770.
TAMHGC *Cryst. Struct. Commun.*, 1977, **6**, 157.
TAMPHG *J. Am. Chem. Soc.*, 1979, **101**, 7729.
TAZCFE *Isr. J. Chem.*, 1977, **15**, 165.
TAZOCO10 *Inorg. Chem.*, 1977, **16**, 271.
TAZRUP10 *Inorg. Chem.*, 1976, **15**, 2788.
TAZTDG *J. Chem. Soc., Dalton Trans.*, 1975, 144.
TBARHC *Inorg. Chem.*, 1971, **10**, 566.
TBCBFE *Chem. Ber.*, 1978, **111**, 3530.
TBIAZR *Inorg. Chem.*, 1979, **18**, 2030.
TBPAHG10 *J. Chem. Soc., Dalton Trans.*, 1978, 253.
TBPCFE *J. Organomet. Chem.*, 1976, **107**, 241.
TCACTC *J. Chem. Soc., Dalton Trans.*, 1977, 1837.
TCACTC01 *Acta Crystallogr., Sect. B*, 1978, **34**, 3359.
TCATPD *Inorg. Chem.*, 1975, **14**, 343.

TCBPNB *Inorg. Chem.*, 1976, **15**, 309.
TCBPZR *Inorg. Chem.*, 1976, **15**, 309.
TCHXPH10 *J. Chem. Soc., Dalton Trans.*, 1977, 1845.
TCMIPD10 *Acta Crystallogr., Sect. C*, 1983, **39**, 186.
TCMNET10 *Phys. Rev. B*, 1979, **19**, 306.
TCMOFM *Transition Met. Chem.*, 1975, **1**, 2.
TCPDNI01 *J. Am. Chem. Soc.*, 1981, **103**, 1942.
TCPMNN10 *Inorg. Chem.*, 1974, **13**, 1037.
TCPNIH11 *J. Am. Chem. Soc.*, 1979, **101**, 5631.
TCPPHG01 *Can. J. Chem.*, 1979, **57**, 2555.
TCTPOS *Inorg. Chem.*, 1969, **8**, 1078.
TCTPPU *Inorg. Chem.*, 1978, **17**, 394.
TCXNTI *J. Chem. Soc., Dalton Trans.*, 1978, 1176.
TCYENI10 *Finn. Chem. Lett.*, 1977, 71.
TCYPSC10 *J. Am. Chem. Soc.*, 1973, **95**, 1488.
TCYPTI10 *J. Am. Chem. Soc.*, 1971, **93**, 3592.
TDACCD10 *Acta Crystallogr., Sect. B*, 1975, **31**, 2531.
TDCURF *Transition Met. Chem.*, 1979, **4**, 82.
TEPPMN01 *Cryst. Struct. Commun.*, 1981, **10**, 1263.
TEPPTB *J. Chem. Soc., Dalton Trans.*, 1980, 1737.
TESTHG *Acta Crystallogr., Sect. B*, 1968, **24**, 935.
TETCPD *J. Am. Chem. Soc.*, 1973, **95**, 8566.
TFMESM *J. Chem. Soc. A*, 1971, 2285.
THMPOS01 *J. Am. Chem. Soc.*, 1977, **99**, 7557.
THUPDC *Bull. Chem. Soc. Jpn.*, 1960, **33**, 861.
TIMCUS *Acta Chem. Scand., Ser. A*, 1974, **28**, 578.
TIOUNB *Inorg. Chem.*, 1969, **8**, 424.
TIUREA01 *Inorg. Chem.*, 1970, **9**, 1111.
TLCSCR *Cryst. Struct. Commun.*, 1980, **9**, 821.
TLTZMO *Inorg. Chem.*, 1981, **20**, 171.
TMAFMN *J. Chem. Soc., Dalton Trans.*, 1979, 1512.
TMAMNB01 *Acta Crystallogr., Sect. B*, 1978, **34**, 1970.
TMDPHG *Cryst. Struct. Commun.*, 1977, **6**, 359.
TMENSN *Finn. Chem. Lett.*, 1977, 75.
TMPCUB01 *J. Am. Chem. Soc.*, 1981, **103**, 5165.
TMPHWE *J. Am. Chem. Soc.*, 1980, **102**, 1431.
TMSCCU *Inorg. Chem.*, 1979, **18**, 761.
TMTCPC *Inorg. Chem.*, 1974, **13**, 1674.
TMTCZN10 *J. Chem. Soc., Dalton Trans.*, 1980, 1945.
TNBPMN *Can. J. Chem.*, 1972, **50**, 3332.
TOPFCO10 *Inorg. Chem.*, 1980, **19**, 1221.
TPACUB *J. Chem. Soc., Chem. Commun.*, 1980, 192.
TPCPTW *J. Am. Chem. Soc.*, 1979, **101**, 7618.
TPCUBF *J. Am. Chem. Soc.*, 1979, **101**, 754.
TPCUMZ *J. Am. Chem. Soc.*, 1972, **94**, 7323.
TPCYCU *J. Am. Chem. Soc.*, 1970, **92**, 2353.
TPHCOA *Inorg. Chem.*, 1980, **19**, 2968.
TPHGDI10 *Acta Crystallogr., Sect. B*, 1978, **34**, 2300.
TPICBO *J. Chem. Soc., Chem. Commun.*, 1980, 80.
TPMCDB10 *J. Chem. Soc., Dalton Trans.*, 1979, 619.
TPPMRH10 *Inorg. Chem.*, 1980, **19**, 2726.
TPPTCC *J. Am. Chem. Soc.*, 1975, **97**, 3952.
TPPTCP01 *J. Chem. Soc. A*, 1970, 2770.
TPRUET21 *J. Cryst. Mol. Struct.*, 1974, **4**, 43.
TPTHCC *Acta Crystallogr., Sect. B*, 1977, **33**, 619.
TPYCLV *Cryst. Struct. Commun.*, 1973, **2**, 421.
TPYRPR *Inorg. Chem.*, 1971, **10**, 1463.
TRENCM *Inorg. Chem.*, 1978, **17**, 457.
TROPRH *Inorg. Chim. Acta*, 1980, **42**, 105.
TROPTH *J. Am. Chem. Soc.*, 1970, **92**, 3626.
TROPUE *J. Cryst. Mol. Struct.*, 1973, **3**, 221.
TTHPHG *J. Chem. Soc., Chem. Commun.*, 1979, 140.
TTPPDB *Zh. Strukt. Khim.*, 1976, **17**, 135.
TTZZCU10 *J. Am. Chem. Soc.*, 1984, **106**, 93.
TUNCPF10 *Acta Crystallogr., Sect. B*, 1974, **30**, 1357.
TURURS01 *Inorg. Chem.*, 1980, **19**, 776.
TXPCPD *Inorg. Chem.*, 1978, **17**, 22.
TZTDAG01 *Inorg. Chem.*, 1978, **17**, 49.
UCHXOS *J. Chem. Soc., Dalton Trans.*, 1979, 562.
UHXAPY10 *Inorg. Chem.*, 1976, **15**, 1827.
URCLNI *Acta Crystallogr., Sect. B*, 1980, **36**, 2251.
URDEAM10 *Inorg. Chem.*, 1976, **15**, 2498.
UREAZN *Cryst. Struct. Commun.*, 1972, **1**, 257.
URMSUL *Acta Crystallogr., Sect. B*, 1978, **34**, 2302.
URSCNI *Kristallografiya*, 1978, **23**, 1196.
URSDUR03 *Inorg. Chem.*, 1983, **22**, 1557.
VCPRUA10 *J. Chem. Soc., Dalton Trans.*, 1983, 2661.
VCPRUE10 *J. Chem. Soc., Dalton Trans.*, 1983, 2661.
VIBONI *J. Organomet. Chem.*, 1981, **215**, 255.
VPHTHC *J. Chem. Soc., Dalton Trans.*, 1980, 2300.
XAXASP *Cryst. Struct. Commun.*, 1978, **7**, 219.
YBAENI *Inorg. Chem.*, 1977, **16**, 1623.
ZEGCET *J. Chem. Soc., Dalton Trans.*, 1982, 1531.
ZEGGUN *Inorg. Chem.*, 1983, **22**, 888.
ZEGNOP *J. Am. Chem. Soc.*, 1984, **106**, 801.
ZEGPEG *Inorg. Chim. Acta*, 1984, **82**, 35.
ZNACAT10 *Acta Crystallogr., Sect. B*, 1968, **24**, 904.
ZTANPB *Inorg. Chem.*, 1975, **14**, 604.
ZZZARD01 *Acta Crystallogr., Sect. C*, 1984, **40**, 781.
ZZZCCG10 *Acta Crystallogr., Sect. B*, 1980, **36**, 1938.

Acknowledgements

We thank the S.E.R.C. for a studentship (to L. B.) and Mrs. Claire Jones for her patient and careful typing of this work.

References

1 L. E. Sutton, 'Tables of Interatomic Distances and Configuration in Molecules and Ions,' *Special Publ.*, The Chemical Society, London, 1958, no. 11.
2 L. E. Sutton, 'Tables of Interatomic Distances and Configuration in Molecules and Ions,' *Special Publ.*, The Chemical Society, London, 1965, no. 18.
3 O. Kennard, 'International Tables for *X*-Ray Crystallography,' Kynoch Press, Birmingham, 1962, vol. 3, pp. 275—276.
4 F. H. Allen, S. Bellard, M. D. Brice, B. A. Cartwright, A. Doubleday, H. Higgs, T. Hummelink, B. G. Hummelink-Peters, O. Kennard, W. D. S. Motherwell, J. R. Rodgers, and D. G. Watson, *Acta Crystallogr., Sect. B*, 1979, **35**, 2331.
5 O. Kennard, D. G. Watson, F. H. Allen, N. W. Isaacs, W. D. S. Motherwell, R. C. Pettersen, and W. G. Town, 'Molecular Structures and Dimensions,' vol. A1, 'Interatomic Distances, 1960—1965,' Oosthoek, Utrecht, 1972.
6 M. D. Harmony, R. W. Laurie, R. L. Kuczkowski, R. H. Schwendemann, D. A. Ramsay, F. J. Lovas, W. J. Lafferty, and A. G. Maki, *J. Phys. Chem. Ref. Data*, 1979, **8**, 619.
7 M. I. Bruce, 'Comprehensive Organometallic Chemistry,' Pergamon, London, 1981, vol. 9, pp. 1209—1520.
8 I. D. Brown, M. C. Brown, and F. C. Hawthorne, BIDICS-1981, Bond Index to the Determinations of Inorganic Crystal Structures, Institute for Materials Research, Hamilton, 1982.
9 D. R. Russell, *Specialist Periodical Reports*, Royal Society of Chemistry, London, 1988, pp. 427—525.
10 F. H. Allen, O. Kennard, D. G. Watson, L. Brammer, A. G. Orpen, and R. Taylor, *J. Chem. Soc., Perkin Trans. 2*, 1987, S1—S19.
11 P. M. Murray-Rust and J. Raftery, *J. Mol. Graphics*, 1985, **3**, 50.
12 P. M. Murray-Rust and J. Raftery, *J. Mol. Graphics*, 1985, **3**, 60.
13 R. Taylor and O. Kennard, *Acta Crystallogr., Sect. B*, 1983, **39**, 517.
14 R. Taylor and O. Kennard, *Acta Crystallogr., Sect. A*, 1985, **41**, 85.
15 R. Taylor and O. Kennard, *J. Chem. Inf. Comput. Sci.*, 1986, **26**, 28.
16 G. Bergerhoff, R. Hundt, R. Sievers, and I. D. Brown, *J. Chem. Inf. Comput. Sci.*, 1983, **23**, 66.

Received 18*th July* 1988; *Paper* 8/02879F