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STEREOCHEMISTRY OF CHROMIUM COMPLEXES: A BIBLIOGRAPHIC LISTING

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Arrangement of the bibliography

Table 1 lists all the chromium complexes whose structures have been determined by X-ray or neutron diffraction and had been published prior to the middle of 1976. The formulae are expressed in terms of abbreviated ligand codes (e.g. acac, cp), a list of which is given in Table 2 and Fig. 2. The complexes in Table 1 and the ligands illustrated in Fig. 2 are both ordered according to increasing ligand electro-negativities, starting with pi-complexes and followed by ligands bonded through C, P, N, S, O and halogen in that order. This brings chemically similar species together and makes the lists easy to search as well as profitable to browse through. Table 2 lists the ligand codes alphabetically with cross references to Fig. 2 and Table 1.

Method of compilation

The information in these tables has been drawn largely from the Organic Crystal Structure Database produced by the Cambridge Crystallographic Data Centre, but it has been supplemented by the addition of 33 carbonyl, cyanide and ammonium complexes that lie outside the range of compounds included in the database. There has been no attempt to include all oxygen, sulphur and halogen complexes. In all other cases the information given in this compilation has been derived directly from the database; only in a few cases was it necessary to consult the original paper. The editing of the database is sufficiently thorough that it has detected numerical errors in 29 of the 147 original papers that publish complete structural information. In a third of these cases it has been possible to correct the errors. Unfortunately, 49 reports of structure determinations contain no atomic coordinates so that in these cases it is impossible to find out more about the stereo-chemistry than the author has chosen to report.

The use of the Cambridge Organic Crystal Structure Database made the preparation of this bibliography remarkably simple. The database, which contains data on all structures containing an organic moiety, was computer searched for compounds containing chromium. Structural information (unit

cell, atomic coordinates, etc.) for these compounds was automatically extracted and used as input to the programs PLOD and GEOM which respectively plot projections of the molecules and print out a comprehensive list of bond lengths and angles. Two or three days work spent in collating these results yielded a collated record of the structural chemistry of chromium complexes that would have taken several weeks of library work to compile by traditional means. Further, this record not only contained a more complete listing of bond distances and angles than was given in the original papers, but was purged of many of the published errors and ambiguities.

List of chromium complexes (Table 1)

The complexes are listed in order of their least electronegative ligand. Thus tricarbonylbenzenechromium comes before pentacarbonyltriphenylphosphinechromium and the ethylenediamine complexes follow both. The complex is described by means of a formula using abbreviated ligand names. The chromium complex is always given first in square brackets. Phase information follows the formula after a hyphen (e.g. "-a" means triclinic form, "-m" means monoclinic form). The alphabetical listing of the ligand abbreviations is given in Table 2.

Following the formula in Table 1 is the formal oxidation state and coordination number of the chromium atom. Since these are not always unambiguous, certain conventions have been adopted for determining the formal charge and number of functional groups of each ligand. All delocalized or alternating double bond systems pi-bonded to the metal are taken as singly coordinating. Likewise C=C groups pi-bonded to the metal are singly coordinating but other double bonded groups (e.g. As=As and O=O) are taken as bidentate. Nitrosyl is taken to have a formal charge of zero and peroxide of −2.

The atoms directly bonded to chromium are listed (CO is listed separately from C) and, for pi-bonded rings, the size of the ring and its heteroatoms (if any) are also given. The stereochemistry is given in part by the order of the ligands in the formula (e.g. [(NCS)2 NH3 (NCS)2 NH3 Cr] is the *trans* isomer, [(NCS)4 (NH3)2 Cr] is the *cis*) and by the number of functional groups in polydentate ligands (given under "Geometry"). Thus 22C and 22T refer respectively to the *cis* and *trans* isomers of complexes with two bidentate ligands, 33C refers to the arrangement of two tridentate ligands with the three functional groups of each ligand mutually *cis*, and 33T refers to the arrangement where each tridentate ligand has its three coordinating atoms planar with the metal.

The bibliographic data for each complex is given in the right-hand side of the entry. It starts with a reference to the original publication in the order: journal coden (ASTM standard — see Table 3), volume, page and year of publication. The accuracy of the determination is indicated by the following code based on the standard error in the length of a typical C—C bond, or, if this is not available, the crystallographic agreement index, *R*.

1 = Error in C—C ≤ 0.005 Å
2 = Error in C—C ≤ 0.010 Å or $R \leq 0.05$
3 = Error in C—C ≤ 0.03 Å or $R \leq 0.15$
4 = Error in C—C > 0.03 Å or $R > 0.15$
5 = No information on accuracy given.

The remaining information refers to the Organic Crystal Structure Database. Class and Refcode refer to the classification and location of the entry in the database. The file status codes have the following meaning:

OK = Full error-free structural information available in the database;
Error in data = The full structural information is in the file but the original publication contains an error which cannot be corrected;
Paper corrected = The original paper contains an error which has been corrected in the database. Equivalent to the status OK;
No coordinates in paper = No atomic coordinates were given in the original publication and therefore they are not available in the database;
Not in file = Complexes which contain no organic fragment are not included in the Organic Crystal Structure Database.

Finally the presence of disorder, the use of neutron diffraction or the determination of the absolute configuration of the complex are noted.

Ligand List (Table 2)

The ligands are listed in alphabetical order of their abbreviations and include to the left, a number referring to the diagram of the ligand in Fig. 2 and to the right, the ligand formula, name and reference to the complexes in Table 1 that contain the ligand. For completeness, the list also includes a number of common ligands not found in the chromium complexes. The diagrams in Fig. 2 are illustrated in the following chemical order:
Pi-bonded rings ordered according to (i) size of the ring, (ii) heterocycles following homocycles, (iii) number of rings fused to the coordinating ring, (iv) increasing substitution of the ring; other C—Cr pi-bonds; C—Cr sigma-bonds starting with carbonyl then in order of increasing electronegativity of the atoms bonded to C; H—Cr; Sn—Cr; As—Cr; P—Cr; N—Cr; S—Cr; O—Cr; Halogen—Cr.

Polydentate ligands follow the monodentate ligands in the same order, thus triphenylphosphine, pi-bonding through a phenyl ring as well as sigma-bonding through P, follows the mondentate pi-bonded rings, whereas monodentate triphenylphosphine appears with the P—Cr group further down the list.

Ligand names are either in the form of mnemonics or formulae. Certain of the mnemonics (e.g. Me, Ph) are written with one upper case and one lower case letter like an element and are used in formulae in the same way as an element symbol. Other mnemonics (e.g. acac) are written only in lower case and stand alone. In formula names, all numbers are to be read as subscripts (e.g. PPh3 represents PPh_3 which is the same as $P(C_6H_5)_3$). Bridging ligands

have names ending in an asterisk (e.g. O*) and those names ending in $1, $2 etc. refer to the same ligand coordinating in different ways (e.g. "cp" is pi-bonded cyclopentadienyl; "cp$1" is sigma-bonded cyclopentadienyl).

Where available, the bond lengths (in picometres = 10^{-2} Å) found in chromium complexes are given in Fig. 2. All chemically equivalent bonds have been averaged. Where two distances are given, they represent the range of observed bond lengths. Unless otherwise shown, C—C bonds in alkyl groups are 154 pm and in benzene rings are 142 pm. C—Cr distances to pi-bonded rings lie between 220 and 230 pm, except in sandwich complexes where they are 208—214 pm.

Nearly half the complexes contain carbonyl groups which, in spite of the relatively poor accuracy of the structure determinations, show a marked correlation between the C—O and Cr—C bond lengths (Fig. 1). For Cr—C—O groups *trans* to a pi-bonded ring, Cr—C = 184 pm, C—O = 115 pm and the Cr—C—O angle deviates by 3.5° (standard deviation) from 180° (modal angle = 178°). For Cr—C—O groups *trans* to a CO group the geometry is slightly different. The Cr—C distance is 190 pm, C—O = 114 pm and the Cr—C—O angle deviates from 180° by 5.1° (standard deviation) (modal angle = 176°). In the pentacarbonyls this larger deviation from linearity is associated with a bending of the equatorial carbonyl groups away from the bulky sixth ligand.

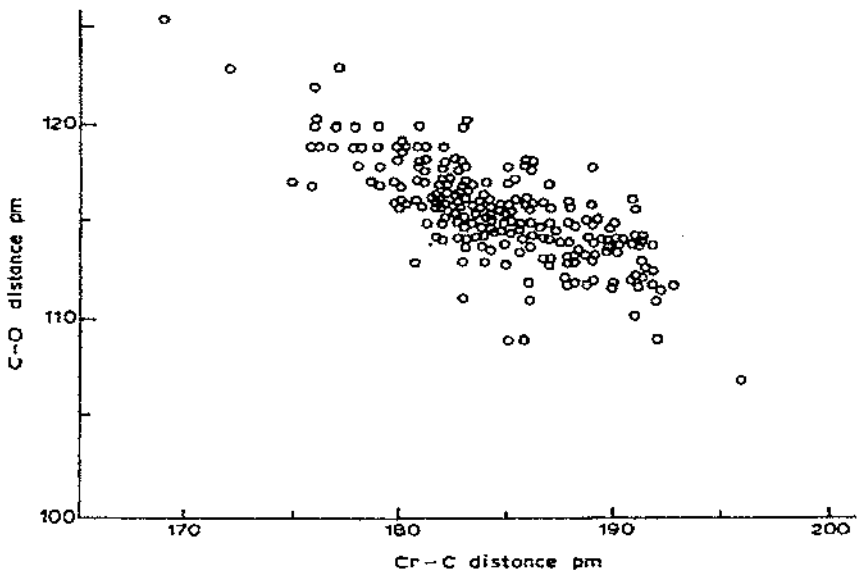


Fig. 1. Observed correlation between Cr—C and C—O distances in chromium carbonyl complexes.

Metal—Metal Bonds

A few binuclear complexes have short Cr—Cr distances, some of which undoubtedly represent metal—metal bonds. A list of these complexes is given in order of increasing metal—metal length.

Cr—Cr distance (pm)	Found in complex number
197	84
198	137–8
228	23
236	227–8
262	18
267	17
295	19
297	196
299	180
328	12

Acknowledgement

This work was carried out during a sabbatical leave spent at the Cambridge Crystallographic Data Centre. The cooperation of the staff of the centre is gratefully acknowledged.

TABLE 1

LIST OF CHROMIUM COMPLEXES IN THE ORGANIC CRYSTAL STRUCTURE DATABASE

Complexes are listed in order of increasing electronegativity of their ligands.
Each complex appears only once under its least electronegative ligand.

Ligand order as follows: Cr-C pi bonds (rings first)
Cr-C sigma bonds (CO first)
Cr, Su, As, P, N, O, I, Br, Cl

SANDWICH COMPLEXES

1 [(bz)2 Cr]

JORCA 5 490 (1966)

Ox.No.= 0 Coord.No.= 2
Size of pi ring = 6

Accuracy = 1
Class = 74

File status = OK
Refcode = DBENCR03

2 [(bz)2 Cr]

JCPSA 40 3129 (1964)

Ox.No.= 0 Coord.No.= 2
Size of pi ring = 6

Accuracy = 5
Class = 74

File status = No coordinates in paper
Refcode = DBENCR02

3 [(bz)2 Cr]

JORCA 1 43 (1963)

Ox.No.= 0 Coord.No.= 2
Size of pi ring = 6

Accuracy = 3
Class = 74

File status = OK
Refcode = DBENCR10

4 [(bz)2 Cr]

JACSA 85 1543 (1963)

Ox.No.= 0 Coord.No.= 2
Size of pi ring = 6

Accuracy = 3
Class = 74

File status = No coordinates in paper
Refcode = DBENCR01

5 [(bz)2 Cr] I

ACBCA 30 838 (1974)

Ox.No.= 1 Coord.No.= 2
Size of pi ring = 6

Accuracy = 3
Class = 74

File status = OK
Refcode = BENCRI

Disordered

6 [(bz)2 Cr] tcnq

DANKA 199 334 (1971)

Ox.No.= 1 Coord.No.= 2
Size of pi ring = 6

Accuracy = 3
Class = 71

File status = OK
Refcode = BCRLQN

7 [(toln)2 Cr] tcnq

CCOMA 1969 649 (1969)

Ox.No.= 1 Coord.No.= 2
Size of pi ring = 6

Accuracy = 3
Class = 74

File status = No coordinates in paper
Refcode = TCRTCQ

8 [(toln)2 Cr] I

ZSTKA 2 162 (1961)

Ox.No.= 1 Coord.No.= 2

Accuracy = 3

File status = OK

SANDWICH COMPLEXES

9 [(tolu)2 Cr] (tcag)2

Ox.No.= 1 Coord.No.= 2
Size of pi ring = 6

ZSTKA 16 147 (1975)

Accuracy = 4 File status = OK
Class = 60 Refcode = DTCRCQ10

Disordered

10 [(PyMe2)2 Cr] - a

Ox.No.= 0 Coord.No.= 2
Size of pi ring = 6 Hetero atom = N

JACSA 98 1044 (1976)

Accuracy = 3 File status = No coordinates in paper
Class = 75 Refcode = DMPICR10

11 [(PyMe2)2 Cr] - o

Ox.No.= 0 Coord.No.= 2
Size of pi ring = 6 Hetero atom = N

JACSA 98 1044 (1976)

Accuracy = 2 File status = No coordinates in paper
Class = 75 Refcode = DMPICR11

COMPLEXES WITH 5 MEMBERED PI BONDED RING

12 [(CO)3 cp Cr]

Ox.No.= 1 Coord.No.= 4
Size of pi ring = 5
Coordinated atoms CO 3,

JACSA 96 749 (1974)

Accuracy = 1 File status = OK
Class = 73 Refcode = CPCOCR

13 [(CO)3 cp Cr SnCl2* Cr cp (CO)3]

Ox.No.= 1 Coord.No.= 5
Size of pi ring = 5
Coordinated atoms CO 3,Sn 1,

JCDTB 1975 230 (1975)

Accuracy = 4 File status = Paper corrected
Class = 73 Refcode = CSNCCR

14 [NO cp (NO)2 Cr]

Ox.No.= 2 Coord.No.= 4
Size of pi ring = 5
Coordinated atoms N 3,

JCSIA 1970 605 (1970)

Accuracy = 3 File status = Paper corrected
Class = 73 Refcode = CPNOCC10

15 [cp NO Cr NO* NH2* Cr NO cp]

Ox.No.= 2 Coord.No.= 4
Size of pi ring = 5
Coordinated atoms N 3,

ACBCA 26 1899 (1970)

Accuracy = 3 File status = OK
Class = 73 Refcode = CPNICR10

Disordered

16 [NO cp Cr (NMe2*)2 Cr cp NO]

Ox.No.= 2 Coord.No.= 4
Size of pi ring = 5
Coordinated atoms N 3,

JCSIA 1970 611 (1970)

Accuracy = 3 File status = OK
Class = 73 Refcode = MACPCC10

Disordered

COMPLEXES WITH 5 MEMBERED PI BONDED RING

17 [NO cp Cr (Nde2*)2 Cr NO cp]

Ox.No.= 2 Coord.No.= 4
Size of pi ring = 5
Coordinated atoms N 3,

JCSIA 1970 611 (1970)

Accuracy = 3 File status = OK
Class = 73 Refcode = RACPCT10

Disordered

18 [NO cp Cr (NO*)2 Cr NO cp]

Ox.No.= 1 Coord.No.= 4
Size of pi ring = 5
Coordinated atoms N 3,

JORCA 64 C10 (1974)

Accuracy = 2 File status = No coordinates in paper
Class = 73 Refcode = NTSCPC

19 [NO cp Cr (SPh*)2 Cr NO cp]

Ox.No.= 2 Coord.No.= 4
Size of pi ring = 5
Coordinated atoms N 1, S 2,

JCSIA 1968 1858 (1968)

Accuracy = 2 File status = OK
Class = 73 Refcode = PSNCPC

20 [cp (NO)2 Cl Cr]

Ox.No.= 2 Coord.No.= 4
Size of pi ring = 5
Coordinated atoms N 2,Cl 1,

JCSIA 1966 1095 (1966)

Accuracy = 3 File status = OK
Class = 73 Refcode = CPNCBC10

Disordered

21 [(Cl)3 cp Cr] (thf)2 diox Li

Ox.No.= 3 Coord.No.= 4
Size of pi ring = 5
Coordinated atoms Cl 3,

JORCA 44 141 (1972)

Accuracy = 3 File status = OK
Class = 67 Refcode = DTLICR

22 [(CO)3 dpful Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 5
Coordinated atoms CO 3,

JCCCA 1975 117 (1975)

Accuracy = 3 File status = No coordinates in paper
Class = 75 Refcode = PFULCR

23 [pmcp Cr (CO*)4 Cr pmcp]

Ox.No.= 1 Coord.No.= 5
Size of pi ring = 5
Coordinated atoms CO 4,

INOCA 13 2540 (1974)

Accuracy = 2 File status = OK
Class = 73 Refcode = PMCPCR10

24 [(CO)3 mapyr Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 5 Hetero atom = N
Coordinated atoms CO 3,

CHBEA 105 301 (1972)

Accuracy = 2 File status = OK
Class = 75 Refcode = CMPYCR

25 [(CO)3 tap Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 5 Hetero atom = S
Coordinated atoms CO 3,

INOCA 4 1306 (1965)

Accuracy = 3 File status = No coordinates in paper
Class = 75 Refcode = TMCRCO

Disordered

COMPLEXES WITH 5 MEMBERED PI BONDED RING

26 [(CO)3 dmcat Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 5 Hetero atom = S
Coordinated atoms CO 3,

ACBCA 29 726 (1973)

Accuracy = 3 File status = OK
Class = 75 Refcode = CHTPCR10

COMPLEXES WITH SIX MEMBERED PI BONDED RING

27 [(CO)3 bz Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

INOCA 4 1314 (1965)

Accuracy = 2 File status = OK
Class = 74 Refcode = BZCRCO

28 [(CO)3 bz Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

AANLA 31 241 (1961)

Accuracy = 2 File status = OK
Class = 74 Refcode = BZCRCO01

29 [(CO)3 bz Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

ACBCA 29 2515 (1973)

Accuracy = 1 File status = OK
Class = 74 Refcode = BZCRCO12
Neutron diffraction

30 [(CO)3 bz Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

ACBCA 29 2515 (1973)

Accuracy = 1 File status = OK
Class = 74 Refcode = BZCRCO13

31 [(CO)2 bdpm Cr]

Ox.No.= 0 Coord.No.= 4 Geometry = 2
Size of pi ring = 6
Coordinated atoms CO 2,As 1,

INOCA 13 1047 (1974)

Accuracy = 2 File status = OK
Class = 74 Refcode = CRCDAM10
Disordered

32 [(CO)3 anis Cr] (C6 H3 (N O2)3)

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

JCSIA 1966 822 (1966)

Accuracy = 3 File status = OK
Class = 60 Refcode = CCATBB

33 [(CO)3 PhCOMe Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

JCSIA 1967 1619 (1967)

Accuracy = 2 File status = OK
Class = 74 Refcode = CRMEBZ

COMPLEXES WITH SIX MEMBERED PI BONDED RING

34 [(CO)3 PhCOMe Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

CHDCA 270 1792 (1970)

Accuracy = 3 File status = OK
Class = 74 Refcode = ACTPCR

35 [(CO)3 Cr biph* Cr (CO)3] - n

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

JACSA 82 2075 (1960)

Accuracy = 4 File status = No coordinates in paper
Class = 74 Refcode = COCRDP

36 [(CO)3 Cr biph* Cr (CO)3] - a

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

AANLA 31 399 (1961)

Accuracy = 4 File status = Paper corrected
Class = 74 Refcode = COCRDP01

37 [(CO)2 CS PhCOOMe Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 2, C 1,

JORCA 94 409 (1975)

Accuracy = 1 File status = OK
Class = 74 Refcode = MBZCRC

38 [(CO)2 PPh3 PhCOOMe Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 2, P 1,

JORCA 101 209 (1975)

Accuracy = 2 File status = OK
Class = 74 Refcode = MBZCRP

39 [(CO)2 Cr (PPh3*)2 Cr (CO)2]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 2, P 1,

JORCA 60 C11 (1973)

Accuracy = 2 File status = No coordinates in paper
Class = 74 Refcode = CTPPCR

40 [(CO)3 acpnoa Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

ACBCA 29 469 (1973)

Accuracy = 4 File status = OK
Class = 74 Refcode = HABENC10

41 [(CO)3 bnbz Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

JORCA 94 47 (1975)

Accuracy = 2 File status = OK
Class = 74 Refcode = BENGLY

42 [(CO)3 bapt Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

JORCA 63 321 (1973)

Accuracy = 3 File status = OK
Class = 74 Refcode = RMBBEN

COMPLEXES WITH SIX MEMBERED PI BONDED RING

43 [(CO)3 hppt Cr] - a

OK.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

JORCA 59 281 (1973)

Accuracy = 4 File status = Error in data
Class = 74 Refcode = MHPBCH11

44 [(CO)3 hppt Cr] - a

OK.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

JORCA 59 281 (1973)

Accuracy = 3 File status = OK
Class = 74 Refcode = MHPBCH10

45 [(CO)3 moacph Cr]

OK.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

ACBCA 29 469 (1973)

Accuracy = 4 File status = OK
Class = 74 Refcode = MABENC10

46 [(CO)3 mohebz Cr]

OK.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

ACBCA 28 3183 (1972)

Accuracy = 3 File status = Error in data
Class = 74 Refcode = MHBCRC10

Absolute configuration

47 [(CO)3 mtolt Cr] (M M2 Ph Et)

OK.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

CCOMA 1969 1491 (1969)

Accuracy = 2 File status = No coordinates in paper
Class = 74 Refcode = CRTOLC

Absolute configuration

48 [(CO)3 otn Cr]

OK.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

JCSIA 1967 228 (1967)

Accuracy = 3 File status = OK
Class = 74 Refcode = TOLCRC10

49 [(CO)3 otolt Cr] (M M2 Ph Et)

OK.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

CCOMA 1969 1491 (1969)

Accuracy = 3 File status = No coordinates in paper
Class = 74 Refcode = PCRTOL

Absolute configuration

50 [(CO)3 tbba Cr]

OK.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

JORCA 78 229 (1974)

Accuracy = 2 File status = Paper corrected
Class = 74 Refcode = HTCRBZ

51 [(CO)3 xmbz Cr]

OK.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

INOCA 4 1298 (1965)

Accuracy = 3 File status = OK
Class = 74 Refcode = XBCRTC

COMPLEXES WITH SIX MEMBERED PI BONDED RING

52 [(CO)3 anap Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

JCSIA 1968 1866 (1968)

Accuracy = 3 File status = OK
Class = 74 Refcode = ANNCCR

53 [(CO)3 nap Cr] - o

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

HCACA 50 1052 (1967)

Accuracy = 3 File status = OK
Class = 74 Refcode = NPHTCR

54 [(CO)3 tcddu Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

ANCBA 82 293 (1970)

Accuracy = 5 File status = No coordinates in paper
Class = 75 Refcode = CRTCDD

55 [(CO)3 abnnn Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

ACBCA 32 653 (1976)

Accuracy = 3 File status = OK
Class = 74 Refcode = ABORCR10

56 [(CO)3 anth Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

JORCA 11 151 (1968)

Accuracy = 2 File status = OK
Class = 74 Refcode = ANTHCR

57 [(CO)3 a2phene9 Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

JCSPA 1968 476 (1968)

Accuracy = 2 File status = OK
Class = 74 Refcode = PHCRCH10

58 [(CO)3 a2phen1 Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

JCDTB 1973 1834 (1973)

Accuracy = 3 File status = Error in data
Class = 74 Refcode = CPHECR

59 [(CO)3 phene Cr] _ o

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

JCSPA 1968 467 (1968)

Accuracy = 2 File status = OK
Class = 74 Refcode = PANCRO11

60 [(CO)3 phene Cr] - m

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

JCDTB 1973 1834 (1973)

Accuracy = 2 File status = OK
Class = 74 Refcode = PANCRO02

COMPLEXES WITH SIX MEMBERED PI BONDED RING

61 [(CO)3 phenm Cr] - m

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

ACCRA 17 800 (1964)

Accuracy = 4 File status = OK
Class = 74 Refcode = PAWCRO

62 [(CO)3 tmaoc Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6
Coordinated atoms CO 3,

ACBCA 30 2360 (1974)

Accuracy = 2 File status = OK
Class = 75 Refcode = BNCYCR10

63 [(CO)3 dmdhpy Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6 Hetero atom = N
Coordinated atoms CO 3,

CHBRA 105 3924 (1972)

Accuracy = 1 File status = OK
Class = 75 Refcode = MHPYCR

64 [(CO)3 3mdhmpy Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6 Hetero atom = N
Coordinated atoms CO 3,

JCDTB 1973 2285 (1973)

Accuracy = 2 File status = OK
Class = 75 Refcode = MEPYCR10

65 [(CO)3 5mdhmpy Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6 Hetero atom = N
Coordinated atoms CO 3,

JCDTB 1973 2285 (1973)

Accuracy = 3 File status = OK
Class = 75 Refcode = MPYRCR10

66 [(CO)3 mebrz Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6 Hetero atom = N
Coordinated atoms CO 3,

CHBRA 105 3437 (1972)

Accuracy = 3 File status = OK
Class = 75 Refcode = MBORCR10

67 [(CO)3 tphp$1 Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 6 Hetero atom = P
Coordinated atoms CO 3,

CHBRA 105 1148 (1972)

Accuracy = 3 File status = OK
Class = 75 Refcode = TPCRCO

COMPLEXES WITH 7 MEMBERED PI BONDED RING

68 [(CO)3 phcht Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 7
Coordinated atoms CO 3,

JCSIA 1968 2704 (1968)

Accuracy = 3 File status = OK
Class = 75 Refcode = PCHCRO10

COMPLEXES WITH 7 MEMBERED PI BONDED RING

69 [(CO)3 trop Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 7
Coordinated atoms CO 3,

CCOMA 1971 119 (1971)

Accuracy = 2 File status = No coordinates in paper
Class = 75 Refcode = TROPCR

70 [(CO)3 ocudp Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 7
Coordinated atoms CO 3,

JCSIA 1969 328 (1969)

Accuracy = 3 File status = OK
Class = 75 Refcode = MCDPCR10

71 [(CO)3 bcudt Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 7
Coordinated atoms CO 3,

JCSIA 1971 1962 (1971)

Accuracy = 3 File status = OK
Class = 75 Refcode = TCUTCR

Disordered

72 [(CO)3 eopax Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 7
Coordinated atoms CO 3,

JCSPA 1966 504 (1966)

Accuracy = 3 File status = OK
Class = 75 Refcode = CRCAAZ

73 [(CO)3 tacht8 Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 7
Coordinated atoms CO 3,

ACBCA 29 477 (1973)

Accuracy = 4 File status = OK
Class = 75 Refcode = TACHCR10

74 [(CO)3 tacht4 Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 7
Coordinated atoms CO 3,

ACBCA 29 477 (1973)

Accuracy = 4 File status = OK
Class = 75 Refcode = TACHTC

75 [(CO)3 hman Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 7
Coordinated atoms CO 3,

CCOMA 1971 220 (1971)

Accuracy = 2 File status = No coordinates in paper
Class = 75 Refcode = HANLCR

COMPLEXES WITH 8 MEMBERED PI BONDED RING

76 [(CO)3 cot Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 8
Coordinated atoms CO 3,

JCSOA 1962 3770 (1962)

Accuracy = 1 File status = Error in data
Class = 75 Refcode = TCOCCR

COMPLEXES WITH 8 MEMBERED PI BONDED RING

77 [(CO)3 tacota Cr]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 8
Coordinated atoms CO 3,

JACSA 90 903 (1968)

Accuracy = 2 File status = OK
Class = 75 Refcode = TBCOCR

78 [(CO)3 Cr dhocl* Cr (CO)3]

Ox.No.= 0 Coord.No.= 4
Size of pi ring = 8
Coordinated atoms CO 3,

JCDTB 1973 1834 (1973)

Accuracy = 3 File status = Error in data
Class = 75 Refcode = HCOTCR10

COMPLEXES WITH Cr-C PI BONDS

79 [(all)3 Cr]

Ox.No.= 3 Coord.No.= 3
Coordinated atoms Pi 3,

ACACB 25 S160 (1969)

Accuracy = 5 File status = No coordinates in paper
Class = 72 Refcode = ALLYCR

80 [(CO)4 anbchx Cr]

Ox.No.= 0 Coord.No.= 6 Geometry = 2
Coordinated atoms Pi 2,CO 4,

JORCA 29 275 (1971)

Accuracy = 3 File status = OK
Class = 75 Refcode = CBTCHR10

81 [(CO)3 nnd PPh3 Cr]

Ox.No.= 0 Coord.No.= 6 Geometry = 2
Coordinated atoms Pi 2,CO 3, P 1,

ACBCA 31 2896 (1975)

Accuracy = 2 File status = OK
Class = 75 Refcode = NBCRCP

82 [(CO)3 tam PPh3 Cr]

Ox.No.= 2 Coord.No.= 5
Coordinated atoms Pi 1,CO 3, P 1,

JORCA 81 389 (1974)

Accuracy = 3 File status = OK
Class = 72 Refcode = BRNCRP

83 [(CO)4 dmnna Cr]

Ox.No.= 0 Coord.No.= 6 Geometry = 2
Coordinated atoms Pi 1,CO 4, O 1,

JCDTB 1974 1876 (1974)

Accuracy = 2 File status = OK
Class = 75 Refcode = MIBOCR

84 [all Cr (all*)2 Cr all]

Ox.No.= 2 Coord.No.= 4
Coordinated atoms Pi 3,Cr 1,

BCSJA 42 545 (1969)

Accuracy = 4 File status = OK
Class = 72 Refcode = TALDCR

COMPLEXES WITH Cr-C PI BONDS

OTHER COMPLEXES WITH CARBONYL LIGANDS

85 [(CO)6 Cr]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms C0 6,

86 [(CO)6 Cr]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms C0 6,

87 [(CO)5 chamvc Cr]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms C0 5, C 1,

88 [(CO)5 dcmc Cr]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms C0 5, C 1,

89 [(CO)5 dmec Cr]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms C0 5, C 1,

90 [(CO)5 dphcp Cr]

Ox.No.= 1 Coord.No.= 6
Coordinated atoms C0 5, C 1,

91 [(CO)5 mmac Cr]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms C0 5, C 1,

92 [(CO)5 mphcc Cr]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms C0 5, C 1,

JACSA 98 7918 (1976)

Accuracy = 1 File status = Not in file

JACSA 98 7918 (1976)

Accuracy = 1 File status = Not in file

Neutron diffraction

CHBMA 103 3149 (1970)

Accuracy = 3 File status = OK
Class = 71 Refcode = CHVICR

JCSIA 1969 334 (1969)

Accuracy = 2 File status = OK
Class = 71 Refcode = DMAPCC

CHBMA 105 67 (1972)

Accuracy = 2 File status = OK
Class = 71 Refcode = EMACCR

AMCHA 81 536 (1969)

Accuracy = 3 File status = No coordinates in paper
Class = 71 Refcode = PCPCCR

CCOMA 1967 1199 (1967)

Accuracy = 3 File status = No coordinates in paper
Class = 71 Refcode = MMACCR

JCDTB 1972 653 (1972)

Accuracy = 1 File status = OK
Class = 71 Refcode = PMPHCR

93 [(CO)5 pnoc Cr]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms CO 5, C 1,

JCSIA 1968 642 (1968)

Accuracy = 4 File status = Paper corrected
Class = 71 Refcode = CRCACP10

94 [(CO)4 anc PPh3 Cr]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms CO 4, C 1, P 1,

JCSIA 1969 1274 (1969)

Accuracy = 3 File status = Paper corrected
Class = 71 Refcode = MCTPCR

95 [(CO)2 CNe CO PMe3 Br Cr]

Ox.No.= 4 Coord.No.= 6
Coordinated atoms CO 3, C 1, P 1, Br 1,

ANCHA 86 667 (1974)

Accuracy = 3 File status = No coordinates in paper
Class = 71 Refcode = BMPCCB

96 [(CO)2 I (CO)2 CNe Cr]

Ox.No.= 4 Coord.No.= 6
Coordinated atoms CO 4, C 1, I 1,

ANCHA 86 667 (1974)

Accuracy = 2 File status = No coordinates in paper
Class = 71 Refcode = MCBICB

97 [(CO)5 Cr H* Re (CO)5]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms CO 5, H 1,

JORCA 54 C22 (1973)

Accuracy = 3 File status = Not in file

98 [(CO)5 Cr AsMe2* Mn (CO)5]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms CO 5, As 1,

CHDHA 105 1486 (1972)

Accuracy = 3 File status = OK
Class = 86 Refcode = CMASCR

99 [((CO)5 Cr)3 As2Ph2**]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms CO 5, As 1,

ACIHA 15 234 (1976)

Accuracy = 3 File status = No coordinates in paper
Class = 86 Refcode = ARBZPC

100 [(CO)4 asf1 Cr]

Ox.No.= 0 Coord.No.= 6 Geometry = 2
Coordinated atoms CO 4, As 2,

JCDTB 1972 2381 (1972)

Accuracy = 3 File status = OK
Class = 86 Refcode = MAPHCR
Disordered

101 [(CO)4 asf6 Cr]

Ox.No.= 0 Coord.No.= 6 Geometry = 2
Coordinated atoms CO 4, As 2,

INOCA 12 1148 (1973)

Accuracy = 1 File status = OK
Class = 86 Refcode = BARCBC

OTHER COMPLEXES WITH CARBONYL LIGANDS

102 [(CO)4 asf5 Cr]

Ox.No.= 0 Coord.No.= 6 Geometry = 2
Coordinated atoms CO 4,As 2,

JCDTB 1972 2378 (1972)

Accuracy = 3 File status = OK
Class = 86 Refcode = HAPPCR

103 [(CO)4 asf4 Cr]

Ox.No.= 0 Coord.No.= 6 Geometry = 2
Coordinated atoms CO 4,As 2,

JCDTB 1972 2381 (1972)

Accuracy = 3 File status = OK
Class = 86 Refcode = ARFECR
Disordered

104 [(CO)4 asf2 Cr]

Ox.No.= 0 Coord.No.= 6 Geometry = 2
Coordinated atoms CO 4,As 2,

JCDTB 1972 2381 (1972)

Accuracy = 3 File status = OK
Class = 86 Refcode = CCREAS10
Disordered

105 [(CO)4 Cr As2Mo4* Cr (CO)4]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms CO 4,As 2,

ICHAA 10 127 (1974)

Accuracy = 2 File status = Paper corrected
Class = 86 Refcode = MDASCR

106 [(CO)3 Cr cnna* Cr (CO)3]

Ox.No.= 0 Coord.No.= 6 Geometry = 3
Coordinated atoms CO 3,As 3,

JCCCA 1974 953 (1974)

Accuracy = 4 File status = No coordinates in paper
Class = 86 Refcode = NNASCR

107 [(CO)5 tphp Cr]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms CO 5, P 1,

CHBEA 106 2227 (1973)

Accuracy = 3 File status = OK
Class = 86 Refcode = PCPBCR

108 [(CO)5 PH3 Cr]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms CO 5, P 1,

JORCA 47 385 (1973)

Accuracy = 3 File status = Not in file
Disordered

109 [(CO)5 PO3Ph3 Cr]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms CO 5, P 1,

INOCA 12 265 (1973)

Accuracy = 2 File status = Error in data
Class = 86 Refcode = PCPOCR10

110 [(CO)5 PPh3 Cr]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms CO 5, P 1,

INOCA 12 265 (1973)

Accuracy = 1 File status = OK
Class = 86 Refcode = PCTPCR10

OTHER COMPLEXES WITH CARBONYL LIGANDS

111 [(CO)5 Cr ppeph* Mn Br (CO)3] - alpha

Ox.No.= 0 Coord.No.= 6
Coordinated atoms C 5, P 1,

INOCA 12 2902 (1973)

Accuracy = 3 File status = Error in data
Class = 86 Refcode = CRPPMN10

112 [(CO)5 Cr ppeph* Mn Br (CO)3] (C H2 Cl2)

Ox.No.= 0 Coord.No.= 6
Coordinated atoms C 5, P 1,

INOCA 12 2902 (1973)

Accuracy = 3 File status = Error in data
Class = 86 Refcode = PEMOCR

113 [(CO)2 PO3Ph3 (CO)2 PO3Ph3 Cr]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms C 4, P 2,

INOCA 11 161 (1972)

Accuracy = 2 File status = OK
Class = 86 Refcode = POTCDR

114 [(CO)4 (PH3)2 Cr]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms C 4, P 2,

INOCA 12 1143 (1973)

Accuracy = 3 File status = Not in file

115 [(CO)4 diphos Cr]

Ox.No.= 0 Coord.No.= 6 Geometry = 2
Coordinated atoms C 4, P 2,

ACBCA 27 1899 (1971)

Accuracy = 3 File status = OK
Class = 86 Refcode = DPETCR

116 [(CO)3 (PH3)3 Cr]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms C 3, P 3,

JOBCA 47 383 (1973)

Accuracy = 3 File status = Not in file

117 [(CO)3 (PH3)4 Cr]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms C 2, P 4,

JCSIB 1 69 (1971)

Accuracy = 2 File status = Not in file

118 [(CO)3 bpppe Cr]

Ox.No.= 0 Coord.No.= 6 Geometry = 3
Coordinated atoms C 3, P 2, N 1,

JACSA 91 7000 (1969)

Accuracy = 3 File status = Paper corrected
Class = 86 Refcode = PEACCR

119 [CO PMePh2 I CO PMePh2 NO Cr]

Ox.No.= 1 Coord.No.= 6
Coordinated atoms C 2, P 2, N 1, I 1,

JCDTB 1976 699 (1976)

Accuracy = 3 File status = OK
Class = 86 Refcode = CPMINC

OTHER COMPLEXES WITH CARBONYL LIGANDS

120 [(CO)4 tmin Cr]

Ox.No.= 0 Coord.No.= 6 Geometry = 2
Coordinated atoms CO 4, N 2,

JCCCA 1975 683 (1975)

Accuracy = 3 File status = No coordinates in paper
Class = 83 Refcode = CIHYCR

121 [(CO)3 dien Cr]

Ox.No.= 0 Coord.No.= 6 Geometry = 3
Coordinated atoms CO 3, N 3,

INOCA 5 1851 (1966)

Accuracy = 3 File status = OK
Class = 76 Refcode = ETCRCO

122 [(CO)5 mbenzot Cr]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms CO 5, S 1,

JOMCA 112 145 (1976)

Accuracy = 3 File status = OK
Class = 85 Refcode = BZESCR

123 [(CO)5 SPMe3 Cr]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms CO 5, S 1,

JCDTB 1973 2205 (1973)

Accuracy = 3 File status = Error in data
Class = 85 Refcode = CMPHSC

124 [(CO)4 Cr (SPh2)2 N (cp)2]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms CO 4, S 2,

ACBCA 30 2717 (1974)

Accuracy = 4 File status = Paper corrected
Class = 73 Refcode = CPHTCR10

125 [(CO)5 I Cr] (P Me2 N)4 Se

Ox.No.= 0 Coord.No.= 6
Coordinated atoms CO 5, I 1,

JCDTB L973 377 (1974)

Accuracy = 3 File status = Not in file

COMPLEXES WITH Cr-C SIGMA BONDS

126 [(CN)6 Cr] KJ

Ox.No.= 3 Coord.No.= 6
Coordinated atoms C 6,

ACAPC 28 623 (1974)

Accuracy = 3 File status = Not in file

127 [(CN)6 Cr] [(NH3)6 Co]

Ox.No.= 0 Coord.No.= 6
Coordinated atoms C 6,

ACBCA 33 59 (1977)

Accuracy = 1 File status = Not in file

COMPLEXES WITH Cr-C SIGMA BONDS

128 [(CN)6 Cr] Na4 (aq)10

Ox.No.= 2 Coord.No.= 6
Coordinated atoms C 6,

129 [(CN)6 Cr]2 Mn3 (aq)x

Ox.No.= 3 Coord.No.= 6
Coordinated atoms C 6,

130 [(CN)6 Cr] Cs2 Li

Ox.No.= 3 Coord.No.= 6
Coordinated atoms C 6,

131 [(CN)6 Cr] [(NH3)6 Co]

Ox.No.= 3 Coord.No.= 6
Coordinated atoms C 6,

132 [(CN)6 Cr] Cs2 Li

Ox.No.= 3 Coord.No.= 6
Coordinated atoms C 6,

133 [(CN)6 Cr]2 Cd3 (aq)x

Ox.No.= 3 Coord.No.= 6
Coordinated atoms C 6,

134 [(Me)6 Cr] Li3 (diox)3

Ox.No.= 3 Coord.No.= 6
Coordinated atoms C 6,

135 [(Ph)5 Cr] Na2 (Et2 O)3 thf

Ox.No.= 3 Coord.No.= 5
Coordinated atoms C 5,

136 [(mpp)4 Cr]

Ox.No.= 4 Coord.No.= 4
Coordinated atoms C 4,

ACAPC 31 104 (1977)
Accuracy = 2 File status = Not in file

ICHAA 7 121 (1973)
Accuracy = 3 File status = Not in file

ACBCA 33 46 (1977)
Accuracy = 3 File status = Not in file
Neutron diffraction

ACACB 28 S74 (1972)
Accuracy = 1 File status = Not in file

INOCA 13 1681 (1974)
Accuracy = 2 File status = Not in file

ACSAA 26 2169 (1972)
Accuracy = 3 File status = Not in file

JOMCA 65 215 (1974)
Accuracy = 3 File status = OK
Class = 71 Refcode = MCRLDX

JORCA 44 127 (1972)
Accuracy = 4 File status = OK
Class = 71 Refcode = SPHENC

JORCA 61 247 (1973)
Accuracy = 4 File status = No coordinates in paper
Class = 71 Refcode = MPPRCR

COMPLEXES WITH Cr-C SIGMA BONDS

137 [(Me)4 Cr * Cr (Me)4] Li4 (thf)4

Ox.No.= 2 Coord.No.= 5
Coordinated atoms C 4,Cr 1,

JORCA 21 159 (1970)

Accuracy = 2 File status = OK
Class = 71 Refcode = LIHCRP

138 [(tmn)2 Cr * Cr (tmn)2] Li4 (Et2 O)4

Ox.No.= 2 Coord.No.= 5 Geometry = 22
Coordinated atoms C 4,Cr 1,

JORCA 27 59 (1971)

Accuracy = 4 File status = OK
Class = 71 Refcode = TMCRLI

139 [(CN)5 NO Cr] [(en)3 Co] (aq)2

Ox.No.= 2 Coord.No.= 6
Coordinated atoms C 5, N 1,

INOCA 9 2397 (1970)

Accuracy = 3 File status = OK
Class = 76 Refcode = ENCOPC

140 [(CN)5 NO Cr] K3

Ox.No.= 2 Coord.No.= 6
Coordinated atoms C 5, N 1,

ACSAA 20 1571 (1966)

Accuracy = 4 File status = Not in file

141 [(tasm)2 (bpy)2 Cr] I

Ox.No.= 3 Coord.No.= 6 Geometry = 22C
Coordinated atoms C 2, N 4,

JCDTB 1973 1497 (1973)

Accuracy = 3 File status = Error in data
Class = 71 Refcode = NSMPCR10

142 [(Ph)2 (bpy)2 Cr]

Ox.No.= 3 Coord.No.= 6 Geometry = 22C
Coordinated atoms C 2, N 4,

JCDTB 1973 73 (1973)

Accuracy = 2 File status = OK
Class = 71 Refcode = DPBPCR

143 [(mcph)2 (bpy)2 Cr] I aq

Ox.No.= 3 Coord.No.= 6 Geometry = 22T
Coordinated atoms C 2, N 4,

JCDTB 1972 2584 (1972)

Accuracy = 3 File status = Paper corrected
Class = 71 Refcode = MOPCBB10

144 [(O2)2 (CN)3 Cr] K3

Ox.No.= 4 Coord.No.= 7 Geometry = 22
Coordinated atoms C 3, O 4,

ARKEA 23 401 (1965)

Accuracy = 3 File status = Not in file

145 [(phdo)3 Cr]

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms C 3, O 3,

HCACA 57 1863 (1974)

Accuracy = 3 File status = No coordinates in paper
Class = 71 Refcode = PDOXCR

COMPLEXES WITH Cr-C SIGMA BONDS

146 [Cl tol thf Cl (thf)2 Cr]

Ox.No.= 3 Coord.No.= 6
Coordinated atoms C 1, O 3,Cl 2,

JCSIA 1967 736 (1967)

Accuracy = 3 File status = OK
Class = 84 Refcode = THFTCC10

COMPLEXES WITH Cr-N BONDS

147 [(NCS)2 NH3 (NCS)2 NH3 Cr] (C5 H14 N1)

Ox.No.= 3 Coord.No.= 6
Coordinated atoms N 6,

BCSJA 30 319 (1957)

Accuracy = 3 File status = No coordinates in paper
Class = 3 Refcode = CHOLRI

148 [(NCS)2 NH3 (NCS)2 NH3 Cr] N Py

Ox.No.= 3 Coord.No.= 6
Coordinated atoms N 6,

ZEKGA 109 29 (1957)

Accuracy = 3 File status = No coordinates in paper
Class = 33 Refcode = PYARRI

149 [(NCS)2 NH3 (NCS)2 NH3 Cr] N H4 aq

Ox.No.= 3 Coord.No.= 6
Coordinated atoms N 6,

ZEKGA 106 476 (1955)

Accuracy = 3 File status = Not in file

Disordered

150 [(NCS)6 Cr] [(aq)2 (aca*)3 Ho] (aq)2

Ox.No.= 6 Coord.No.= 6
Coordinated atoms N 6,

INOCA 11 2818 (1972)

Accuracy = 2 File status = Error in data
Class = 81 Refcode = NICHOC10

151 [(NH3)6 Cr] (Cu Br5)

Ox.No.= 3 Coord.No.= 6
Coordinated atoms N 6,

INOCA 10 2604 (1971)

Accuracy = 2 File status = Not in file

152 [(NH3)6 Cr] (Fe F6)

Ox.No.= 3 Coord.No.= 6
Coordinated atoms N 6,

ACBCA 28 529 (1972)

Accuracy = 1 File status = Not in file

153 [(NH3)6 Cr] (Mn F6)

Ox.No.= 3 Coord.No.= 6
Coordinated atoms N 6,

ACBCA 28 529 (1972)

Accuracy = 1 File status = Not in file

COMPLEXES WITH Cr-N BONDS

154 [(NH3)6 Cr] (Cu Br3 Cl2)

Ox.No.= 3 Coord.No.= 6
Coordinated atoms N 6,

CCOMA 1969 1294 (1969)

Accuracy = 2 File status = Not in file

155 [(NH3)6 Cr] (Hg Cl5)

Ox.No.= 3 Coord.No.= 6
Coordinated atoms N 6,

JCDTB 1975 2591 (1975)

Accuracy = 2 File status = Not in file

156 [(NH3)6 Cr] [(CN)5 Ni] (aq)2

Ox.No.= 3 Coord.No.= 6
Coordinated atoms N 6,

INOCA 13 2387 (1974)

Accuracy = 2 File status = Not in file

157 [(NH3)6 Cr] (Zn Cl4) Cl

Ox.No.= 3 Coord.No.= 6
Coordinated atoms N 6,

ACBCA 32 2907 (1976)

Accuracy = 2 File status = Not in file

158 [(NH3)6 Cr] (Cu Cl5)

Ox.No.= 3 Coord.No.= 6
Coordinated atoms N 6,

BCSJA 34 295 (1961)

Accuracy = 4 File status = Not in file

159 [(bg)3 Cr] aq

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms N 6,

ACBCA 32 842 (1976)

Accuracy = 1 File status = OK
Class = 79 Refcode = BGUCRM

160 [(en)3 Cr] [(en)3 Co] Cl6 (aq)6

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms N 6,

ACBCA 32 194 (1976)

Accuracy = 2 File status = OK
Class = 76 Refcode = COCRCL
Disordered

161 [(en)3 Cr] [O (CN)2 OH (CN)2 Mo] aq

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms N 6,

INCOA 14 2035 (1975)

Accuracy = 2 File status = OK
Class = 76 Refcode = CRENOH
Disordered

162 [(en)3 Cr] La (C4 H4 O6)2 (aq)3

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms N 6,

CHLTA 1976 339 (1976)

Accuracy = 4 File status = No coordinates in paper
Class = 76 Refcode = LENCRT

163 [(en)3 Cr][(CN)6 Co](aq)6

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms N 6,

INOCA 7 2333 (1968)

Accuracy = 3 File status = OK
Class = 76 Refcode = BTDHCO

164 [(en)3 Cr]Cl3 (aq)3

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms N 6,

ACBCA 31 2069 (1975)

Accuracy = 1 File status = OK
Class = 76 Refcode = CRTENC
Disordered

165 [(en)3 Cr][(CO)5 Mi](aq)1.5

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms N 6,

INOCA 7 1362 (1968)

Accuracy = 3 File status = OK
Class = 76 Refcode = EDCBCH

166 [(hbg)3 Cr](C10 H15 O4 S)3 (aq)3

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms N 6,

JACSA 91 7199 (1969)

Accuracy = 4 File status = No coordinates in paper
Class = 79 Refcode = BIGCBC
Absolute configuration

167 [(13pn)3 Cr][(CN)5 Mi](aq)2

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms N 6,

INOCA 13 2387 (1974)

Accuracy = 3 File status = OK
Class = 83 Refcode = CRTMCN01

168 [(13pn)3 Cr][(CO)5 Mi](aq)2

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms N 6,

INOCA 13 2387 (1974)

Accuracy = 3 File status = OK
Class = 76 Refcode = CRTMCN01

169 [(dtmsn)3 NO Cr]

Ox.No.= 2 Coord.No.= 4
Coordinated atoms N 4,

JCCCA 1972 567 (1972)

Accuracy = 3 File status = No coordinates in paper
Class = 83 Refcode = SINOCR

170 [(NPi2)3 Cr]

Ox.No.= 3 Coord.No.= 3
Coordinated atoms N 3,

CCOHA 1971 411 (1971)

Accuracy = 3 File status = No coordinates in paper
Class = 83 Refcode = CRPBAH

171 [(sen)2 en Cr](Cl O4)

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms N 4, S 2,

INOCA 15 1183 (1976)

Accuracy = 3 File status = Error in data
Class = 76 Refcode = MCBACR

COMPLEXES WITH Cr-N BONDS

172 [sac (en)2 Cr] (Cl O4)

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms N 4, S 2,

INOCA 12 2690 (1973)

Accuracy = 2 File status = Error in data
Class = 76 Refcode = HCBNCB

173 [(his$3 pen Cr] aq

Ox.No.= 3 Coord.No.= 6 Geometry = 33C
Coordinated atoms N 3, S 1, O 2,

JCCCA 1976 280 (1976)

Accuracy = 2 File status = No coordinates in paper
Class = 82 Refcode = LDHPCH

174 [(tsn)2 Cr] sa (aq)5

Ox.No.= 3 Coord.No.= 6 Geometry = 33T
Coordinated atoms N 2, S 2, O 2,

DANKA 200 1349 (1971)

Accuracy = 4 File status = Error in data
Class = 79 Refcode = BACRSC

175 [(NH3)5 Cr OH* Cr (NH3)5] Cl5 (aq)

Ox.No.= 3 Coord.No.= 6
Coordinated atoms N 5, O 1,

INOCA 12 2928 (1973)

Accuracy = 3 File status = Not in file

176 [(NH3)5 Cr O* Cr (NH3)5] Cl4 (aq)2

Ox.No.= 3 Coord.No.= 6
Coordinated atoms N 5, O 1,

BCSJA 45 2406 (1972)

Accuracy = 3 File status = Not in file

177 [(NH3)5 Cr O* Cr (NH3)5] Cl4 (aq)2]

Ox.No.= 3 Coord.No.= 6
Coordinated atoms N 5, O 1,

JACSA 93 1512 (1971)

Accuracy = 2 File status = Not in file

178 [ox (en)2 Cr] [(ox)2 en Cr] (aq)2

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms N 4, O 2,

JCSIA 1970 1862 (1970)

Accuracy = 2 File status = OK
Class = 76 Refcode = CRENOI
Disordered

179 [(aesal)2 Cr] I

Ox.No.= 3 Coord.No.= 6 Geometry = 33T
Coordinated atoms N 4, O 2,

ACBCA 27 1505 (1971)

Accuracy = 4 File status = Error in data
Class = 78 Refcode = AESCRI

180 [(phen)2 Cr (OH*)2 Cr (phen)2] I4 (aq)4

Ox.No.= 3 Coord.No.= 6 Geometry = 22C
Coordinated atoms N 4, O 2,

INOCA 14 1127 (1975)

Accuracy = 3 File status = Paper corrected
Class = 83 Refcode = XPHOCR
Disordered

181 [(phen)2 Cr (OH*)2 Cr (phen)2] Cl4 (aq)6

Ox.No.= 3 Coord.No.= 6 Geometry = 22C
Coordinated atoms N 4, O 2,

ACBCA 29 12 (1973)

Accuracy = 3 File status = Error in data
Class = 83 Refcode = HPENCR
Disordered

182 [(NH3)12 Cr4 (OH*)6] Br6 (aq)2

Ox.No.= 3 Coord.No.= 6
Coordinated atoms N 4, O 2,

ACSAA 24 275 (1970)

Accuracy = 3 File status = Not in file

183 [(en)6 Cr4 (OH*)6] (N3)6 (aq)4

Ox.No.= 3 Coord.No.= 6 Geometry = 22C
Coordinated atoms N 4, O 2,

JACSA 91 193 (1969)

Accuracy = 3 File status = No coordinates in paper
Class = 76 Refcode = ENCRNI

184 [(aq)2 acpysc Cr] O H (N O3)2 aq

Ox.No.= 3 Coord.No.= 7 Geometry = 5
Coordinated atoms N 3, O 4,

JCCCA 1975 799 (1975)

Accuracy = 2 File status = No coordinates in paper
Class = 84 Refcode = DAPSCR

185 [(gly)3 Cr] aq

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms N 3, O 3,

INOCA 10 1468 (1971)

Accuracy = 1 File status = OK
Class = 82 Refcode = TGLYCR

186 [(quin)3 Cr] MeOH

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms N 3, O 3,

CCOMA 1968 1170 (1968)

Accuracy = 3 File status = No coordinates in paper
Class = 83 Refcode = QUICRM

187 [O (O2)2 bpy Cr] - o

Ox.No.= 6 Coord.No.= 7 Geometry = 222
Coordinated atoms N 2, O 5,

ACSAA 22 1439 (1968)

Accuracy = 2 File status = OK
Class = 83 Refcode = OPYICR

188 [O (O2)2 bpy Cr] - a

Ox.No.= 6 Coord.No.= 7 Geometry = 222
Coordinated atoms N 2, O 5,

ACSAA 22 1439 (1968)

Accuracy = 4 File status = No coordinates in paper
Class = 83 Refcode = OPYICR01

189 [O (O2)2 phen Cr]

Ox.No.= 6 Coord.No.= 7 Geometry = 222
Coordinated atoms N 2, O 5,

ARKEA 24 111 (1965)

Accuracy = 3 File status = OK
Class = 83 Refcode = OCRPOL

COMPLEXES WITH Cr-N BONDS

190 [O2 aq O2 en Cr] aq

Ox.No.= 4 Coord.No.= 7 Geometry = 222
Coordinated atoms N 2, O 5,

AHKBA 24 47 (1965)

Accuracy = 3 File status = OK
Class = 76 Refcode = OBTDCR

191 [ox (en)2 Cr] [(ox)2 en Cr] (aq)2

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms N 2, O 4,

JCSIA 1970 1862 (1970)

Accuracy = 2 File status = OK
Class = 76 Refcode = CRENOI
Disordered

192 [(odab1)2 Cr] PyH (aq)3

Ox.No.= 3 Coord.No.= 6 Geometry = 33C
Coordinated atoms N 2, O 4,

HCACA 51 580 (1968)

Accuracy = 4 File status = OK
Class = 83 Refcode = PPAACR

193 [(dhazb)2 Cr] PyH

Ox.No.= 3 Coord.No.= 6 Geometry = 33T
Coordinated atoms N 2, O 4,

HCACA 48 317 (1965)

Accuracy = 4 File status = No coordinates in paper
Class = 83 Refcode = CRPAZB

194 [(hnbb)2 Cr]2 (PyH)2 Py

Ox.No.= 3 Coord.No.= 6 Geometry = 33T
Coordinated atoms N 2, O 4,

HCACA 48 317 (1965)

Accuracy = 4 File status = No coordinates in paper
Class = 83 Refcode = PACRPS

195 [ensal (aq)2 Cr] Cl

Ox.No.= 3 Coord.No.= 6 Geometry = 4T
Coordinated atoms N 2, O 4,

JCSIA 1970 3296 (1970)

Accuracy = 3 File status = OK
Class = 78 Refcode = CRASAL

196 [(gly)2 Cr (OH$)2 Cr (gly)2]

Ox.No.= 3 Coord.No.= 6 Geometry = 22C
Coordinated atoms N 2, O 4,

INOCA 12 342 (1973)

Accuracy = 2 File status = Error in data
Class = 82 Refcode = HGLYCR10

197 [aq Cr trienta$ Cr aq] (aq)6

Ox.No.= 3 Coord.No.= 6 Geometry = 5
Coordinated atoms N 2, O 4,

ACBCA 30 1987 (1974)

Accuracy = 3 File status = OK
Class = 76 Refcode = ATTHAC

198 [(thf)2 (dtmsa)2 Cr]

Ox.No.= 2 Coord.No.= 4
Coordinated atoms N 2, O 2,

JCCCA 1972 567 (1972)

Accuracy = 3 File status = No coordinates in paper
Class = 83 Refcode = TPSICR

COMPLEXES WITH Cr-N BONDS

199 [(O2)2 O Py Cr]

Ox.No.= 6 Coord.No.= 6 Geometry = 22C
Coordinated atoms N 1, O 5,

ABKBA 22 29 (1964)

Accuracy = 3 File status = OK
Class = 83 Refcode = PYBOCR

200 [Cl (aq)2 Cl en Cr] Cl

Ox.No.= 3 Coord.No.= 6 Geometry = 2
Coordinated atoms N 2, O 2,Cl 2,

ACSAA 23 343 (1969)

Accuracy = 4 File status = OK
Class = 76 Refcode = EDTCRC
Disordered

201 [Cl en Cl en Cr] Cl2 (H5 O2)

Ox.No.= 3 Coord.No.= 6 Geometry = 22T
Coordinated atoms N 4,Cl 2,

BCSJA 33 354 (1960)

Accuracy = 3 File status = OK
Class = 76 Refcode = CEDCRC

202 [dien (Cl) 3 Cr]

Ox.No.= 3 Coord.No.= 6 Geometry = 3
Coordinated atoms N 3,Cl 3,

JCSIA 1970 803 (1970)

Accuracy = 3 File status = OK
Class = 76 Refcode = AMZCCR

203 [(NMe3)2 (Cl)3 Cr]

Ox.No.= 3 Coord.No.= 5
Coordinated atoms N 2,Cl 3,

JCSIA 1971 3636 (1971)

Accuracy = 3 File status = OK
Class = 83 Refcode = TMAMCR10

COMPLEXES WITH Cr-S BONDS

204 [(SCN)6 Cr] K3 (aq)x

Ox.No.= 3 Coord.No.= 6
Coordinated atoms S 6,

ZFKHA 27 106 (1953)

Accuracy = 5 File status = Not in file

205 [(dtbanz)3 Cr]

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms S 6,

BISCA 38 1106 (1968)

Accuracy = 4 File status = No coordinates in paper
Class = 85 Refcode = DTBZCR

206 [(etxan)3 Cr]

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms S 6,

ACBCA 30 2788 (1974)

Accuracy = 1 File status = OK
Class = 80 Refcode = ETXACR10

COMPLEXES WITH Cr-S BONDS

207 [(mordtc)3 Cr] (C Cl2 H2)

JCDTB 1975 2517 (1975)

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms S 6,

Accuracy = 3 File status = OK
Class = 80 Refcode = HOTCCR

208 [(oexan)3 Cr]

ACBCA 28 972 (1972)

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms S 6,

Accuracy = 3 File status = OK
Class = 80 Refcode = CREXAN

209 [(pyrdtc)3 Cr]2 Br

INOCA 15 369 (1976)

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms S 6,

Accuracy = 3 File status = OK
Class = 80 Refcode = PYTCCR

COMPLEXES WITH Cr-O BONDS

210 [aq ox aq ox Cr] K (aq)3

ACCRA 4 35 (1951)

Ox.No.= 3 Coord.No.= 6 Geometry = 22T
Coordinated atoms O 6,

Accuracy = 5 File status = No coordinates in file
Class = 01 Refcode = KOXACR

211 [(acac)3 Cr] (tu)2

CSCMC 2 477 (1973)

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms O 6,

Accuracy = 2 File status = OK
Class = 60 Refcode = ACRTOR

212 [(acac)3 Cr]

ACAM1 1969 30 (1969)

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms O 6,

Accuracy = 5 File status = No coordinates in paper
Class = 77 Refcode = ACACCR01

213 [(acac)3 Cr]

ACCRA 19 131 (1965)

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms O 6,

Accuracy = 3 File status = OK
Class = 77 Refcode = ACACCR

214 [(atc)3 Cr]

JACSA 92 7620 (1970)

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms O 6,

Accuracy = 5 File status = No coordinates in paper
Class = 77 Refcode = CRACAM
Absolute configuration

COMPLEXES WITH Cr-O BONDS

215 [(cat)3 Cr]2 K6 (aq)3

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms O 6,

JACSA 98 1767 (1976)

Accuracy = 2 File status = OK
Class = 84 Refcode = KCATCR

216 [(mal)3 Cr] [(12pn)3 Co] (aq)3

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms O 6,

JCDTB 1976 251 (1976)

Accuracy = 4 File status = OK
Class = 76 Refcode = COHRCH10
Absolute configuration
Disordered

217 [(ox)3 Cr] (N H4)3 (aq)2

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms O 6,

ACCRA 5 499 (1952)

Accuracy = 5 File status = No coordinates in file
Class = 81 Refcode = AMOXCR

218 [(propn)3 Cr]

Ox.No.= 3 Coord.No.= 6 Geometry = 222
Coordinated atoms O 6,

ACBCA 31 916 (1975)

Accuracy = 2 File status = OK
Class = 84 Refcode = PRDOCR

219 [(acac)2 Cr (O2PPh2*) Cr (acac)2]

Ox.No.= 3 Coord.No.= 6 Geometry = 22C
Coordinated atoms O 6,

INOCA 4 99 (1965)

Accuracy = 3 File status = OK
Class = 77 Refcode = PHACCR

220 [(bracac)2 Cr (OEt*)2 Cr (bracac)2]

Ox.No.= 3 Coord.No.= 6 Geometry = 22C
Coordinated atoms O 6,

ACAM1 4 11 (1976)

Accuracy = 5 File status = No coordinates in paper
Class = 77 Refcode = EXBACR

221 [(bracac)2 Cr (OMe*)2 Cr (bracac)2]

Ox.No.= 3 Coord.No.= 6 Geometry = 22C
Coordinated atoms O 6,

ACAM1 4 11 (1976)

Accuracy = 5 File status = No coordinates in paper
Class = 77 Refcode = MXBACR

222 [(clacac)2 Cr (OMe*)2 Cr (clacac)2]

Ox.No.= 3 Coord.No.= 6 Geometry = 22C
Coordinated atoms O 6,

INOCA 15 1179 (1976)

Accuracy = 1 File status = OK
Class = 77 Refcode = MXCACR10

223 [(mal)2 Cr (OH*)2 Cr (mal)2] Na4 (aq)5

Ox.No.= 3 Coord.No.= 6 Geometry = 22C
Coordinated atoms O 6,

ACAM1 4 11 (1976)

Accuracy = 5 File status = No coordinates in paper
Class = 81 Refcode = SCRMAL

COMPLEXES WITH Cr-O BONDS

224 [(ox)2 Cr (OH*)2 Cr (ox)2] Na4 (aq)6

Ox.No.= 3 Coord.No.= 6 Geometry = 22C
Coordinated atoms O 6,

ACAN1 4 11 (1976)

Accuracy = 5 File status = No coordinates in paper
Class = 81 Refcode = SCBIOI

225 [(aq Cr (ac*)2)3 O**] Cl (aq)6

Ox.No.= 3 Coord.No.= 6
Coordinated atoms O 6,

ACBCA 26 673 (1970)

Accuracy = 3 File status = Error in data
Class = 81 Refcode = CRACOP11
Disordered

226 [(aq Cr (ac*)2)3 O**] Cl (aq)6

Ox.No.= 3 Coord.No.= 6
Coordinated atoms O 6,

NATUA 205 694 (1965)

Accuracy = 4 File status = No coordinates in paper
Class = 81 Refcode = CRACOP

227 [aq Cr (ac*)4 Cr aq]

Ox.No.= 2 Coord.No.= 6
Coordinated atoms O 5,Cr 1,

ACBCA 27 1664 (1971)

Accuracy = 1 File status = OK
Class = 81 Refcode = CRAQAC11

228 [aq Cr (ac*)4 Cr aq]

Ox.No.= 2 Coord.No.= 6
Coordinated atoms O 5,Cr 1,

ACCRA 6 501 (1953)

Accuracy = 4 File status = No coordinates in file
Class = 81 Refcode = CRAQAC

229 [Cl (OHMe)2 Cl (OHMe)2 Cr] Cl

Ox.No.= 3 Coord.No.= 6
Coordinated atoms O 4,Cl 2,

JCCCA 1975 190 (1975)

Accuracy = 2 File status = No coordinates in paper
Class = 84 Refcode = CMBTAC

TABLE 2

Alphabetical list of ligand abbreviations

Fig. 2	Abbreviation	Formula	Name	Chromium complex no.
29	abnbn	$C_{13}H_{14}O_2$	η-exo-2-acetoxybenznorbornenyl	55
211	ac	$C_2H_3O_2$	acetato	
212	ac *	$C_2H_3O_2$	μ-acetato	225—8
221	acac	$C_5H_7O_2$	2,4-pentanedionato [acetylacetonato]	211—3, 219
53	acn	C_3H_3N	1-2-η-acrylonitrile	
18	acphob	$C_8H_8O_2$	η-o-hydroxyacetophenone	40
154	acpysc	$C_{11}H_{15}N_7O_2$	2,6-diacetylpyridine-bis (semicarbazone)	184
157	aesal	$C_9H_{11}N_2O$	2-aminoethylsalicylideneiminato	179
166	ala	$C_3H_6NO_2$	α-alaninato	
54	all	C_3H_5	1-3-η-allyl	79, 84
58	all *	C_3H_5	μ-1-3-η-allyl	84
27	anap	$C_{10}H_9N$	5-10-η-aminonaphthalene	52
9	anis	C_7H_9O	1-6-η-anisole	32
30	anth	$C_{14}H_{10}$	1-5, 14-η-anthracene	56
196	aq	H_2O	aquo	184, 190, 195, 197, 200, 210, 225—8
197	aq *	H_2O	μ-aquo	
104	asf1	$C_6H_{14}As_2F_2$	1,2-bis(dimethylarsino)-1,1-difluoroethane	100
103	asf2	$C_6H_{13}As_2F_3$	1,2-bis(dimethylarsino)-1,1,2-trifluoroethane	104
102	asf4	$C_6H_{12}As_2ClF_3$	1,2-bis(dimethylarsino)-1,1,2-trifluoro-2-chloroethane	103
105	asf5	$C_7H_{13}As_2ClF$	1,3-bis(dimethylarsino)-2-chloro-1,1,3,3-tetrafluoropropane	102
107	asf6	$C_{12}H_{26}As_2$	1,3-bis(dimethylarsino)-2,2,4,4-tetracyclobutane	101
98	AsMe2	C_2H_6As	dimethylarsino	
99	AsMe2 *	C_2H_6As	μ-dimethylarsino	98
100	As2Me4	$C_4H_{12}As_2$	1,1,2,2-tetramethyl-diarsine	
101	As2Me4 *	$C_4H_{12}As_2$	μ-1,1,2,2-tetramethyl-diarsine	105
109	As2Ph2 **	$C_{12}H_{10}As_2$	μ_3-arsenobenzene	99
167	asn	$C_6H_7N_2O_3$	asparaginato	
226	atc	$C_{12}H_{17}O_2$	3-acetylcamphorato	214
165	bala	$C_3H_6NO_2$	β-alaninato	
43	bcudp	$C_{11}H_{10}$	η-bicyclo(4.4.1) undecapentene	70
44	bcudt	$C_{11}H_{14}$	1-4-η-bicyclo(4.4.1) undeca-1,3,5-triene	71
59	bdn	C_4H_6	1-2-η, 3-4-η-butadiene	
14	bdpm	$C_{25}H_{22}As_2$	bis(diphenylarsino)methane	31
76	benz	C_7H_7	benzyl	
140	bg	$C_6H_6N_5$	biguanidato	159
21	bbbz	$C_{10}H_{14}O_2$	1,2-bis(1-hydroxyethyl)benzene	41
143	bigua	$C_2H_{11}N_5$	biguanidine	

TABLE 2 (continued)

Fig. 2	Abbreviation	Formula	Name	Chromium complex no.
12	biph *	$C_{12}H_{10}$	μ-1,2,6-η, 1',2',6'-η-biphenyl	35—6
139	biu	$C_2H_2N_3O_2$	biureto	
48	bman	$C_{16}H_{14}$	1,6.8,13-bis-methano (14) annulene	75
57	bn	C_4H_8	2-3-η-but-2-ene	
118	bpppe	$C_{30}H_{33}NP_2$	N,N-bis(2-phenylphosphinoethyl)-ethylamine	118
147	bpy	$C_{10}H_8N_2$	2,2'-bipyridine	141—3, 187—8
231	Br	Br	bromo	95
232	Br *	Br	μ-bromo	
219	bracac	$C_5H_6BrO_2$	3-bromopropane-2,4-dionato	220—1
80	Bt	C_4H_9	t-butyl	
75	Bu	C_4H_9	n-butyl	
183	buxan	$C_5H_9OS_2$	n-butylxanthato	
7	bz	C_6H_6	η-benzene	1—6, 27—30
223	cat	$C_6H_4O_2$	chatecholato	215
83	chamvc	$C_{10}H_{17}NO$	cyclohexylamino-(1-methoxy-vinyl)carbene	87
233	Cl	Cl	chloro	146, 200—3, 229
234	Cl *	Cl	μ-chloro	
220	clacac	$C_5H_6ClO_2$	3-chloropropane-2,4-dionato	222
72	CMe	C_2H_3	methylmethinyl	95—96
88	CN	CN	cyano	126—33, 139—40, 144
108	cnma *	$C_9H_{27}As_9$	cyclonona(methylarsine)	106
89	CNMe	C_2H_3N	methylisonitrile	
64	CO	CO	carbonyl	12—3, 22, 24—78, 80—3, 85—125
65	CO *	CO	μ-carbonyl	23
92	COOME	$C_2H_3O_2$	methoxycarbonyl	
49	cot	C_8H_{10}	1-6-η-cycloocta-1,3,5-triene	76
1	cp	C_5H_5	η-cyclopentadienyl	12—21
66	cp $1	C_5H_5	cyclopentadien-7-yl	
91	CS	CS	thiocarbonyl	
82	demc	$C_6H_{13}N$	diethylamino(methyl)-carbene	88
171	dhazb	$C_{12}H_8N_2O_2$	o,o'-dihydroxy-*trans*-azobenzene	193
51	dhocl *	$C_{14}H_{14}$	*trans*-6a, 12a-dihydrooctalene	78
106	diars	$C_{10}H_{16}As_2$	o-phenylbis(dimethylarsine)	
150	dien	$C_4H_{13}N_3$	4,5-diamino-3-azapentane[diethyltriamine]	121, 202
206	diox	$C_4H_8O_2$	dioxane	
116	diphos	$C_{26}H_{24}P_2$	1,2-bis(diphenylphosphine)-ethane	115

TABLE 2 (continued)

Fig. 2	Abbreviation	Formula	Name	Chromium complex no.
6	dmcht	$C_{11}H_{12}S$	1-3, 9-10-η-5,7-dimethyl-4H-cyclohepta(c)thiophene	26
36	dmdhpy	$C_7H_{11}N$	η-1,4-dimethyl-1,2-dihydropyridine	63
90	dmec	$C_5H_{11}NO$	dimethylamino(ethoxy)carbene	89
216	dmg	$C_4H_6N_2O_2$	diethylglyoximato(2-)	
63	dmnbn	C_9H_{14}	7,7-dimethoxynorborn-2-ene	83
204	dmso	C_2H_6OS	dimethylsulfoxide	
2	dpful	$C_{18}H_{14}$	1-5α-η-diphenylfulvene	22
70	dphcp	$C_{15}H_{10}$	2,3-diphenylcyclopropenylidene	90
185	dtbenz	$C_7H_5S_2$	dithiobenzato	205
137	dtmsa	$C_6H_{18}NSi_2$	di(trimethylsilyl)amido	169, 198
227	edta	$C_6H_4N_2O_8$	ethylenediaminetetraacetato	
142	en	$C_2H_8N_2$	ethylenediamine	160—5, 171—2, 178, 183, 190—1, 200—1
158	ensal	$C_{16}H_{14}N_2O_2$	N,N′-ethylenebis(salicylideneiminato)	195
45	eopaz	$C_{18}H_{16}O_2$	η-1-ethoxy-3-oxo-3a-phenyl-3,3a-dihyroxoazulene	72
73	Et	C_2H_5	ethyl	
184	etdtc	$C_5H_{10}NS_2$	N,N′-diethylthiocarbamato	
52	etn	C_2H_4	η-ethylene	
179	etxan	$C_3H_5S_3$	ethylthioxanthato	206
209	form	CHO_2	formato	
164	gly	$C_2H_4NO_2$	glycinato	185, 196
155	glygly	$C_3H_7N_2O_2$	glycylglycinato	
95	H	H	hydrido	
96	H*	H	μ-hydrido	97
222	hacac	$C_5H_8O_2$	2,4-pentadione	
141	hbg	$C_2H_7N_5$	biguanide	166
217	hdmg	$C_4H_7N_2O_2$	dimethylglyoximato(1-)	
39	hebrz	$C_{12}H_{30}B_3N_3$	η-hexaethylborazine	66
169	his $1	$C_6H_8N_3O_2$	histidinyl-NO	
146	his $2	$C_6H_9N_3O_2$	histidinyl-NN′	
156	his $3	$C_6H_8N_3O_2$	histidinyl-NN′O	173
61	hmbchx	$C_{12}H_{18}$	2-3,5-6-η_2-hexamethylbicyclo-(2.2.0)hexa-2,5-diene	80
25	hmbz	$C_{12}H_{18}$	hexamethylbenzene	51
23	hmpt	$C_{11}H_{16}O$	η-o-(1-hydroxyl-1-methylpropyl) toluene	42
172	hnhb	$C_{16}H_9N_3O_4$	(2-hydroxynaphthalene-1-azo)-(2′-hydroxy-4′-nitrobenzene)	194
24	hppt	$C_{16}H_{18}O$	η-o-(1-hydroxyl-1-phenylpropyl)-toluene	43—4
218	h2 dmg	$C_4H_8N_2O_4$	dimethylglyoxime	
210	h2 ox	$C_2H_2O_4$	oxalic acid	
32	h2 phene1	$C_{14}H_{12}$	9-14-η-1,4-dihydrophenanthrene	58
33	h2 phene9	$C_{14}H_{12}$	1-4,11-12-η-9,10-dihydrophenanthrene	57

TABLE 2 (continued)

Fig. 2	Abbreviation	Formula	Name	Chromium complex no.
228	h4 edta	$C_6H_8N_2O_8$	ethylenediaminetetraacetic acid	
229	I	I	iodo	96, 125
230	I *	I	μ-iodo	
214	mal	$C_3H_2O_4$	malonato(2-)	216, 223
56	mall	C_4H_7	1-3-η-2-methylallyl	
71	Me	CH_3	methyl	134, 137
4	mepyr	C_5H_7N	N-methylpyrrole	24
81	mmac	C_3H_7N	methylamino(methyl)carbene	91
85	mmc	C_3H_6O	methyl(methoxy)carbene	94
19	moacph	$C_9H_{10}O_2$	η-o-methoxyacetophenone	45
20	mohebz	$C_9H_{12}O_2$	η-o-methoxy(1'-hydroxyethyl) benzene	46
69	moph	C_7H_7O	2-methoxyphenyl	143
182	mordtc	$C_5H_8NOS_2$	morphilino-dithiocarbamato	207
84	mphtc	C_8H_8S	methyl(phenylthio)carbene	92
78	mpp	$C_{10}H_{13}$	2-methyl, 2-phenylpropyl	136
16	mtolt	$C_8H_7O_2$	η-m-toluate	47
119	N	N	nitrido	
26	nap	$C_{10}H_8$	1-5,10-η-naphthalene	53
60	nbd	C_7H_8	1-2-η,3-4-η-norbornadiene	81
62	nbdl	C_7H_7	norbornadien-7-yl	
129	NCO	CNO	isocyanato	14
130	NCS	CNS	isothiocyanato	147—50
124	NH	NH	imido	
125	NH *	NH	μ-imido	
133	NHMe2	C_2H_7N	dimethylamine	
126	NH2	NH_2	amido	15
127	NH2 *	NH_2	μ-amido	
128	NH3	NH_3	amine	147—9, 151—8, 175—7, 182
131	NMe *	CH_3N	μ-methylimido	
132	NMe2 *	C_2H_6N	μ-dimethylamido	16—7
134	NMe3	C_3H_9N	trimethylamine	203
120	NO	NO	nitrosyl	14—20, 119, 139—40, 169
121	NO *	NO	μ-nitrosyl	15, 18
122	NO2	NO_2	nitro	
136	NPi2	$C_6H_{14}N$	diisopropylaminato	170
123	N3	N_3	azido	
190	O	O	oxo	187—9, 199
191	O *	O	μ-oxo	176—7
192	O **	O	μ_3-oxo	225—6
193	O ***	O	μ_4-oxo	
173	odabl	$C_{18}H_{13}BrN_4O_3$	1-(4-bromophenyl)-3-methyl-5-pyraxolone-4-diazo-(3-methyl-anthanilate)	192

TABLE 2 (continued)

Fig. 2.	Abbreviation	Formula	Name	Chromium complex no.
202	OEt	C_2H_5O	ethoxo	
203	OEt *	C_2H_5O	μ-ethoxo	220
180	oexan	$C_5H_5OS_2$	O-ethylxanthato	208
194	OH	HO	hydroxo	
195	OH *	HO	μ-hydroxo	175, 180—3, 196, 223—4
201	OHMe	CH_4O	methanol	229
198	OMe	CH_3O	methoxo	
199	OMe *	CH_3O	μ-methoxo	221—2
188	ONO	NO_2	nitrito	
189	ONO_2	NO_3	nitrato	
15	otn	C_7H_9N	η-o-toluidine	48
17	otolt	$C_8H_7O_2$	η-o-toluate	49
213	ox	C_2O_4	oxalato(2-)	178, 191, 210, 217, 224
207	O2	O_2	peroxo	144,187—90, 199
208	O2 *	O_2	μ-peroxo	
225	O2PPh2 *	$C_{12}H_{12}O_2P$	μ-diphenylphosphinato	219
162	pen	$C_5H_9NO_2S$	penicillammato	173
67	Ph	C_6H_5	phenyl	135, 142
42	phcht	$C_{13}H_{12}$	exo-7-phenylcyclohepta-1,3,5-triene	68
10	PhCOMe	C_8H_8O	η-acetophenone	34
11	PhCOOMe	$C_8H_8O_2$	η-methylbenzoate	33, 37—8
94	phdo	$C_9H_9O_2$	2'-(2-phenyl-1,3-dioxolano)	145
149	phen	$C_{12}H_8N_2$	1,10-phenanthroline	180—1, 189
31	phene	$C_{14}H_{10}$	1-4,11-12-η-phenanthrene	59—61
138	phlen	$C_8H_{11}N$	α-phenylethylamine	
110	PH3	H_3P	phosphine	108, 114, 116—7
79	Pi	C_3H_7	i-propyl	
3	pmcp	$C_{10}H_{30}$	η-pentamethylcyclopentadiene	23
112	PMePh2	$C_{13}H_{13}P$	methyldiphenylphosphine	119
111	PMe3	C_3H_9P	trimethylphosphine	95
86	pmoc	C_8H_8O	phenyl(methoxy)carbene	93
74	Pn	C_3H_7	n-propyl	
113	PO3 Ph3	$C_{18}H_{15}O_3P$	triphenoxyphosphine	109, 113
186	ppdtc	$C_7H_{14}NS_2$	N,N-di-n-propyldithiocarbamato	
117	ppeph *	$C_{34}H_{33}P_3$	μ-phenyl-bis(2-diphenylphosphinoethyl)phosphine	111—2
114	PPh3	$C_{18}H_{15}P$	triphenylphosphine	38, 110
13	PPh3 *	$C_{18}H_{15}P$	μ-η-triphenylphosphine	39
215	propon	$C_3H_3O_2$	1,3-propanedionato	218
135	Py	C_5H_5N	pyridine	199

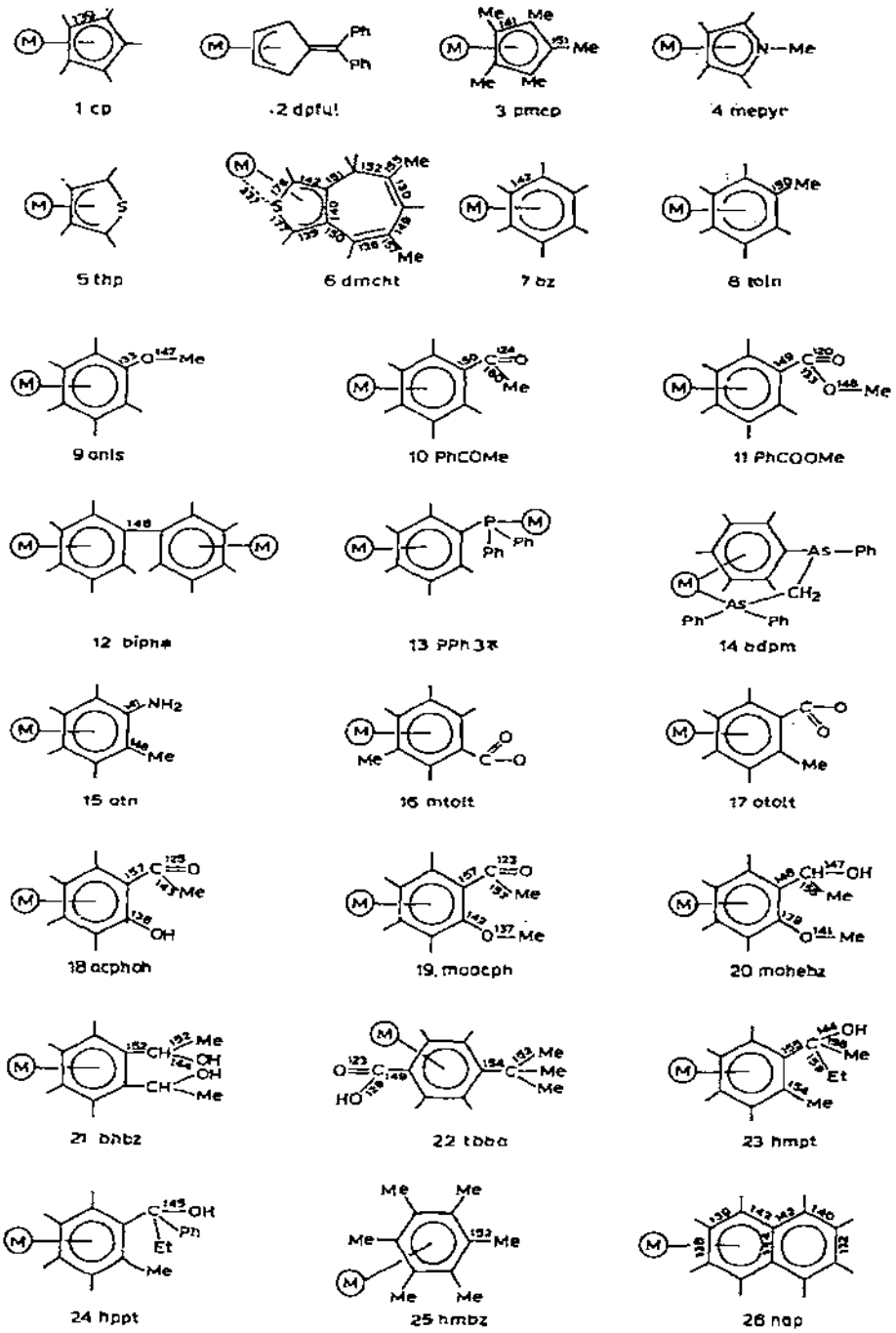
TABLE 2 (continued)

Fig. 2	Abbreviation	Formula	Name	Chromium complex no.
35	PyMe2	C_7H_9N	η-2,6-dimethylpyridine	10—1
181	pyrdtc	$C_5H_6NS_2$	pyrrolidinecarbodithioato	209
170	quin	C_9H_7NO	quinolinato	186
187	sac	$C_2H_2O_2S$	mercaptoacetato(2-)	172
178	sbenzet	$C_9H_{12}S$	benzylethylsulphide	122
163	sc	CH_5N_3O	semicarbazide	
175	SCN	CNS	thiocyanato	204
160	sen	C_2H_6NS	mercaptoethylamine	171
97	SnCl2 *	Cl_2Sn	μ-dichlorostanno	13
177	SPh *	C_6H_5S	μ-benzthiolato	19, 124
176	SPMe3	C_3H_9PS	trimethylphosphinesulphide	123
77	sty	C_8H_9	styrenyl	
22	tbba	$C_{11}H_{14}O_2$	4-t-butylbenzoic acid	50
28	tcddn	$C_{10}H_{12}$	2-5-η-tricyclo(4.3.1.0)-deca-2,4-diene	54
205	thf	C_4H_8O	tetrahydrofuran	146, 198
5	thp	C_4H_4S	thiophene	25
46	tmcht4	$C_{12}H_{14}S$	4-9-η-4,5,7-trimethyl-4H-cyclohepta(b)-thiophene	74
47	tmcht8	$C_{12}H_{14}S$	3-7-η-5,7,8-trimethyl-8H-cyclohepta(b)thiophene	73
50	tmcotn	$C_{12}H_{16}$	1-6-η-1,3,5,7-tetramethylcyclooctatetraene	77
148	tmim	$C_{10}H_{20}N_4$	NN′N″N‴ tetramethylbis(imidazolidin-2-ylidene)	120
55	tmm	C_4H_6	trimethylmethane	82
93	tmn	C_4H_8	tetramethylene	138
34	tmnoc	$C_{10}H_{24}$	1,3,3,5-tetramethyl-7-(1′,2′-naphtho)bicyclo(3.2.1)octene	62
87	tmsm	$C_4H_{11}Si$	trimethylsilylmethyl	141
68	tol	C_7H_7	tolyl	146
8	toln	C_7H_8	η-toluene	7—9
115	tphp	$C_{23}H_{17}P$	2,4,6-triphenylphosphorin	107
40	tphp $1	$C_{23}H_{17}P$	η-2,4,6-triphenylphosphorin	67
151	tren	$C_6H_{18}N_4$	2,2′2″-triaminotriethylamine	
152	trien	$C_6H_{18}N_4$	triethylenetetramine	
153	trienta *	$C_{18}H_{24}N_4O_{12}$	triethylenetetraminehexaacetato	197
41	trop	C_7H_6O	η-tropone	69
224	tropn	$C_7H_5O_2$	tropolonato	
159	tsc	CH_5N_3S	thiosemicarbazide	
161	tsn	$C_5H_5N_3O_2S$	thiosemicarbazone	174
174	tu	CH_4N_2S	thiourea	
200	ur	CH_4N_2O	urea	
168	val	$C_5H_9NO_2$	valine	
144	12pn	$C_3H_{10}N_2$	1,2-propanediamine	
145	13pn	$C_3H_{10}N_2$	1,3-propanediamine	167—8
37	3edhmpy	$C_8H_{13}N$	η-3-ethyl-1,2-dihydro-1-methylpyridine	64
38	5edhmpy	$C_8H_{13}N$	η-5-ethyl-1,2-dihydro-1-methylpyridine	65

TABLE 3

List of ASTM Journal Codens used in Table 1

AANLA	Accad. Naz. Lincei, Rend. Sci. Fiz. Mat. e Nat.
ACACB	Acta Cryst., A
ACAM1	Amer. Cryst. Ass. Mtg. (Spring)
ACAPC	Acta Chem. Scand., A
ACBCA	Acta Cryst., B
ACCRA	Acta Cryst.
ACIEA	Angew. Chem. Internat. Edn.
ACSAA	Acta Chem. Scand.
ANCEA	Angew. Chem. (German Edn.)
ARKEA	Ark. Kemi.
BCSJA	Bull. Chem. Soc. Japan
CCOMA	Chem. Comm.
CHBEA	Chem. Berichte
CHDCA	C.R. Acad. Sci. Paris, C
CMLTA	Chem. Letters
CSCMC	Cryst. Structure Comm.
DANKA	Doklady Akad. Nauk SSSR
HCACA	Helv. Chim. Acta
ICHAA	Inorg. Chim. Acta
INOCA	Inorg. Chem.
JACSA	J. Amer. Chem. Soc.
JCCCA	J. Chem. Soc., Chem. Comm.
JCDTB	J. Chem. Soc., Dalton Trans.
JCMLB	J. Cryst. Mol. Structure
JCPSA	J. Chem. Phys.
JCSIA	J. Chem. Soc., A
JCSOA	J. Chem. Soc.
JCSPA	J. Chem. Soc., B
JORCA	J. Organometallic Chem.
NATUA	Nature
RISCA	Ricerca Scientifica
ZFKHA	Zh. Fiz. Khim.
ZSTKA	Zh. Strukt. Khim.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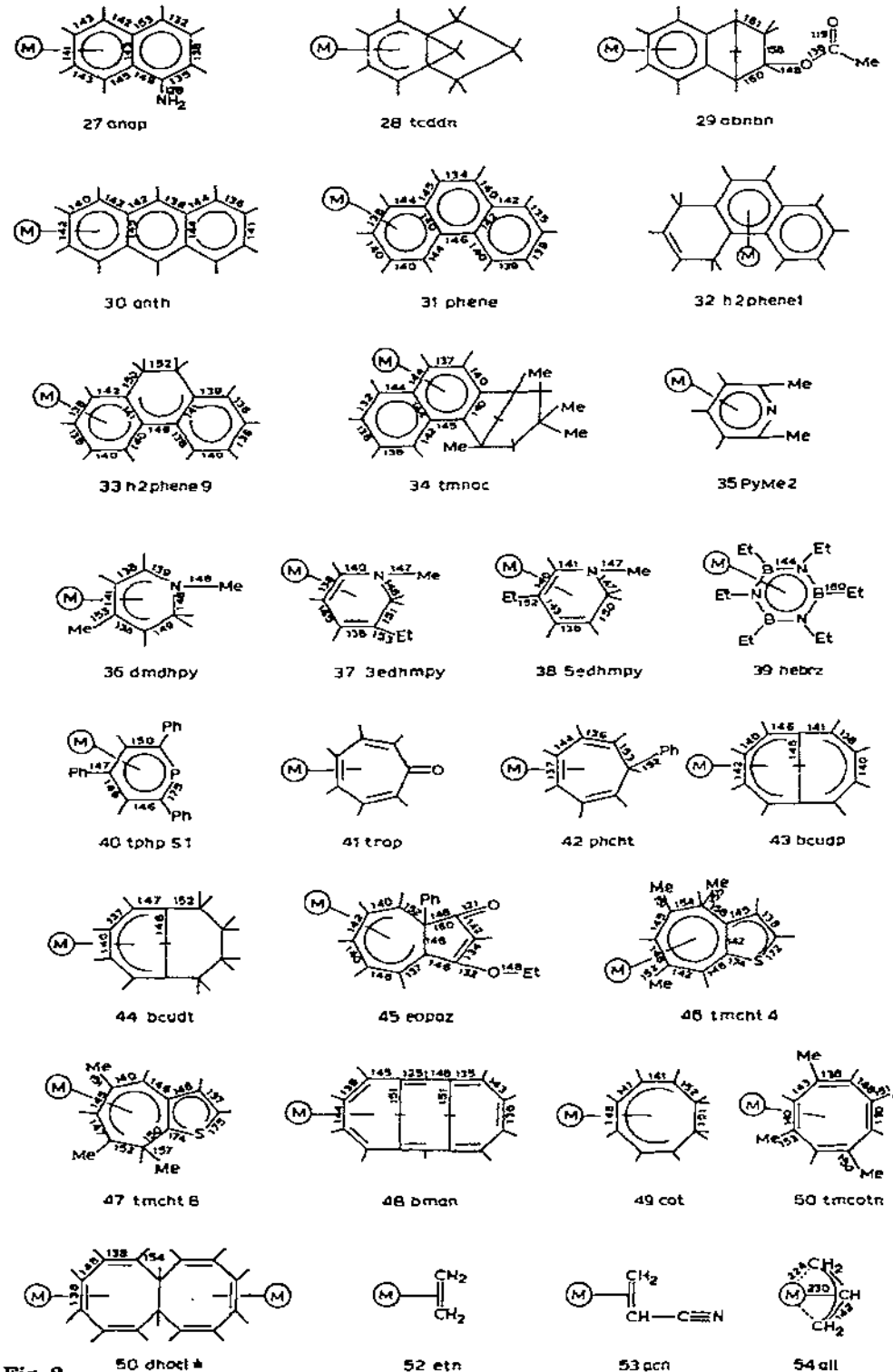
5 thp
6 dmcht
7 bz
8 toln
9 anis
10 PhCOMe
11 PhCOOMe
12 biph
13 PPh3
14 bdpm
15 atn
16 mtolt
17 otolt
18 acphoh
19. moacph
20 mohebz
21 bhbz
22 tbba
23 hmpt
24 hppt
25 hmbz
26 nap

Fig. 2.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38 5edhmpy
39 hebrz
40 tphp 51
41 trop
42 phcht
43 bcudp
44 bcudt
45 eopaz
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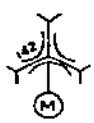
47 tmcht 8
48 bman
49 cot
50 tmcotn
50 dhoct a
52 etn
53 acn
54 all

Fig. 2.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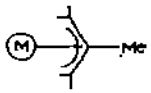
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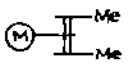
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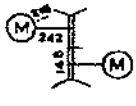
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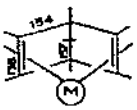
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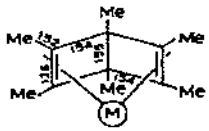
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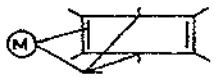
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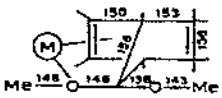
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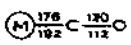
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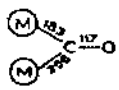
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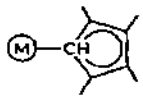
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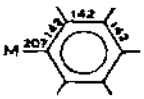
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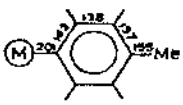
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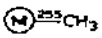
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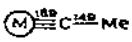
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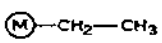
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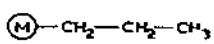
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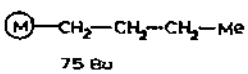
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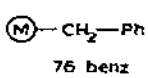
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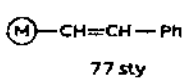
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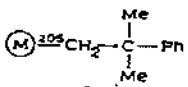
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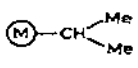
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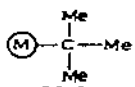
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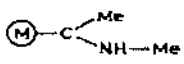
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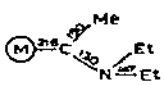
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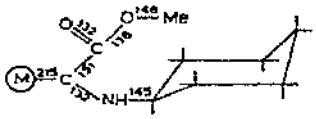
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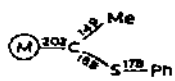
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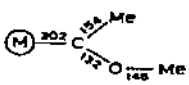
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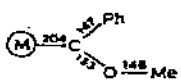
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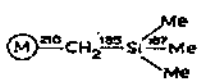
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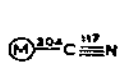
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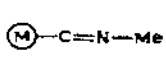
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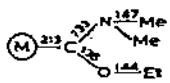
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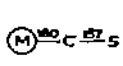
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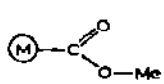
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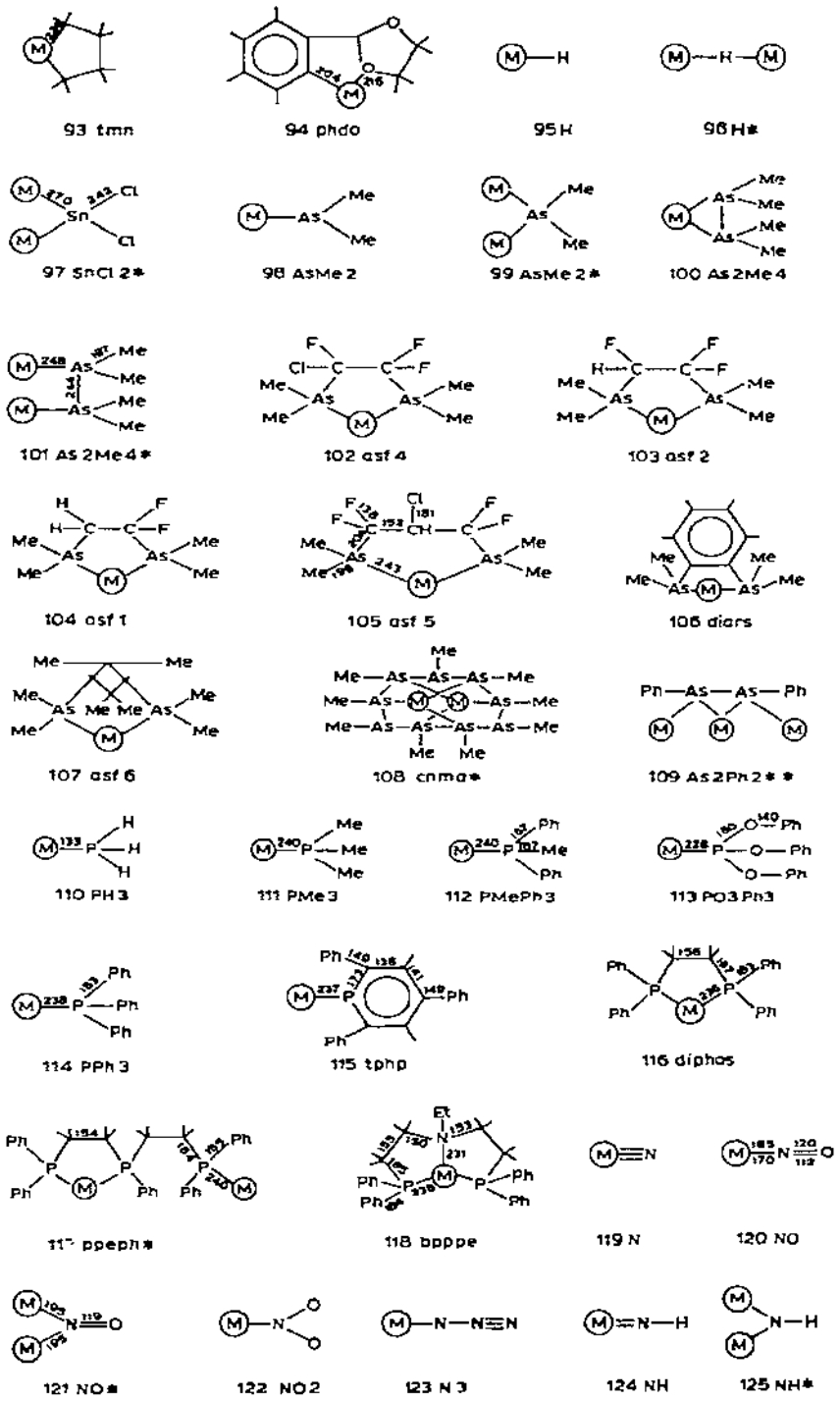
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118 bpppe
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121 NO*
122 NO 2
123 N 3
124 NH
125 NH*

Fig. 2.

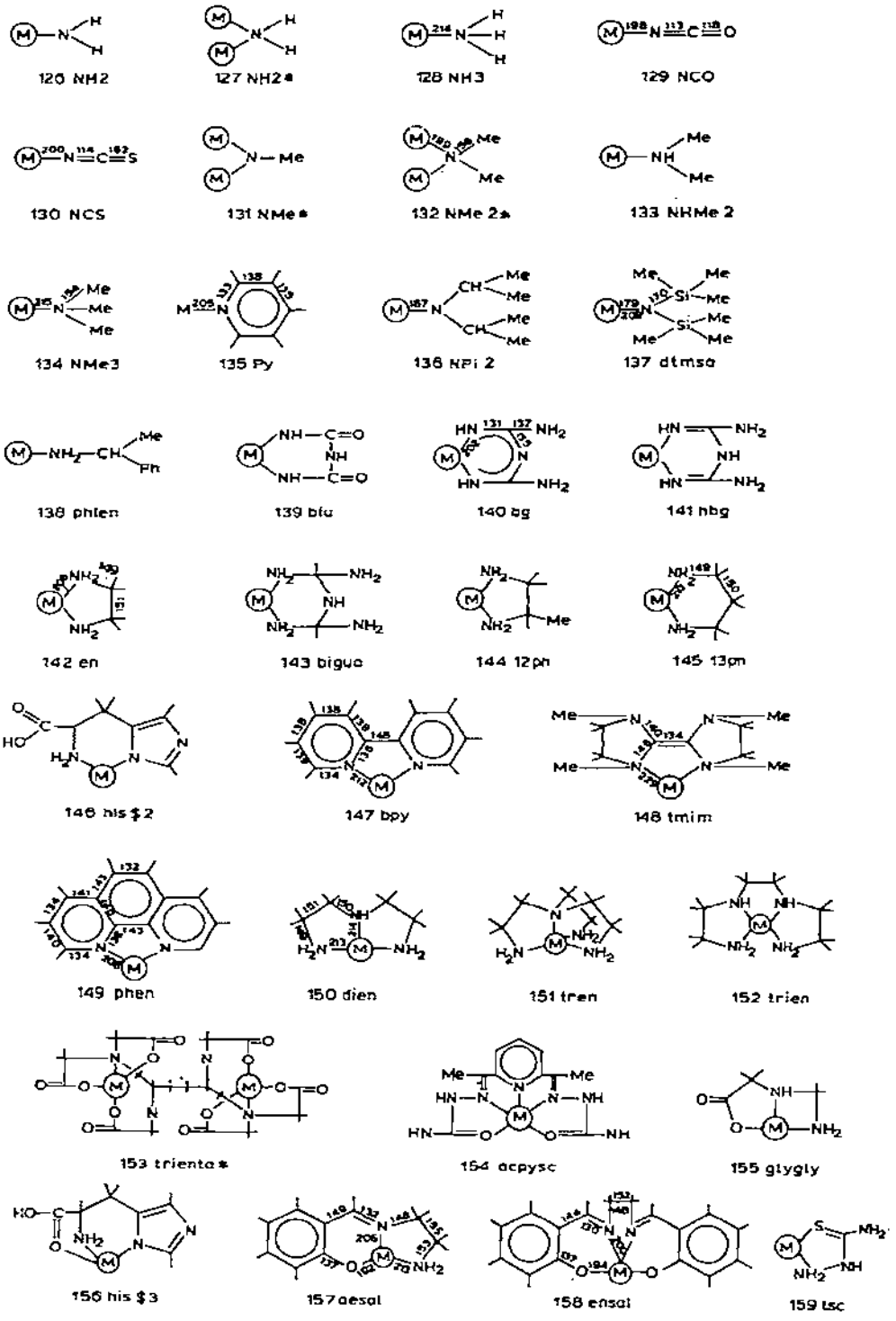
126 NH2
127 NH2*
128 NH3
129 NCO
130 NCS
131 NMe*
132 NMe 2*
133 NHMe 2
134 NMe3
135 Py
136 NPi 2
137 dtmso
138 phten
139 biu
140 bg
141 hbg
142 en
143 biguo
144 12pn
145 13pn
146 his $2
147 bpy
148 tmim
149 phen
150 dien
151 tren
152 trien
153 trienta*
154 acpysc
155 glygly
156 his $3
157 aesal
158 ensal
159 tsc

Fig. 2.

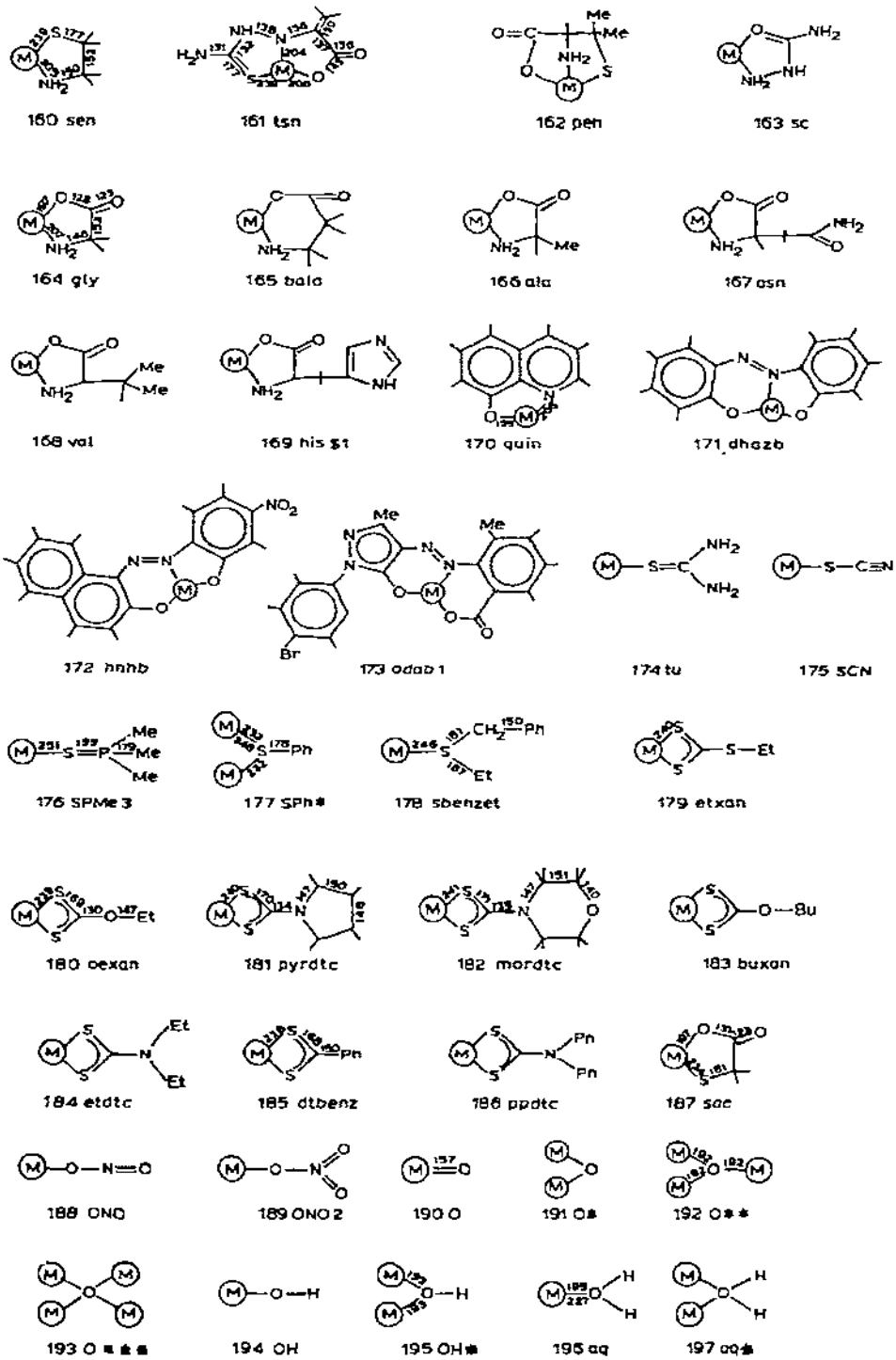
160 sen
161 tsn
162 pen
163 sc
164 gly
165 bala
166 ala
167 asn
168 val
169 his $1
170 quin
171 dhazb
172 hnnb
173 odab1
174 tu
175 SCN
176 SPMe3
177 SPh*
178 sbenzet
179 etxan
180 oexan
181 pyrdtc
182 mordtc
183 buxan
184 etdtc
185 dtbenz
186 ppdtc
187 sac
188 ONO
189 ONO2
190 O
191 O*
192 O**
193 O***
194 OH
195 OH*
196 aq
197 aq*

Fig. 2.

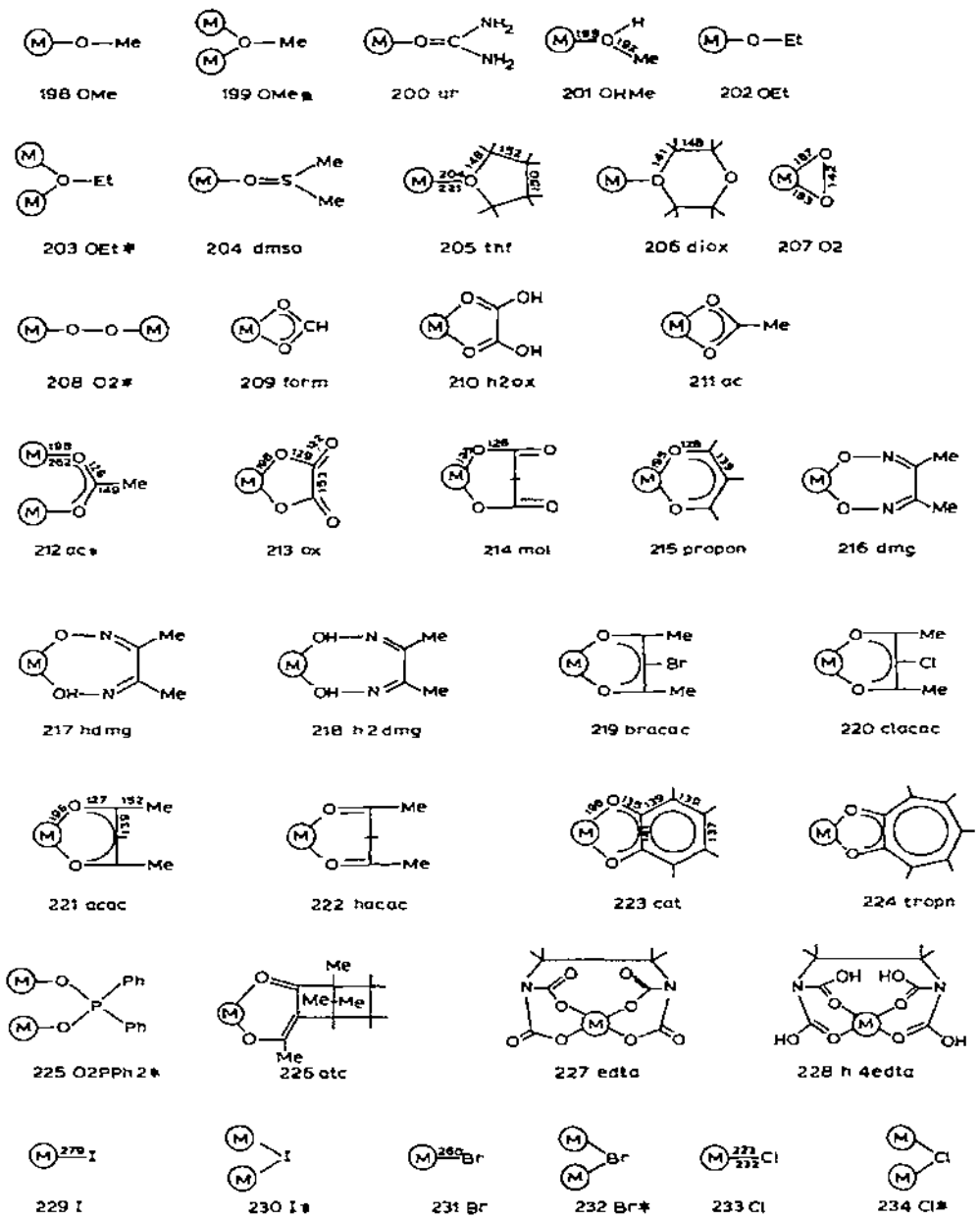

Fig. 2. Structural diagrams of ligands listed alphabetically in Table 2. The distances (in pm) are the mean values (or range of values) found in the Cr complexes.