Appendix D

# Supplemental Data for Table 9-1. Selected 1,2-$C_2B_{10}H_{12}$ Derivatives

| Compound[a] | Information[b] | References |
|---|---|---|
| Parent | Review of C—H···X solid state interactions X = O, N, S, F. Cl, Br, I, C≡CR, Cp, arene | [8] |
| | X, inclusion complexes with cyclotriveratrylene (CTV) | [9,10] |
| | X, H inclusion complexes with *p*-$CMe_3$-calix[5]arene | [11] |
| | H (plastic crystals) | [26] |
| | H, B molecular dynamics, magic angle spinning | [1846] |
| | Molecular dynamics in plastic crystals | [1852] |
| | B, paramagnetic effects of $Sm^{2+}$ | [40] |
| | B, solid state | [41] |
| | $^{10}B$ NMR, solid-state isomerization | [32] |
| | $J_{C,B}$, $J_{C,C}$, $J_{B,B}$ NMR coupling constants | [42] |
| | *C* (quadrupole coupling, $^{13}C$ relaxation) | [35] |
| | *D* (rotational motion in solid; spin-spin and spin-lattice relaxation times) | [49] |
| | IR (C—H, H-bonding with solvents) | [55] |
| | IR (*D* exchange at CH and BH) | [60] |
| | IR and broadband dielectric loss spectra, glassy crystals | [61] |
| | MS | [74,52] |
| | Angle-resolved photoemission and inverse photoemission films on Cu(100); close-packed ordering | [80] |
| | Photoemission spectra, MO binding energies, adsorption on metal surfaces | [81] |
| | Reflection-absorption IR; adsorption and dehydrogenation on Pt(111) surface | [82] |
| | p$K_a$, metallation equilibrium constants | [88–90] |
| | Dipole moment | [99–103] |
| | X-ray fluorescence | [104] |

*Continued*

| Compound | Information | References |
|---|---|---|
| | DTA, plastic crystallinity | [105] |
| | Dielectric permittivity | [106] |
| | Glassy crystal dynamics | [107] |
| | Molecular films, photoemission and inverse photoemission studies | [108] |
| | Plasma-enhanced CVD → $B_xCH_y$ thin films; electrical transport of amorphous hydrogenated boron carbide | [1894] |
| | Ionic fragmentation following photon-induced B 1 s and C 1 s excitation versus energetics of decomposition | [109] |
| | Additive in polysiloxane-based scintillators for neutron detection | [1559] |
| | Hot-wire deposition on n-type crystalline silicon, for thermal neutron detection | [1647,1850] |
| | Plasma-enhanced CVD → amorphous hydrogenated boron carbide films; p–n heterojunction devices that show improved performance following irradiation with 200 keV $He^+$ ions | [1932] |
| | Reaction with $C_{60}$ in mass spectrometer → $C_{60}$-$C_2B_{10}H_{11}$ | [1664] |
| | Pulsed discharge plasma → hard coating for Madison Symmetric Torus | [1665] |
| | Photo-fragmentation, double cation formation photoelectron-photoion-photoion coincidence (PEPIPICO) spectroscopy; MS (time-of-flight mass analysis) | [1766] |
| | Addition to aqueous solution of β-cyclodextrin inclusion complexes with napahthalene increases luminescence | [1774] |
| $C_2B_{10}D_{12}$ (FF) | Decomposition to boronize tokomak walls for plasmas | [116] |
| | S | [118] |
| **Nontransition metal derivatives** | | |
| $(1,2\text{-}C_2B_{10}H_4)_n$ nanoparticles (FF) | Enhanced yield of $C_2H_6$ in catalytic hydrogenation of $C_2H_4$ | [1871] |
| 1,2-$C_2B_{10}H_{12}$@{[Cp*Fe($\eta^5$-$P_5$)]$_{12}$($CuBr)_{18.8}$} carborane encapsulated in supramolecule | S, X | [1822] |
| 1-R-2-R′-3-C(H): R, R′ = H, Me carbenes | | [114] |
| (15-crown-5)$_3$ $Na_2^{2+}(1,2-C_2B_{10}H_{11})_2^{2-}$ (FF) | S, X, B, H, IR | [120] |
| $K^+\{H_{10}B_{10}C_2[K^+C(CH_2)_2O(CH_2)_2X-10-(nido-7,8-C_2B_9H_{11})]_2^-\}$X = O, S crown ethers | S, H, B, C, IR, MS | [1928] |
| 1,1′-(1,2-$C_2B_{10}H_{11})_2$ (FF) | IR (C—H intensity) | [51] |
| 1,1′-1,2-$C_2B_{10}H_{11}$-1,7-$C_2B_{10}H_{11}$ (FF) | IR (C—H intensity) | [51] |
| $(C_2B_{10}H_4)_n$ nanoparticle coating on Mo-graphite accelerates decomposition of $NH_3$ at 700 K | Scanning tunneling microscopy, tunneling current-voltage | [1789] |
| Adamantane-δ-cyclodextrin-1,2-$C_2B_{10}H_{12}$ inclusion complex (FF) | Fluorescence | [1656] |
| 1-cRGD-$C_2B_{10}H_{11}$ conjugates on β-cyclodextrin coated surfaces cRGD = cyclic Arg-Gly-Asp peptide supramolecular connector for biological surfaces | FTIR, water contact angle, quartx crystal microbalance (QCM), bioactivity | [1836] |

| Compound | Information | References |
|---|---|---|
| 1,2-$C_2^{10}B^{11}B_9H_{12}$ (4 isotopologues) (FF) | Microwave spectra | [1565] |
| | Implantation on a 28-nm logic *p*-type field effect transistor (pFET) metal oxide semiconductor | [1569] |
| (graphene oxide)[C(O)—$C_2B_{10}H_{11}]_n$ | S, IR, E, TEM, SCM, atomic force microscopy, electron force microscopy | [1728] |
| $Au_n(HSC_2B_{10}H_{11})_m^{n-}$ gold nanoclusters/ nanoparticles | S, H, B, Li, IR, UV, STM, TGA, cell toxocity | [1601] |
| ***Alkyl derivatives*** | | |
| 1-Me | S | [124–129] |
| | S (1 − $MeC_2B_{10}H_{11}^{\bullet}$ radical) | [1398] |
| | IR (C—H, H-bonding with solvents) | [55] |
| | p$K_a$, metallation equilibrium constants | [89,90] |
| | DTA, plastic crystallinity | [105] |
| 1-Me-2-$CHMeCH_2Me$ | S | [135] |
| 1-Me-2-*n*-$C_5H_{11}$ | S, H, C, B, IR | [1484] |
| 1-$CH_2$-$C_5Me_4H$ | S, X, H, B, C | [1556] |
| | DTA, plastic crystallinity | [105] |
| 1,2-*cyclo*-$(CH_2)_2$-9-Cl | S, H | [146] |
| 1-(CHMe—$C_5H_4$R) R = H, *o*-Me, *p*-Me | S, H, B, C, IR | [912] |
| 1-*cyclo*-$C_3H_5$-2-R R = H, CH(OH)Ph | X, H, B, C, MS | [1452] |
| 1-*n*-$C_4H_9$ | $\Delta H_{formation}$ | [1348] |
| | $\Delta H_{evaporation}$, vapor pressure | [88] |
| 1-*i*-$C_4H_9$ | $\Delta H_{evaporation}$, vapor pressure | [88] |
| | $\Delta H_{formation}$ | [1425] |
| 1-$(CH_2)_2CHMe_2$ | S | [151] |
| 1-*n*-$C_5H_{11}$ | $\Delta H_{evaporation}$, vapor pressure | [88] |
| | $\Delta H_{formation}$ | [1350,1351] |
| | $\Delta H_{evaporation}$, vapor pressure | [88] |
| 1,2-($CR_2$-$C_5H_5)_2$ $R_2 = Me_2$, $(CH_2)_5$ | S, X[$(CH_2)_5$], H, B | [1361] |
| 3-R R = β-pinenyl, camphenyl, D-limonenyl | S, H, B, C, MS | [1604] |
| 3-$(CH_2)_3SiMe_3$-*n*-I *n* = 6,9 | S, H, B, C, MS | [1604] |
| 1-R-2-$(CH_2)_4C_7H_8$ norbornyl R = Ph, Me | S, H, B, C, MS | [1719] |
| 1-γ-$C_7H_7$-2-R R = H, Me, γ-$C_7H_7$ tropenyl | S, H, UV, IR | [155] |
| 1-$C_7H_6$-2-$C_5H_4$ | Hyperpolarizability; NLO | [157] |
| $HCB_{10}H_{10}C—(CH_2)_2—CB_{10}H_{10}C—(CH_2)_2—CB_{10}H_{10}CH$ (FF) | S | [776] |
| $HCB_{10}H_{10}C—(CH_2)_4—CB_{10}H_{10}CH$ (FF) | S | [776] |
| 9-Me | S | [131,160] |
| | $\Delta H_{combustion}$, $\Delta H_{formation}$ | [131] |
| 9,12/8,10/3,6-$Me_2$ | S(insertion of carbenes), H, B, IR, MS | [161] |
| 9,12-$Me_2$ | S, H, B, C, MS | [162] |
| | S, H, IR | [169] |

*Continued*

| Compound | Information | References |
|---|---|---|
| B-Et | S (electrophilic alkylation) | [163,164] |
| 9-Et | S | [170–173] |
| 8,9,12-$Et_3$ | S | [172] |
| 8,9,10,12-$Et_4$ | S | [172] |
| B-$Et_7$ | S (electrophilic alkylation) | [163] |
| 9-*n*-$C_3H_7$ | S | [175] |
| *n*-(*n*-$C_3H_7$) *n*=8, 9 | S (electrophilic alkylation) | [176] |
| 9-$CHMe_2$ | S | [171,175] |
| *n*-$CHMe_2$ *n*=4, 8, 9 | S (electrophilic alkylation) | [176] |
| B-$CHMe_2$ | S (electrophilic alkylation) | [163] |
| 9-*n*-$C_4H_9$ | S | [160–171] |
| 9-$CH_2CHMe_2$ | S | [171] |
| 9-*n*-$C_6H_{13}$ | S | [175] |
| **Haloalkyl Derivatives** | | |
| 1-$CH_2F$ | S | [178] |
| 1-$C(CF_3)$[NHOC(O)$CMe_3$]C(O)OMe-2-Me amino acid ester | S, X | [448] |
| 1-$CH_2CH{=}CHCH_2R$ R=*n*-$C_6F_{13}$, *i*-$C_3F_7$ | S, H, B, C, F, IR, MS | [181] |
| | IR | [127,183] |
| | Dipole moment | [1342] |
| 1-(3′-$ClC_3H_6$)$C_2B_{10}H_{11}$ | S, X, H, B, C, IR, MS | [1694] |
| 1,2-(3′-$ClC_3H_6$)$_2C_2B_{10}H_{10}$ | S, X, H, B, C, IR, MS | [1694] |
| 1-CHClPh-2-R R=Me, Ph | S, X(Me), H, B, C, IR, MS | [186] |
| 1-*cyclo*-$CRCH_2CCl_2$ R=H, Me cyclopropanes | S, IR | [1206] |
| 1-$CH_2$-*cyclo*-$CHCH_2CCl_2$ R=H, Me cyclopropanes | S, IR | [1206] |
| 1,2-$(CH_2Cl)_2$ | S | [141,151] |
| 1-$CH_2Br$ | S | [143,187,188] |
| 1-$CH_2Br$ | DTA, plastic crystallinity | [105] |
| | Dipole moment | [1342] |
| [$(CH_2)_3Cl$]$HC_2B_{10}Me_8H_2$ (FF) | S, X, H, B, C, MS | [190] |
| 1-$CHBrCH_2Br$ | S | [1186] |
| [$Br(CH_2)_3$]$HC_2B_{10}Me_8H_2$ (FF) | S, H, B, C, MS | [194] |
| 1-$(CH_2)_4$I-2-R R=Me, Ph | S, H, B, C, IR | [524] |
| 1-R-2-$(CH_2)_3Br$ R=H, Me, $(CH_2)_3Br$ | S, H, B, C, IR, MS | [195] |
| 1-$CH_2Br$-2-R R=Li, D, C(O)OH, SH | S, H, C, IR | [196] |
| B-$(CH_2Br)_2$ | S | [197] |
| | Dipole moment | [1342] |
| 1,2,9,12-$(Br_2CH_2CH_2CH_2)_4$ | S, H, B, C, MS, IR | [1891] |
| 8,9,10,12-$(Br_2CH_2CH_2CH_2)_4$ | S, H, B, C, MS, IR | [1891] |

| Compound | Information | References |
|---|---|---|
| 9,12-[$(CH_2)_3X]_2$ X = Cl, Br | S, H, B, C, IR, MS | [1898] |
| 8,9,10,12-[$(CH_2)_3X]_4$ X = Cl, Br | S, X(Cl), H, B, C, IR, MS | [1898] |
| **Aryl Derivatives** | | |
| 1-Ph | H (C—H-acceptor H-bonds) | [212] |
| | p$K_a$, C—H thermodynamic and kinetic acidity | [91] |
| | Deposition of $C_2B_{10}H_{12}$ on Si substrate to reduce impurities in plasma | [1855] |
| *n*-Ph *n* = 1, 2, 3, 7 | UV, IR | [213] |
| *n*-Ph *n* = 3, 4 | S (oxidation of dianions) | [214] |
| 1,2-$Ph_2$ | S | [126,216] |
| 1-Ph-2-deoxyribose anomers | S, X, H, B, C, IR, MS, cytotoxicity | [1799] |
| 1-($C_6H_4$-*m*-R) R = $NO_2$, $NH_2$, Me | H (C—H-acceptor H-bonds) | [212] |
| 1-($C_6H_4$-*p*-R) R = $NO_2$, $NH_2$, Me, OMe | H (C—H-acceptor H-bonds) | [212] |
| 1-($C_6H_4$-*p*-R) R = $NO_2$, $NH_2$ precursors to Ph-C≡C-terminated imide oligomers | S, H, C, IR | [1933] |
| 1-$C_6H_4$(2′-OMe) | S, H, B, C, MS | [223] |
| 1-$C_6H_4$(2′-R) R = $NO_2$, $NH_2$ | S, H, B, C, MS | [223] |
| 1-*p*-$C_6H_4$Me | S, H, C, MS | [226] |
| 1-*m*/*p*-$C_6H_4$Me | p$K_a$ | [227] |
| 1-CHCl-$C_6H_4$-*p*-R R = H, Br, OMe, CN, $NO_2$ | S, H, B, C, IR, MS | [228] |
| 1-CH(OH)-$C_6H_4$-*p*-R R = H, Br, OMe, CN, $NO_2$ | S, H, B, C, IR, MS | [228] |
| 1-CHR-$C_4H_2$XE E = O, S R = OH, Cl; X = H, Br | S, H, B, C, IR, MS | [228] |
| 1,2-(*p*-$C_6H_4Me)_2$ | S | [437] |
| 1-*p*-$C_6H_4$-C(O)-*cyclo*-$NC_5H_9$R R = H, C(O)OEt | S, X[C(O)OEt], H, IR, MS | [230] |
| 1-*p*-$C_6H_4$-C(O)NH$(CH_2)_2$-*cyclo*-$NC_5H_{10}$ | S, H | [230] |
| 1-*p*-$C_6H_4$-$OCH_2$Ph, 1-*p*-$C_6H_4$-$OCH_2$C(O)NHAr Ar = Ph, 3-C(O)Ph$C_6H_4$ potent inducers of β5, β1, and β2 activities of 20S proteasome | S, H, C, IR, MS | [1526] |
| 1-R-2-$C_6H_4$-*p*-B$F(C_6H_2Me_3)_2^-$ K(18-crown-6)$^+$ R = Me, Ph enhanced Lewis acidity of triarylboranes | S,X(Ph),H,B,C | [1360] |
| $HCB_{10}H_{10}C—CB_{10}H_{10}C$—*o*-$C_6H_4$Me (FF) | S, H, B, C, IR, MS | [149] |
| 1-Me-2-$CH_2$(*p*-$C_6H_4)_n$C(O)Me *n* = 1, 2 | S, H, B, C, IR, MS, fluorescence | [233] |
| $C_6H_3$-1,3,5-[(*p*-$C_6H_4)_n$-$C_6H_3$-3,5-$(CH_2—CB_{10}H_{10}C—Me)_2]_3$ *n* = 0, 1 | S, H, B, C, IR, MS, TGA, DSC | [233] |
| $C_6H_3$-1,3,5-[(*p*-$C_6H_4$)-$CH_2—CB_{10}H_{10}C—C_7H_{15}]_3$ *n* = 1,2 | S, H, B, C, IR, MS, TGA, DSC | [233] |
| 1,2-$R_2$-8/9-CH═HR′ $R_2$ = $Me_2$, $(CH_2Ph)_2$, $(CH_2)_3$ R′ = Ph, *m*/*p*-$C_6H_4$Me, $C_6H_4$OMe, $C_6H_4$F, $C_6H_4$Cl, $C_6H_4$Br, $C_{10}H_7$, C(O)Et, OC(O)Me | S, H, B, C, MS | [1926] |
| 3-Ph | S, H, IR | [169] |
| 3-$C_6H_4$-*o*-OMe | Pd-catalyzed demethylation with 2-MeOPhMgBr | [238] |
| 9-$C_6H_4$-*o*-OMe | Pd-catalyzed demethylation of 1,2-$C_2B_{10}H_{11}$-3-$C_6H_4$-OMe with 2-MeOPhMgBr | [238] |
| 1,2-$Me_2$-3-Ph | S, H, IR | [169] |

*Continued*

| Compound | Information | References |
|---|---|---|
| 1,2-$Me_2$-3,6-$Ph_2$ | S, H, IR | [169] |
| 3-($C_6H_4$-*p*-Ph) | S, H, B(2d), C, IR | [234] |
| 3-($C_6H_4$-*o*-Ph) C–H—π intramolecular H-bonding | S, X, H, B, C, IR, MS | [239] |
| 3-*m*/*p*-$C_6H_4Me$ | S, C (detailed assignments) | [44] |
| | E | [73] |
| *n*-*m*/*p*-$C_6H_4Me$ $n=3$, 4 | S (oxidation of dianions) | [214] |
| 4-$C_6H_4Me$ | X | [214] |
| 9-$C_6H_4Me$ | S | [171] |
| 9-$C_6H_4$-*p*-OPh | S, H, B, C, IR, S | [229] |
| 9,12-($C_6H_4$-*p*-Me)$_2$ | S, H, B, C, IR, S | [229] |
| 9-*m*/*p*-$C_6H_4$-R R=C(O)Me, Br, Hg[C(O)$OCF_3$], $NO_2$ | S, H | [241] |
| 9,12-[$(CH_2)_3$Ph]$_2$ | S, H, B, C, IR, MS | [1898] |
| 8,9,10,12-[$(CH_2)_3$Ph]$_4$ | S, X(Cl), H, B, C, IR, MS | [1898] |
| 1,2-$Me_2$-9-$C_6H_4$-R R=*o*/*m*/*p*-OMe, *p*-OEt, *m*-$CMe_3$, *o*/*p*-Br, *m*/*p*-Cl, *p*-F, *p*-C(O)Me | S, X, H, B, C | [1868] |
| 1-Ph-2-(*p*-$C_6H_4Br$) | S, X, H, B, IR | [228] |
| 1,2-*cyclo*-*o*-$(CH_2)_2C_6H_4$ | S | [135] |
| 1-$CH_2Ph$ | S\\ | [135] |
| 1-$C_6H_4$-R R=C6H4-*o*-Me, $C_6H_4$-*o*-$CHMe_2$, $C_{10}H_7$ (naphthyl), $C_{14}H_{13}$ (phenanthrenyl) | S(Ni-catalyzed coupling of *o*-carborane with aryl iodides), H, B, C, MS | [1888] |
| $C_6H_4$(1,-1,2-$C_2B_{10}H_{11}$)$_2$ | S(Ni-catalyzed coupling of *o*-carborane with aryl iodides), H, B, C, MS | [1888] |
| 1-Me-2-Ph | S(Ni-catalyzed coupling of *o*-carborane with aryl iodides), X, H, B, C, MS | [1888] |
| 1,2-$R_2$ R=$C_6H_3$-*o*/*m*-Me, $C_{10}H_7$ | S(Ni-catalyzed coupling of *o*-carborane with aryl iodides), X(Cl,$CF_3$,Me,OMe,Ph), H, B, C, MS | [1888] |
| 1,2-($CH_2Ph$)$_2$-8,9,10,12-$Et_4$ | S | [172] |
| 1-$CH_2C_5H_4NMe^+$ | S, H, B, C, IR, MS | [243] |
| 1-$CH_2$(*cyclo*-$C_6H_{11}$) | S, H, B, C, IR, MS | [243] |
| 1-$CMe_2C_5H_4$ | S, H, B, C, IR | [869] |
| 1,2-($CH_2Ph$)$_2$ | S, H, B | [246] |
| 1-$CH_2$R R=$C_6H_6$, MePh, *p*-$MeC_6H_4Me$ | S | [178] |
| 1-(*o*-$C_6H_4$X-$CH_2$)-2-$SiMe_2CMe_3$ X=Cl, Br | S, X, H, B, C | [247] |
| $(Me_3C)Me_2Si—CB_{10}H_{10}C—CH_2—$*o*-$C_6H_4—(CH_2)_2—$*o*-$C_6H_4—CH_2—CB_{10}H_{10}C—SiMe_2CMe_3$ (FF) | S, X, H, B, C | [247] |
| 1-Me-2-(2′,3′-$C_6H_3Cl_2$) | S, X, H, MS | [258] |
| 1,2-*cyclo*-$C_8H_6$ (naphtho-*o*-carborane) | S | [248] |
| 1-$C_{13}O_2H_8$-2-$CHMe_2$ 5,6-benzocoumarin | S, X, H, B, IR | [1817] |
| 1-$C_{13}O_2H_7$[C(O)OEt]-2-$CHMe_2$ 5,6-benzocoumarin | S, X, H, B, IR | [1817] |
| 1-$CHMe_2$-2-$C_9H_6$(O)RC(O)OEt R=O, OH coumarin derivatives | S | [1874] |

| Compound | Information | References |
|---|---|---|
| [1-$CHMe_2$-2-$C_9H_6$(O)RC(O)OEt(O)$^-$]$_n$$M^+$ M = K, $n$ = 1; M = Li, $n$ = 2; M = Mg, $n$ = 3 coumarin derivatives | S, H, B, IR, MS | [1874] |
| 1,2-*cyclo*-$C_6H_4$(OR)R′ R = Me, Et; R′ = H, Me, $CMe_3$ prepared via carboryne insertion into aromatic rings | S, X, H, B, C | [1510] |
| 1-(1-$C_{10}H_7$)-2-(*p*-$C_6H_4NO_2$) $C_{10}H_7$ = naphthyl | S, H, B, C, S | [251] |
| 1,2-*cyclo*-*o*-$CH_2$-$C_6H_4$-$C_6H_4$-$CH_2$-diphenyldimethylene-*o*-carborane | S, X, H, B, C, IR | [250] |
| $C_{14}H_{18}$-9,10-($CB_{10}H_{10}Ph)_2$ anthracene aggregation-induced emission, crystallization-induced emission, aggregation-caused quenching, multichromism | S, X, H, B, C, MS, UV, photoluminescence | [1872] |
| 1-$C_{14}H_9$ (phenanthrene) aggregation-induced photoluminescence | UV, luminescence | [1543] |
| 1-$C_{14}H_{19}$-9,12-(*p*-$C_6H_4$—C≡CH)$_2$ 9′-phenanthrene color-tunable dual emission (normal and aggregation-induced) | S, H, B, C, UV, fluorescence | [1821] |
| 1-$C_{14}H_{19}$ 9′-phenanthrene color-tunable dual emission (normal and aggregation-induced) | S, H, B, C, UV, fluorescence | [1821] |
| Aggregation-induced emission of *o*-carborane BODIPY-phenanthrene-tolane dyes | | [1777] |
| $(Me_3Si)_4C_{22}H_8$($C_6H_4$-*p*-$CH_2$—$CB_{10}H_{10}C$—$SiMe_2CMe_3)_2$ $C_{22}H_8$ = pentacenyl (FF) | S, X, H, B, C, MS | [1472] |
| *Cyclo*-($C_2B_{10}H_{10}$—1,3-$CH_2$—$C_6H_4$—$CH_2)_n$ $n$ = 2,4 (FF) | S, X, H, B, C, IR, MS | [158] |
| $PhCH_2$—$CB_{10}H_{10}C$—*p*-$C_6H_4$—$CB_{10}H_{10}C$—$CH_2Ph$ (FF) | S, X, H, B, C, MS | [1536] |
| $HCB_{10}H_{10}C$—*m*-$C_6H_4$—$CB_{10}H_{10}CH$ (FF) | S, H, B, C, MS | [1536] |
| $HCB_{10}H_{10}C$—*p*-$C_6H_4$—$CB_{10}H_{10}CH$ (FF) | S, H, B, C, MS | [1536] |
| *Syn*/*anti*-1′,2′,3′-$C_6H_3$($CB_{10}H_{10}C$—$CH_2Ph)_3$ (FF) | S, X(acetone-encapsulated[*syn*]), H, B, C, MS | |
| $MeCB_{10}H_{10}C$—(*p*-$C_6H_4$)—$CB_{10}H_{10}CMe$ (FF) | S, X, H, MS | [258] |
| $HCB_{10}H_{10}C$—(*p*-$C_6H_4$)—$CB_{10}H_{10}C$—(*p*-$C_6H_4$) —$CB_{10}H_{10}CH$ (FF) | S, X | [260] |
| 1′,3′,5′-($HCB_{10}H_{10}C)_3C_6H_3$ benzene-centered (FF) | S, H, B, C, MS | [259] |
| *o*-$C_6H_4$($CH_2$—$CB_{10}H_{10}CH)_2$ (FF) | S, X | [159] |
| *Zn*(porphyrin){$C_6H_3$[$OCH_2C_6H_3$($OCH_2C_6H_3$-{$OCH_2C_6H_3$[$O(CH_2)_3SiMe_2(CH_2)_3$-$CB_{10}H_{10}CMe\}_2)_2]_2\}_4$ dendrimer (FF) | S, H, B, C, MS, IR, UV(emission), diffusion coefficients from diffusion-ordered NMR (DOSY) | [1866] |
| 9-$CH_2$-Ph | S | [170,171] |
| 1-R-9-($CH_2$-$C_6H_4$-*p*-C(O)Me) R = H, Me | S, H, B, C, IR | [265] |
| 1′,3′,5′-$C_6H_3$[$C_6H_4$-*p*-$CH_2$-9-(RR′$C_2B_{10}H_9$)]$_3$ R = H, Me, *n*-$C_7H_{13}$, Si(CH=$CH_2)_3$; R′ = *n*-$C_7H_{13}$, Si(CH=$CH_2)_3$ (FF) | S, H, B, C, IR | [265] |
| *Cyclo*-[-($CH_2)_3$—$CB_{10}H_8$(9,12-$R_2$)C—]$_4$ R = H, Me trimethylene-linked carboracycle (FF) | S, X, H, B, C, MS | [266] |

*Continued*

| Compound | Information | References |
|---|---|---|
| *Cyclo*-[-$CH_2C_6H_4CH_2$—$CB_{10}H_{10}C$—]$_4$ xylylene-linked carboracycle (FF) | S, X, H, B, C, MS | [266] |
| *Cyclo*-{—$CH_2$—$CB_{10}H_8$[9,12-$(C_6H_4R)_2$] C—$CH_2$}$_4$R′$_4$ R = H, OMe; R′ = $CH_2$, $(CH_2)_2$, $NC_5H_3(CH_2)_2$ (FF) | S, X, H, B, C, MS | [240] |
| *Cyclo*-{—$CB_{10}H_8$[9,12-$(C_6H_4R)_2$]C—}$_6$R′$_6$ R = H, OMe; R′ = $(CH_2)_3$, $(CH_2)_4$, $NC_5H_3(CH_2)_2$] carboracycle (FF) | S, X[H, $(CH_2)_2$], H, B, C, MS | [240] |
| $(HCB_{10}H_{10}C)_2C_6H_4$ distorted benzene ring (FF) | S, X, H, B, C | [267] |
| 1-($PhC_5H_2N$—$C_5H_4N$)-2-R R = Ph, Me bipyridyl | S, H, B, C | [273] |
| $RCB_{10}H_{10}C$–$PhC_3N_3$—$C_5H_3N$—$C_3N_3Ph$—$CB_{10}H_{10}CR$ R = Ph, Me triazinyl (FF) | S, H | [273] |
| 1-[2′-*cyclo*-1′,3′,5′-$C_3N_3$-4′,6′-$(NR_2)_2$]-2-R′ R = Me, Et, *n*-$C_3H_7$, *N*-morpholinyl; R′ = H, Me. Et, *n*-$C_3H_7$ triazines | S, H, IR, inhibition of topoisomerase in human cancer cell lines | [1889] |
| *Cyclo*-1,3,5-$C_3N_3$-2,4-$(CB_{10}H_{10}CR)_2$-6-NR′$_2$ R = Me, Et, *n*-$C_3H_7$; R′ = H, Me. Et, *n*-$C_3H_7$, *N*-morpholinyl triazines (FF) | S, H, IR, inhibition of topoisomerase in human cancer cell lines | [1889] |
| 1-C(O)$NCH_2$-$C_6H_4$-*p*-*cyclo*-$CN_4CH$ tetrazinyl | S, X, H, B, C, MS | [1910] |
| 1-C(O)$NCH_2$-$C_6H_4$-*p*-*bicyclo*-$C_{10}N_2H_{13}OH$ Diels-Alder product | S, H, B, C, MS, UV | [1910] |
| 2,6-$(PhCB_{10}H_{10}CCH_2)_2$-*cyclo*-$NC_5H_3$ lutidine (FF) | S, X, H, B, C, IR, MS | [1314] |
| 1,2-$C_2B_{10}H_{12}$·*o*-$C_6H_4(OMe)_2$] (FF) | S, X | [276] |
| $(C_6H_4)_2$-2,2′-$(CB_{10}H_{10}CH)_2$ (FF) | S, X, H, B, C, UV, E, MS | [1773] |
| $C_6H_4$-1,3-$(CB_{10}H_{10}CH)_2$ (FF) | S, H, B, C, UV, E, MS | [1773] |
| $C_6H_4$-1,4-$(CB_{10}H_{10}CH)_2$ (FF) | S, X, H, B, C, UV, E, MS | [1773] |
| $C_6H_4$-1,2-$(CB_{10}H_{10}CH)_2$ (FF) | X(revised) | [1773] |
| 1-[3′-R-4′,5′-$(MeO)_2C_6H_2$]-2-$C_6H_4$R′ R = H, MeO R′ = MeO, OH | S, H, C, inhibition of hypoxia-induced HIF-1α accumulation | [1737] |
| 1-R-2-$C_6H_2(OMe)_3$ R = $C_6H_2(OH)(OMe)$, $C_6H_4(OMe)$ | S, H, B, C, IR, MS, inhibition of hypoxia-induced HIF-1α mediated transcriptoonal activity | [1864] |
| 1,2-[C═$H_6$(*n*-$C_6H_{13})_2]_n$ photoluminescent polyfluorene polymer | UV, photoluminescence; solvent effects on emission | [1577] |
| —[$C_{13}H_6$(*n*-$C_6H_{13})_2$—$CB_{10}H_{10}C$—$C_{13}H_6$ (*n*-$C_6H_{13})_2]_n$— polyfluorene derivatives | S, UV, photoluminescence, density-voltage-luminescence | [1610] |
| 1-R-2-$CH_2C_6H_4CH_2$-$SiMe_2CH$═CH-$C_{13}H_8$ $C_{13}H_8$ = fluorenyl R = Me, Ph | S, X(Me), H, B, C, MS, UV, fluorescence emission | [1788] |
| 1-R-2-$C_{13}H_6$-9′,9″-(*n*-$C_8H_{17})_2$ $C_{13}H_8$ = fluorenyl R = H, $CH_2C_6H_4CH_2$, $CH_2$-anthracenyl | S, H, B, C, MS, UV, fluorescence emission | [1788] |
| $C_{14}H_6$-9,10-$(CB_{10}H_{10}CR)_2$ R = Me, Ph $C_{14}H_6$ = anthracenyl | S, X, H, B, C, MS, UV, fluorescence emission | [1788] |
| 1-CHPhNHR R = $C_{22}H_9$, $C_{26}H_{10}$ perylenes | S, X($C_{22}H_9$), UV(absorption, emission; π–π interactions) | [1585] |
| 1,3,5-$C_6H_3$(*p*-$C_6H_4)_3${$OCH_2C_6H_3$[$OCH_2$-$C_2HN_3$—$(CH_2)_3$—$CB_{10}H_{10}CMe$)]$_2$}$_3$ dendrimer | S, H, B, C, IR, MS, accumulation in SK-Hep1 cancer cells | [1603] |
| 1,2-*cyclo*-RC═CR′—CR″═CR‴ R, R′ = Et; R″ = Me, R‴ = Ph benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), X, H, B, C, MS | [1605] |

| Compound | Information | References |
|---|---|---|
| 1,2-*cyclo*-RC═CR′—CR″═CR‴ R, R′ = Et; R″ = Et, R‴ = Ph benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′—CR″═CR‴ R, R′ = Et; R″ = Ph, R‴ = Et benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′—CR″═CR‴ R, R′ = Et; R″ = $CMe_3$, R‴ = Ph, *n*-$C_4H_9$ benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), X, H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′—CR″═CR‴ R, R′ = Et; R″ = $CHMe_2$, R‴ = Me benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′—CR″═CR‴ R, R′ = Et; R″ = Me, R‴ = $CHMe_2$ benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′—CR″═CR‴ R, R′ = Et; R″ = Me, R‴ = Et benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′—CR″═CR‴ R, R′ = Et; R″ = Et, R‴ = Me benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′—CR″═CR‴ R, R′ = Et; R″ = $CH_2$-OMe, R‴ = Ph | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), X, H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′—CR″═CR‴ R, R′ = Et; R″ = $CH_2NMe$, R‴ = Ph benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′—CR″═CR‴ R, R′ = Et; R″ = $CH_2CH═CH_2$, R‴ = Ph benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), X, H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′—CR″═CR‴ R, R′ = Et; R″, R‴ = C(O)OMe benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′—CR″═CR‴ R, R′ = Et; R″ = *n*-$C_4H_9$, R‴ = $SiMe_3$ benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), X, H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′—CR″═CR‴ R, R′ = Et; R″ = Ph, R‴ = Me, *n*-$C_4H_9$, $(CH_2)_3Cl$ benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′—CR″═CR‴ R, R′ = Et; R″, R‴ = Ph benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′—CR″═CR‴ R, R′, R″ = *n*-$C_4H_9$; R‴ = Ph benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′—CR″═CR‴ R, R′ = *n*-$C_4H_9$; R″ = Ph, R‴ = Me benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), X, H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′—CR″═CR‴ R, R″ = Ph; R′ = Me, R‴ = *n*-$C_4H_9$ benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R′, R″, R‴ = *n*-$C_3H_7$ benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| {benzo[b]acrid-12(7H)-one}-N-$CH_2C_2B_{10}H_{11}$ derivatives for BNCT | S, H, C, MS, cell uptake in U87 human glioblastoma, cytotoxicity | [1768] |
| 1,2-*bicyclo*-$C_8H_6$, $C_{12}H_8$ (isomers) | S(cycloaddition of alkylbenzenes to carboryne), X($C_{12}H_8$ isomers), H, B, C, MS | [1611] |
| 1,2-*bicyclo*-$C_6H_4RR'$ R,R′ = H, Me, $CMe_3$, *n*-$C_4H_9$, $SiMe_3$ | S(cycloaddition of alkylbenzenes to carboryne), X(Me, isomers; $CMe_3$; $SiMe_3$), H, B, C, MS | [1611] |
| 1,2-*bicyclo*-$C_6H_4CH_2$ R = Me, $CMe_3$ | S(cycloaddition of alkylbenzenes to carboryne), X, H, B, C, MS | [1611] |
| 1-$CH_2C_6H_4$-*p*-$CH═CH_2$ | free radical copolymerization with PEG-b-PLA Block copolymer → PM micelles for BNCT | [1612] |
| 1,2-*bicyclo*-$CH_2CH_2C_6H_3R$— R = H, Me | S(from carboryne), X, H, B, C | [1621] |
| 1,2-*tricyclo*-$C_{12}H_{12}$ 2 isomers | S(from carboryne), X, H, B, C | [1621] |

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| Compound | Information | References |
|---|---|---|
| 1,2-*bicyclo*-CH═CH-$C_6H_3$R— R = H, Me | S(from carboryne), X, H, B, C | [1621] |
| 1-CHR$C_4H_5$ R = Me, Ph Diels-Alder reactions of *o*-carboryne with fulvenes | S, H, B, C | [1792] |
| 1,2-*bicyclo*-$C_4H_4$C═$CPh_2$-9,12-$Me_2$ Diels-Alder reactions of *o*-carboryne with fulvenes | S, H, B, C | [1792] |
| 1,2 *bicyclo*-$C_4H_2R_2$C═$CPh_2$ $R_2$ = μ-O, $Br_2$, $H_2$ reactions of *o*-carboryne with fulvenes | S, X, H, B, C | [1792] |
| 1,2-*cyclo*-C(CH═O)C(═$CPh_2$)C(CH═O) Diels-Alder reactions of *o*-carboryne with fulvenes | S, X, H, B, C | [1792] |
| 1,2-*bicyclo*-$C_4H_2R_2$C═$CPh_2$ $R_2$ = C(py)NNHCpy, $CH_2$CH═$CHCH_2$, NC(O)NPhC(O)N | S, X[C(py)NNHCpy, NC(O)NPhC(O)N], H, B, C | [1792] |
| 1-Me-2-*m*-$BrC_6H_4$ | S, H, B, C | [1651] |
| 1-Me-2-$C_6H_4$-$C_5NH_4$ (2 isomers) | S, H, B, C | [1651] |
| ($MeC_6H_4CHMe_2$)$RuS_2$Ru[(μ-S)$_2C_2B_{10}H_{10}$]$_2$(μ-CH═CR R = *cyclo*-$C_6H_{12}$, C(O)Ph, and related derivatives (FF) | S, X, H, B, C, IR, MS | [1653] |
| 1-$C_6H_4$—O—$CH_2$C(O)NH$C_6H_4$—C(O)$C_6H_4$-*o*/*m*-R R = $OCH_2$C≡CH, OH | S, H, C, IR, MS, HIF-1α inhibition, fluorescence imaging | [1654] |
| 1-R-2-$C_6H_4$-*p*-$OCH_2$C(O)NH-$C_6H_3$R′R″ R, R″ = H, Me, Et, $CMe_3$, *n*-$C_4H_9$; R′ = C(O)OMe, C(O)OEt. C(O)OH, C(O)Ph, $B(OH)_2$ HIF-1α inhibitors | S | [1659] |
| 1,2-($C_{10}H_7$)$_2$ dinaphthyl charge-transfer multiple photoluminescence | S, luminescence | [1697] |
| 1,2-[$C_6H_5$Cr(CO)$_3$]$_2$-3-Ph | S, H, B, C, Raman | [1698] |
| 1-*p*-$C_6H_4$—$OCH_2$C(O)NH—$C_6H_3$R(OH) | | |
| R = C(O)OMe, $B(OH)_2$ phenoxyacetanilides | S, H, inhibition of HIF-1 transcriptional activity | [1714] |
| 1-*p*-$C_6H_4$—$OCH_2$-*cyclo*-$CONC_6H_3$—C(O)R R = OMe, OH benzoxazoles | S, H, inhibition of HIF-1 transcriptional activity | [1714] |
| 1-$C_6H_4$-*p*-O-CH═CH-C(O)NH—$C_6H_3$(OH)-$BO_2C_2H_2Me_4$ phenoxyacetanilide | S, H, C, IR, MS, inhibition of hypoxia-induced HIF-1 transcriptional activity | [1879] |
| 1′,3′-(1,2-$C_2B_9H_{11}$)$_2C_6H_3$-5′-$OCH_2$C(O)NH$C_6H_3$-(OH)$BO_2C_2H_2Me_4$ phenoxyacetanilide (FF) | S, H, C, IR, MS, inhibition of heat shockprotein (HSP) 60 chaperon activity | [1879] |
| 9-[I-*p*-$C_6H_4$Me] | S, H, B, C | [1715] |
| 1-[CH(OH)-*p*-$C_6H_4$OMe]-*n*-R *n* = 9,12 R = $^{18}$F, $^{19}$F | S, H, B, C, F | [1715] |
| 1′,4′-(R$CB_{10}H_{10}$C)$_2C_6H_4$ R = 3′,5′-($F_3C$)$_2C_6H_3$, Ph, *p*-$C_6H_4$-*n*-$C_4H_9$, *p*-$C_6H_4$-$NMe_2$ (FF) through-space charge transfer, emission color tuning | S, X(=3′,5′-($F_3C$)$_2C_6H_3$, *p*-$C_6H_4$-*n*-$C_4H_9$, *p*-$C_6H_4$-$NMe_2$), H, B, C, UV, photoluminescence, solid state and solution | [1741] |
| 1-*p*-$HOC_6H_4$-2-R R = Et, $CH_2$—CH═$CH_2$, *n*-$C_3H_7$ | S, H, MS, estrogen receptor β selectivity in MCF-7 cell line | [1749] |
| 1,2,7-*tricyclo*-CH($CMe_3$)$CH_2$—C═C($SiMe_3$)—$C_6H_3$R R = H, F, Br | S(Zr-promoted cyclization), X, H, B, C, MS | [1752] |
| $C_6H_2$-1′,6′-$Br_2$-2′,5′-($CB_{10}H_{10}$C-$C_6H_4$-*o*-Br)$_2$ (FF) | S, H, B, C, MS | [1754] |
| 1-{$C_6H_3$-3′,5′-[$C_6H_2$-2″,4″,6″-($CHMe_2$)$_3$]$_2$}-2-P($CHMe_2$)$_2$ terphenyl | S, H, IR | [1841] |
| 1,3-*cyclo*-R R═$CH_2C_6H_2$($OCH_2O$), $CH_2C_{10}H_6$Br, $CH_2C_4H_2$BrS, C(O)$C_6H_4$Br | S(Pd-catalyzed regioselective intramolecular coupling), H, B, C, MS | [1849] |

| Compound | Information | References |
|---|---|---|
| 1,4-*cyclo*-$CH_2C_6H_3$R-2-Me R = H, F, Me, OMe | S(Pd-catalyzed regioselective intramolecular coupling), X(H), H, B, C, MS | [1849] |
| 1,4-R-2-R′ R = *cyclo*-$CH_2C_4H_2S$, $CH_2C_6H_2(OCH_2O)$, $CH_2C_6H_4$; R′ = Me, Ph, $CH_2$Ph | S(Pd-catalyzed regioselective intramolecular coupling), H, B, C, MS | [1849] |
| $C_6H_4$-1,3-$[CH_2OC_6H_3$-1,3-$(CB_{10}H_{10}CR)_2]_2$ R = Ph, Me (FF) | S, H, B, C, IR, fluorescence emission | [1856] |
| $XC_5H_3$-1,3-$(CH_2$-1′,2′-$CB_{10}H_{10}CPh)_2$ X = CH, N (FF) | S, X(CH), H, B, C, IR, fluorescence emission | [1856] |
| 1,2-*tricyclo*-(RC—CR′)-N($SiMe_3$)($C_6H_3$R″) R = H, Me, Ph R′ = H, Me R′ = H, Me, OMe, F, Cl, Br, $CHMe_2$ | S([2 + 2] dearomative cycloaddition of indoles to carboryne), X, H, B, C, MS | [1886] |
| 1-$C_5H_{11}$—12-$C_6H_4$-*p*-R R = C≡C—$C_6H_4$-$OC_8H_{17}$, N=CH—$C_6H_4$—$OC_8H_{17}$, N=N—$C_6H_4$—C(O)O—$C_5H_{11}$* | S, H, B, C, dielectric constant, liquid crystal behavior, polarizability, X-ray powder diffraction | [1919] |
| 1-$C_5H_{11}$—O—$C_6H_4$-$C_2B_{10}H_{10}$-12-L—$C_6H_4$—*p*-$OC_5H_{11}$ L = $CH_2CH_2$, CH=CH (FF) | S, H, B, C, dielectric constant, liquid crystal behavior, polarizability, X-ray powder diffraction | [1919] |
| 1-$CH(C_6H_4$-*p*-$OH)_2$ | S, H, C. S | [1925] |
| 1-R-2-$C_6H_4$-*m*-$B(C_6H_2Me_3)_3$ R = Ph, $B(C_6H_2Me_3)_3$ | S, X, H, B, C, MS, UV, DSC, E, fluorescence | [1912] |
| 1-R-2-$C_6H_4$-*p*-$B(C_6H_2Me_3)_3$ R = Ph, $B(C_6H_2Me_3)_3$ | S, X[$(B(C_6H_2Me_3)_3]$, H, B, C, MS, UV, DSC, E, fluorescence | [1912] |
| **Haloaryl Derivatives** | | |
| 1-Ph-2-R R = $C_6F_5$, *p*-$C_6H_4CF_3$, *p*-$C_6F_4$Me, *p*-$C_6H_4CF_3$ | S, X, H, B, F, E, IR, UV | [1580] |
| 1,2-$(_p$-$C_6R_4CF_3)_2$ R = H, F | S, X, H, B, F, E, IR, UV | [1580] |
| 1-$C_6H_4NH_2$-12-$C_5H_{11}$ | S, H, B, MS | [1767] |
| 1-$C_6H_4NO_2$-12-$C_5H_{11}$ | S, H, B, MS | [1767] |
| 1-($C_8H_{17}$—O—$C_6H_4$—*p*-$C_6H_4$)—12-$C_5H_{11}$ liquid crystal | S, H, B, MS | [1767] |
| 1-$CH_2$=CH-12-$C_6H_4$-*p*-$OC_5H_{11}$ | S, H, B, MS | [1767] |
| 1,4-$(MeC_2B_{10}H_{10})_2C_6F_4$ (FF) | S | [282] |
| 1-$C_6F_4$Cl-2-R R = Me, Ph | S | [282] |
| (*m*-$C_6H_4$F)$HC_2B_{10}Cl_{10}$ (FF) | S, F | [283] |
| 9-$C_6H_4$F | S | [171] |
| 9-*m*/*p*-$C_6H_4$F | S | [284] |
| 9,12-(3′,5′-$C_6H_3F_2)_2$ supramolecular C–H..F | S, X, H, B, C, F, IR | [285] |
| 1-*p*-$C_6H_4$Cl | Dipole moment | [103] |
| B-$(C_6H_4Cl)_n$ *n* = 2, 3 | S | [197] |
| 1,2-$(p$-$C_6H_4X)_2$ X = Cl, Br, I | S | [288] |
| 1-*p*-$C_6H_4$Br | S | [289,129] |
| | Dipole moment | [103] |
| 1-*m*/*p*-$C_6H_4$Br | S | [279] |
| 1-(*p*-$C_6H_4$Br)-2-Ph | S, X, H, B, IR | [242] |

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| Compound | Information | References |
|---|---|---|
| 1,2-(*p*-$C_6H_4$—C≡C—*p*-$C_6H_4$-$OCH_2CHCH_2O)_2$ cross-linking reagent for preparation of translucent hydrogels of poly(γ-glutamic acid); water-sensitive luminescence from aggregation-induced emission of *o*-carborane | S, H, B, C, MS | [1512] |
| 1,2-(*p*-$C_6H_4$—C≡CR)$_2$ R = $C_6H_3$-3′,5′-$(CF_3)_2$, *p*-$C_6H_4CF_3$, Ph, *p*-$C_6H_4$Me, *p*-$C_6H_4$OMe, $C_6H_2$-3′,4′,5′-$(OMe)_3$, *p*-$C_6H_4NMe_2$ multicolor tuning | S, UV, photoluminescence (aggregation-induced emission) | [1539] |
| B-$(C_6H_4Br)_n$ *n* = 1, 2, 4 | S | [197] |
| B-$C_6H_4I$ | S | [197] |
| **Alkenyl Derivatives** | | |
| 1-CH═CHR R = H, Cl, I | S | [293] |
| 1-CH═CH-B[$C_6H_2Me_3$]$_2$ $C_6H_2Me_3$ = mesityl | S, H, C, MS, NLO | [1485] |
| 1-B$(C_6H_2Me_3)_2$-2-R R = H, Ph $C_6H_2Me_3$ = mesityl | S, X(H, Ph), H, B, C, MS, UV, E | [1878] |
| 1-CH═C═$CH_2$ | S | [295] |
| 1-CH═CH($C_5H_4$)FeCp | S, H, B, IR | [1843] |
| 1′,2′-$(C_2B_9H_{11}$-9-$)_2C_2H_2$ (FF) | S(Pd-catalyzed cross-coupling), H, B, C, IR, MS | [1724] |
| 1-Me-2-CH═C═$CH_2$ | S | [296] |
| 1-Me-2-CH═CHMe | X | [297] |
| 1-Me-2-CH═CH-CH═$CH_2$ | S, X | [298] |
| 8,9,10,12-$(CH_2CH═CH_2)_4$ | S, X, H, B, C, IR, MS | [1549] |
| 1,2-[$(CH_2)_4CH═CH_2]_2$ Ru-catalyzed metathesis → 1,2-cyclic derivatives | S, H, B, IR, MS | [1509] |
| 1,2-$(SiMe_2CH_2CH═CH_2)_2$ Ru-catalyzed metathesis → 1,2-cyclic derivatives | S, H, B, IR, MS | [1509] |
| 1,2-$(SiMe_2(CH_2)_4CH═CH_2)_2$ Ru-catalyzed metathesis → 1,2-cyclic derivatives | S, H, B, IR, MS | [1509] |
| 1,2-[$C(O)OCH_2CH═CH_2]_2$ Ru-catalyzed metathesis → 1,2-cyclic derivatives | S, H, B, IR, MS | [1509] |
| 1,2-*cyclo*-[$(CH_2)_nC═C(CH_2)_n$ | S, X(*n* = 4), H, B, IR, MS | [1509] |
| 1,2-*cyclo*-[$SiMe_2(CH_2)_nC═C(CH_2)_n$ *n* = 0,1,4 | S, X(*n* = 0,1), H, B, IR, MS | [1509] |
| μ,μ′-1,1′,2,2′-[$C(O)OCH_2CH═CHCH_2OC(O)]_2(C_2B_{10}H_{10})_2$ (FF) | S, X, H, B, IR, MS | [1509] |
| 1,2-*cyclo*-{CMe[*cyclo*-$C(CH_2)_nC$]CMe} *n* = 3–5 | S, X(*n* = 4), H, B, C, MS | [1514] |
| {[1,2-*cyclo*-C(*n*-$C_4H_9$)═C($C_5H_4N$)Ni] $C_2B_{10}H_{10}\}_2Cl^+$ (2N → Ni) (FF) | S, X, H, B, C, MS | [1514] |
| 1-Me-2-R R = $(CH_2)_2CH═CH_2$, $CH_2CH═CH_2$, $CH_2CH═CHMe$ | S (lithium iodide catalyzed alkylation) | [139] |
| 1-CH═CH—$C_{14}H_9$ $C_{14}H_9$ = anthracene | S(Wittig reaction), X, H | [199] |
| 1,2-*cyclo*-(—CMe═CH—CH═CMe—) dimethylbenzocarborane | S, X, H, C, MS | [304] |
| 1,2-*cyclo*-(—CR═CR′—CR═CR′—) R, R′ = Et, *n*-$C_3H_7$, *n*-$C_4H_9$, Ph, Me, C≡C$C_4H_9$, $CMe_3$, C(O)OMe benzocarboranes | S(Ni-mediated 2 + 2 + 2 *cyclo*addition of carboryne with alkynes), X(R = Me, R′ = Ph), H, B, C, MS | [305] |
| 1,2-*cyclo*-(—$CH_2$—C═C—$CH_2$—) dihydrobenzocarborane | S | [306] |

| Compound | Information | References |
|---|---|---|
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R′ = Et; R″ = Me, R‴ = Ph benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), X, H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R′ = Et; R″ = Et, R‴ = Ph benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R′ = Et; R″ = Ph, R‴ = Et benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R′ = Et; R″ = $CMe_3$, R‴ = Ph, *n*-$C_4H_9$ benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), X, H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R′ = Et; R″ = $CHMe_2$, R‴ = Me benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R′ = Et; R″ = Me, R‴ = $CHMe_2$ benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R′ = Et; R″ = Me, R‴ = Et benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R′ = Et; R″ = Et, R‴ = Me benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R′ = Et; R″ = $CH_2$-OMe, R‴ = Ph | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), X, H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R′ = Et; R″ = $CH_2NMe$, R‴ = Ph benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R′ = Et; R″ = $CH_2CH═CH_2$, R‴ = Ph benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), X, H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R′ = Et; R″, R‴ = C(O)OMe benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R′ = Et; R″ = *n*-$C_4H_9$, R‴ = $SiMe_3$ benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), X, H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R′ = Et; R″ = Ph, R‴ = Me, *n*-$C_4H_9$, $(CH_2)_3Cl$ benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R′ = Et; R″, R‴ = Ph benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R′, R′ = *n*-$C_4H_9$; R‴ = Ph benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R′ = *n*-$C_4H_9$; R″ = Ph, R‴ = Me benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), X, H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R″ = Ph; R′ = Me, R‴ = *n*-$C_4H_9$ benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-RC═CR′-CR″═CR‴ R, R′, R″, R‴ = *n*-$C_3H_7$ benzocarboranes | S($NiCl_2$-catalyzed or $FeCl_3$-promoted), H, B, C, MS | [1605] |
| 1,2-*cyclo*-[CEt═CEt-C(═$NC_6H_3Me_2$)] | S, H, C | [307] |
| 1,2-*cyclo*-(—$PhMeC_4H_3$—CH═$CH_2$—) | S, X, H | [308] |
| 1,2-(*cyclo*-$CH_2CHRCR'═CR''$) R = 2-py, C(O)OMe; R′ = Et, *n*-$C_4H_9$, Me. Ph. *n*-$C_3H_7$; R″ = Et, *n*-$C_3H_7$, *n*-$C_4H_9$, *p*-$C_6H_4Me$, Ph | S(Ni-mediated cycloaddition), X[2-py, Me, Ph; C(O)OMe, Et, Et] H, B, C, MS | [309] |
| 1-R R═*cyclo*-(2-$C_6H_9$), $CMe_2$-CMe═$CH_2$, $CH_2CMe═CMe_2$, $CH_2C(CHMe_2)═CH_2$, β-pinene | S, H, C, MS | [310] |
| 2-Me-*cyclo*-1,3-CMe═$C(CH_2)_nC═CMe'$— *n* = 3–5 | S(Pd/N-cocatalyzed cycloaddition of 1,3-dehydro-*o*-carborane with alkynes), X(*n* = 4), H, B, C, MS | [1533] |

*Continued*

| Compound | Information | References |
|---|---|---|
| 1,3-*bicyclo*-$C_6H_2RR'$ R, R′ = H, F, Cl, $SiMe_3$, $CMe_3$, Me, $CF_3$; RR′ = $Me_2$ | S, X(Me/$Me_2$), H, B, C, MS | [1795] |
| 1,2-*cyclo*-$CHRCH_2$ R = *n*-$C_4H_9$, *n*-$C_6H_{13}$, $CH_2Ph$, Ph, $C_6H_4Ph$, $C_6H_4Br$, 2-naphthyl | S, X(Ph), H, B, C, MS | [1791] |
| 1,2-*cyclo*-CR═CPh R═Me, *n*-$C_4H_9$, $(CH_2)_3Cl$, $CH_2OMe$, $SiMe_3$ | S, H, B, C, MS | [1791] |
| 1,2-*cyclo*-C(*n*-$C_4H_9$)═C($SiMe_3$) | S, H, B, C, MS | [1791] |
| 1,2-*cyclo*-[$Me_2Si$—$CH(CHPh_2)$—$SiMe_2$ | S, H, C, P, Si, MS | [313,314] |
| 1,2*cyclo*-[$Me_2Si$—$CH_2CMe$═$CMeCH_2$—$SiMe_2$] | S, H, C, P, Si, MS | [314] |
| 1,2-*cyclo*-($Me_2Si$—RC═CR′—$SiMe_2$) R, R′ = H, Me, Et, Ph, $SiMe_3$, C(O)OMe | S, H, X(Ph, $SiMe_3$), C, P, Si, MS | [313–315] |
| 1,2-*cyclo*-[$Me_2Si$—NH-C(═CHMe)—$SiMe_2$] enamine | S, H, C, Si, IR, MS | [316] |
| 1,2-*cyclo*-($Me_2Si$—NR—$SiMe_2$) R═$CH_2$-9-anthracenyl, CH═CHPh, CH═$CHCHPh_2$, CH═$CHCH_2Ph$, *cyclo*-[C═$CHCH_2(C_6H_4)$], C($SiMe_3$)═$CH_2$ | S, X[$CH_2$-9-anthracenyl, *cyclo*-C═$CHCH_2(C_6H_4)$], H, C, Si, IR, MS | [316] |
| 1-CH═$CH_2$-2-$SiMe(OMe)_2$ | S | [317] |
| 1,2-*cyclo*-$(C_3H_3)_2C_2B_{10}H_{10}^-$ (FF) | S, H | [311] |
| 1-R-2-CH═$CH_2$ R═Me, $CH_2CH$═$CH_2$, *n*-$C_3H_7$, $CH_2Ph$ | S | [135] |
| 1-R-2-$(CH_2)_n$C═$CH_2$ R═H, Me; *n*═1, 2 | S, X(Me; *n*═1) | [318] |
| 1-CF═CXY-2-Me X,Y═F, Cl, *n*-$C_4H_9$, Ph, $CF_3$, $SC_4H_9$, SPh, $NEt_3$ | S, H, F | [1497] |
| 1-CH═CH-Ph | S | [77] |
| 1,2-$(CH_2CH$═$CH_2)_2$ | S, H, B, C | [319] |
| 1-CH═$CH_2$-2-$CH_2CH_2OH$ | S, X, H, B, C, IR | [320] |
| 1-$CH_2CH_2NMe_2CH_2CH$═$CH_2^+$ $Br^-$ | S, X, H, B, C, IR | [320] |
| 1-$CH_2CH$═$CH_2$-2-$OCH_2OCH_2Me$ | S, H, B, C, IR, MS | [321] |
| 1-CH[$C_6H_4$-*p*-$O(CH_2)_2Cl$]═CEtPh precursor to *nido*-$C_2B_9$ Tamoxifen analogue | S, X, H, B, C, MS | [1455] |
| 1-*cis*/*trans*-C(*p*-$C_6H_4OH$)═CPhEt Tamoxifen analogues; ER breast cancer growth inhibitors APP | S, X, H, B, C, IR, MS | [1532] |
| 1,2-*cyclo*-norbornadiene (3 isomers) | S, X(1 isomer), H, C, MS | [254] |
| 1,2-*cyclo*-[—C═C—$CMe_2CH_2$—S—$CH_2CMe_2$—] | S, H, C | [254] |
| 2/3/9-CH═$CH_2$ | Photoionization mass spectrum | [148] |
| 3-CH═$CH_2$ | S | [324] |
| 1,2-*cyclo*-SCH═C[C(O)$C_5H_4FeCp$]S | S, X, H, B, C, IR, MS | [1583] |
| 1-SCH═CHC(O) $C_5H_4FeCp$ 2 *cis*/*trans* isomers | S, X, H, B, C, IR, MS | [1583] |
| 1,2-$[SCH$═$CHC(O)OMe]_2$ 3 *cis*/*trans* isomers | S, H, B, C, IR, MS | [1583] |
| 1-SCH═CHC(O)OMe 2 *cis*/*trans* isomers | S, H, B, C, IR, MS | [1583] |
| 1,2-$R_2$-8/9-CH═CHR′ $R_2$═$Me_2$, $(CH_2Ph)_2$, $(CH_2)_3$ R′═Ph, *m*/*p*-$C_6H_4Me$, $C_6H_4OMe$, $C_6H_4F$, $C_6H_4Cl$, $C_6H_4Br$, $C_{10}H_7$, C(O)Et, OC(O)Me | S, H, B, C, MS | [1926] |
| 1-$CH_2C_6H_4$-*p*-CH═$CH_2$-2-R R═Ph, Me, H, $CH_2C_6H_4CH$═$CH_2$ fluorescent styrene derivatives | S, X, H, B, C, IR, MS, UV | [1608] |

| Compound | Information | References |
|---|---|---|
| —[—CHRCH$_2$—]—R = $C_6H_4$-*p*-$CH_2CB_{10}H_{10}CR$ R = Me, Ph polystyrene oxidation resistance on graphene oxides; catalyst support (FF) | S, H, B, C, IR, TGA, TEM | [1905] |
| 1-$CH_2C_6H_4$-*p*-CH=$CH_2$ | Free radical copolymerization with PEG-b-PLA Block copolymer→PM micelles for BNCT | [1612] |
| 1,2-*cyclo*-[CHRCH$_2$C(=R′$SiMe_3$)] R = *n*-$C_4H_9$, H, $CH_2COMe$, $CH_2NMe_2$ R′ = $C_6H_4X$ (X = H, Me, $CHMe_2$, $CF_3$, OMe, $NMe_2$, $CMe_3$), $C_6H_3X_2$ (X = Me, OMe), $C_6H_2Me_3$, $C_6F_5$, $C_{10}H_8$ (naphthalene), $C_4H_3S$, *n*-$C_4H_9$, $SiMe_3$, $SiEt_3$, $SiMe_2CMe_3$ metal-mediated cyclotrimerization | S, X[R = *n*-$C_4H_9$; R′ = *n*-$C_4H_9$, Ph, $C_6H_4Me$, $C_6F_5$, $C_4H_3S$, $C_6H_4CF_3$, $C_6H_3Me_2$, $C_6H_4CHMe_2$ (R = H), $SiMe_3$], H, C, B, MS | [1699] |
| 3-CR=C=$CH_2$ R = Me, Et, $CHMe_2$, $SiMe_3$, $CMe_3$, C≡C-*n*-$C_3H_7$ | S(ene reactions of 1,3-$C_2B_{10}H_{10}$), H, B, C, MS | [1890] |
| 3-CR=C=CHEt R=$CHMe_2$, $SiMe_3$, $CMe_3$, C≡C-*n*-$C_3H_7$ | S(ene reactions of 1,3-$C_2B_{10}H_{10}$), H, B, C, MS | [1890] |
| 3-CR=C=CH(*n*-$C_3H_7$) R = *n*-$C_4H_9$, C≡C-*n*-$C_3H_7$, $SiMe_3$ | S(ene reactions of 1,3-$C_2B_{10}H_{10}$), H, B, C, MS | [1890] |
| 3-C(C≡C-$CHMe_2$)=C=$CMe_2$ | S(ene reactions of 1,3-$C_2B_{10}H_{10}$), H, B, C, MS | [1890] |
| 3-R R=C($CH_2CF_3$)=C=CH$(CH_2)_5$Me, C$(CH_2)_6$Me=$CHCF_3$ | S(ene reactions of 1,3-$C_2B_{10}H_{10}$), H, B, C, MS | [1890] |
| 3-R R=$CH_2$C(=$CH_2$)–C≡CEt, C[C(=$CH_2$Me]=C=CHCMe | S(ene reactions of 1,3-$C_2B_{10}H_{10}$), H, B, C, MS | [1890] |
| 1-R-4,5-(*trans*-CH=CHR′)$_2$ R = $SiMe_3$, Et, $CHMe_2$, Ph, $CH_2Ph$, $C_6H_4Cl$ R′ = Ph, 2/3/4-$MeC_6H_4$, 3,4-$(F_3C)C_6H_4$, 4-$C_6H_4$, 4-$PhC_6H_4$, 2-naphthyl | S (Pd-catalyzed direct dialkenation of B-H bonds, X (R = $SiMe_3$, R′ = 3-$F_3CC_6H_4$; R = 4-$ClC_6H_4$, R′ = Ph), H, B, C | [1897] |
| 9,12-$(CH_2$=$CHCH_2)_2$ | S, H, B, C, MS, IR | [1891] |
| 1,2,9,12-$(CH_2$=$CHCH_2)_4$ | S, H, B, C, MS, IR | [1891] |
| 1-R-8,9,10,12-$(CH_2CH$=$CH_2)_4$ R = Me, Ph | S, H, B, C, IR, MS | [1898] |
| 9,12-$(CH_2CH$=$CHPh)_2$ | S, H, B, C, IR, MS | [1898] |
| 8,9,10,12-$(CH_2CH$=$CHPh)_2(CH_2CH$=$CH_2)_2$ | S, H, B, C, IR, MS | [1898] |
| 8,9,10,12-$(CH_2CH$=$CH_2)_4$ | S, X, H, B, C, IR, MS | [1898] |
| **Alkynyl Derivatives** | | |
| 1-C≡C$SiMe_3$-2-Si$(CMe_3)Me_2$ | S, H, B, C, IR, MS | [159] |
| | S | [328,329] |
| 1-Me-2-$(CH_2)_2$C≡C—$SiMe_2CMe_2CHMe_2$ | S (lithium iodide catalyzed alkylation) | [139] |
| 1-CH=CH—C≡CH | S, H, B, C, IR, MS | [1915] |
| —[—$C_6H_4$—$CB_{10}H_{10}$C—$C_6H_4$—C≡C—Ar—C≡C—]$_n$ polymers Ar = 2,5-$C_6H_2(OC_6H_{17})_2$, 2,5-$C_6H_2(OC_{16}H_{33})_2$, N-(*n*-$C_4H_9$)-carbazole, 2,5-$C_6H_2(C_8F_{17})_2$ aggregation-induced emission (FF) | S, H, B, C, UV, fluorescence | [332] |
| {—C≡C-Ar-C≡C-*p*-$C_6H_4$-[*cyclo*-C=C(*n*-$C_4H_9$)-C(*p*-$C_6H_4$-)=C(*n*-$C_4H_9$)]$C_2B_{10}H_{10}$}- Ar = $C_6H_2(OR)_2$, $C_8H_{17}$, $CF_3$ benzocarborane polymers (FF) | S, H, B, C, UV, photoluminescence | [1525] |
| [-(*p*-$C_6H_4$)—$CB_{10}H_{10}$C—*p*-$C_6H_4$—C≡C—$C_{20}H_{10}(OC_8H_{17})_2$- C≡C—]$_n$ $C_{20}H_{10}$ = binaphthyl chiral conjugated polymers (FF) | S, H, B, C, IR, photoluminescence, CD | [333] |

*Continued*

| Compound | Information | References |
|---|---|---|
| 1,2-$R_2$-9-$OPO_2(C_{20}H_{12})$ R = H, Me $C_{20}H_{12}$ = binaphthyl Rh-catalyzed asymmetric hydrogenation of prochiral olefins | S, H, B, C, P | [1391] |
| 1-$C_6H_4$—O—$CH_2C(O)NHC_6H_4$—$C(O)C_6H_4$-*o*/*m*-R R = $OCH_2C{\equiv}CH$, OH | S, H, C, IR, MS, HIF-1α inhibition, fluorescence imaging | [1654] |
| 1-[$C_6H_4$—C≡C—$C_6H_4$—DPP]-2-[$C_6H_4$—C≡C—$C_6H_4$-BODIPY] DPP = diketopyrrolopyrrole BODIPY = extended borondipyrrolemethane Through-space electronic energy transfer across proximal molecular dyads | S, UV(absorption, fluorescence | [1683] |
| 1-[C≡C—$C_6H_4$-*p*-$C(C_4EtMe_2N){=}C(C_4EtMe_2N$-$BF_2$)]-2-[$C_6H_4$-*p*-$C(C_4EtMe_2N){=}C(C_4EtMe_2N$-$BF_2$) BODIPY (boron dipyrromethen) dyads for low-energy photosensitization | S, X, H, B, C, IR, MS, UV(fluorescence), E | [1847] |
| 3-C≡C—$C_6H_4$—*p*-C≡C—$OSi(CHMe_2)_2$ | S, H, B, C, IR, MS | [1930] |
| 3-C≡C—$C_6H_4$—*p*-C≡C—R R = H, $C_6H_4$-*p*-BODIPY, $C_6H_4$-*p*-C(O)OEt, $C_6H_4$-*p*-$CH_2OH$ | S, H, X($C_6H_4$-BODIPY), B, C, IR, MS | [1930] |
| [$C_2B_{10}H_{10}$-9-($C_6H_4$-C≡C)-12-$C_6H_4$—C≡C-$C_6H_2(OR)_2$—]$_n$ luminescent polymer (FF) | S, H, B, C, UV, luminescence | [1696] |
| 3-$(CH_2)_n$$C_{16}H_9$ $C_{16}H_9$ = pyrene | S, H, B, C, MS | [1796] |
| 4-CR=CR′H R, R′ = Ph, Et, SPh, *p*-$C_6H_4$X X = Me, C(O)OMe, $CHMe_2$, F, Cl, Br, $CF_3$, OMe, SMe Ir-catalyzed alkyne hydroboration with the carborane cage | S, X[Ph,Ph; C(O)OMe, C(O)OMe],H, B, C, MS | [1805] |
| 1,4-*cyclo*-C(O)O-CPh=CEt | S, X, H, B, C, MS | [1805] |
| 1,4-*cyclo*-C(O)O-IrCp*(DMSO) | S, X, H, B, C, MS | [1805] |
| **Alcohols and Hydroxy Derivatives** | | |
| 1,2-$(OLi)_2$ | S, X, H, B | [1730] |
| | S[from $B_{10}H_{12}(MeCN)_2$ and RC≡CH with homogeneous Ag catalyst, high yield] | [1760] |
| | S | [345] |
| 1-Me-3-OH | S | [346,347] |
| 1-CHMeOH-2-R R = Me, Ph | S | [348] |
| 1,2-*cyclo*-$CH_2CH(OH)CH_2$ | S, H, IR | [311] |
| 1-R-3-OH R = Et, $CHMe_2$, Ph | S | [134] |
| *n*-OH *n* = 3, 4 | S | [1487] |
| 1-R R = H, OH, $CH_2OH$, $(CH_2)_3OH$ | $K_a$ association constant with β-cyclodextrin | [1921] |
| 1,2-$R_2$ R = H, OH, $CH_2OH$, $(CH_2)_3OH$ | $K_a$ association constant with β-cyclodextrin | [1921] |
| 1-CRR′OH R = H, Me, naphthyl, *n*-$C_6H_{13}$, *n*-$C_4H_9$, R″C=CH | S, H, B, C | [350] |
| 1-$CH_2CH_2OH$-2-Me | S | [352] |
| 1-$CH(OH)C_5H_4$N-2-R R = Me, Ph | S, X(Me), H, B, C, IR, MS | [186] |
| 1-CHR(OH)R-2-R′ R = H, Me, Ph, $CH{=}CH_2$, CH=CHMe, *p*-$C_6H_4OMe$, α-$C_4H_3(O)$, *o*-$C_6H_4Cl$, γ-$NC_5H_4$, β-$NC_5H_4$; R′ = Me, Ph, $CH{=}CH_2$ | S | [353] |
| 1-R-2-R′ R = H, R′ = OH, $CH_2OH$, $NH_2$; R = R′ = OH complexes with β-cyclodextrin | $K_a$ (association constants) | [1404] |

| Compound | Information | References |
|---|---|---|
| 1-C(OH)CR═$CH_2$ R = C(O)OMe, C(O)OEt, C(O)$OCH_2$Ph, C(O)OPh,C(O)H, C(O)Me, C(O)$OCH_2CF_3$, CN, C(O)OMe anti-proliferative activity; BNCT for brain and breast cancer | S | [1244] |
| 1-C(OH)C[C(O)OMe]═CHPh anti-proliferative activity; for brain and breast cancer | S | [1244] |
| 1-R-2-Ph R = glycosyl-containing groups | S, H, IR | [355] |
| | S | [356,144] |
| | MS (fragmentation patterns) | [1505] |
| | E (water-based electrolytes) | [1809] |
| 1-C(OH)R-2-Me R = 9-anthracenyl, 4-pyridyl crystal engineering of carborane alcohols | S, X, H, B, C, MS, IR | [1540] |
| 1-C(OH)R-2-Ph R═CH═CHPh, 2-furanyl crystal engineering of carborane alcohols | S, X, H, B, C, MS, IR | [1540] |
| 1-($CH_2$-O-*m*-$C_6H_4$COH) | S | [1400] |
| 1-$C_6H_4$-*m*/*p*-OH | p$K_a$, $\sigma^-$ (inductive mechanism) | [358] |
| *n*-*p*-$C_6H_4$OH *n* = 1, 3, 9 | p$K_a$, hydrophobicity, estrogen receptor binding affinity | [359] |
| *n*-*p*-$C_6H_4$OH *n* = 1, 3, 12 | Partition coefficients (log P)]; Hansch-Fujita hydrophobic parameters; drug design | [1478] |
| 1,2-$(C_6H_4OH)_2$ | Dipole moments | [1459] |
| [$(CH_2)_3$OH]$HC_2B_{10}Me_8H_2$ (FF) | S, H, B, C, MS | [190] |
| 1-$(CH_2)_n$OH *n* = 1–4 | S | [127] |
| 1,2-[$(CH_2)_n$OH]$_2$ *n* = 1–4 | S | [364] |
| 1,2-{CH(OH)-[2,2]paracyclophane-2-R}$_2$ | S, H, IR | [367] |
| 1-Me-2-*cyclo*-$C_6H_{10}$OH | S, H, B, C, IR | [369] |
| 1-Ph-2-$CH_2$CH(OH)$CH_2$Cl | S, IR (actual spectrum) | [370] |
| 1-Me-2-$CH_2$C(OH)$(CH_2)_2$Me | S, IR (actual spectrum) | [370] |
| 1-R-2-R′ R = $(CH_2)_2$OH, $C_2(CH_2CH_2OH)_2$; R′ = H, $CHMe_2$, CMe═$CH_2$ | IR | [371] |
| 1-CH(OMe)CHPhOH-2-$CHMe_2$ | S, IR | [1499] |
| 1-$CH_2$OCH($CH_2OCH_2$Ph)$_2$-2-$(CH_2)_3$X X = Br, $CH_2$Ph | S, H, B | [1335] |
| 1-$CH_2$OCH($CH_2$OH)$_2$-2-$(CH_2)_3$SH glycerol | S, H, B | [1335] |
| 1-$CH_2$OCH($CH_2$OH)$_2$-2-SPt(terpyridyl)$^+$ $OSO_3CF_3^-$ glycerol | S, H, B, C, Pt, MS | [1335] |
| 1-Me-2-$(CH_2)_3$R R = OH, OTs, $N_3$ | S, H, B, C, IR, MS | [1624] |
| 1-Me-2-$(CH_2)_3$-*cyclo*-$N_3C_2$H-$CH_2$-(5-TDGP) TDGP = thio-C-glocopyranose | S, H, B, C, IR, MS | [1624] |
| 1,2-[$(CH_2)_3$-*cyclo*-$N_3C_2$H-$CH_2$-(5-TDGP)]$_2$ TDGP = thio-C-glocopyranose | S, H, B, C, IR, MS | [1624] |
| 1-CHOH-$C_5H_4$FeCp | X(polymorph) | [1631] |
| 1-CHOH-$C_5H_5$N inter- and intramolecular N-H and O-H bonds | S, X, H, B, C, IR, MS, UV | [1630] |

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| Compound | Information | References |
|---|---|---|
| 1,2-(CHOH-$C_5H_5N)_2$ inter- and intramolecular N-H and O-H bonds | S, X(two polymorphic forms), H, B, C, IR, MS, UV | [1630] |
| *Rac*/*R*/*S*-1-CH(OH)$C_5H_4N$ supramolecular chirality; O-H—N homochiral helical networks | S, X, H, B, C,MS | [1838] |
| 1-R-2-$C_6H_4$-*p*-$OCH_2C(O)NH$-$C_6H_3R'R''$ R, R″ = H, Me, Et, $CMe_3$, *n*-$C_4H_9$; R′ = C(O)OMe, C(O)OEt. C(O)OH, C(O)Ph, $B(OH)_2$ HIF-1α inhibitors | S | [1659] |
| 1-HO-2-C(OH)$R_2$ R = *n*-$C_4H_9$, Me | S, X(*n*-$C_4H_9$), H, B | [1735] |
| 1,2-RR′-9-OH R, R′ = H, Me | S, IR (actual spectra) | [374] |
| 9-CH(OH)Ph | S | [375] |
| 9-*p*-$C_6H_4OH$ | S (RMgX), H | [376] |
| 9,12-(*p*-$C_6H_4OH)_2$ | S, X, H, B, C, MS | [240] |
| 1-$CH_2CR(OH)(C_5H_4)$FeCp R = H, Me | S, H, B, IR | [1843] |
| 9-$(CH_2)_n$CH(OH)$(C_5H_4)$FeCp *n* = 0, 1 | S, H, B, IR | [1843] |
| 9-$CH_2CR(OH)(C_5H_4)$FeCp R = H, Me | S, H, B, IR | [1843] |
| 1,2,9,12-$(CH_2CH_2CH_2OH)_4$ | S, H, B, C, MS, IR | [1891] |
| 8,9,10,12-$(CH_2CH_2CH_2OH)_4$ | S, H, B, C, MS, IR | [1891] |
| 9,12-$[(CH_2)_3OH]_2$ | S, H, B, C, IR, MS | [1898] |
| 8,9,10,12-$[(CH_2)_3OH]_4$ | S, X(Cl), H, B, C, IR, MS | [1898] |
| 8,9,10,12-$[CH_2CH_2C(O)OH]_4$ | S, H, B, C, IR, MS | [1898] |
| **Alkoxy and Aryloxy Derivatives** | | |
| 1,2-[—*cyclo*-MeC═CH-B(OEt)—] | S, H, IR | [378] |
| 1-$B(OMe)_2$-2-$CHMe_2$ | S | [1397] |
| 1-R-3-OR′ R = H, Me; R′ = Me, Et | S | [134] |
| 1-$CH(OEt)_2$-2-R R = H, Me | S | [380] |
| 1,2-$Me_2$-B-OMe | S, IR | [381] |
| 3-$OCH_2CH{=}CH_2$ | S, H, B, C, MS | [177] |
| RR′C[$CH_2$-1-1,2-$C_2B_{10}H_{11}]_2$ R = dimethoxytrityl, R′ = phosphoramidtite (FF) | S, H, C | [1375] |
| RR′C[$CH_2$-X-$CH_2$-1-1,2-$C_2B_{10}H_{11}]_2$ X = $CH_2$, O; R = dimethoxytrityl, R′ = phosphoramidite (FF) | S, H, C, P | [1375] |
| 1-$(CH_2)_n$-triazol-X X = derivative of thymidine, citidine, adenosine, guanosine | S, X(X = thymidine), H, B, C, MS, IR | [1853] |
| 1-$(CH_2)_n$-triazol-X-*cyclo*-$C_4O(CH_2OR)$-OP[O$(CH_2)_2CN]N(CHMe_2)_2$ phosphoramidites X = derivative of thymidine, citidine, adenosine, guanosine; R = dimethoxytriyl chloride, 4-dimethylaminopyridine, $SiMe_2CMe_3$; building-blocks for synthesis of carborane-modified oligonucleotides | S, H, B, C, MS, IR | [1853] |
| Harminium$^+$ $B[(OCH_2)_2(C_2B_{10}H_{10})]_2^-$ | Enthalpy of solution in $H_2O$ and MeOH | [1857] |
| *Aldehydes* | | |
| 1-CHO-2-R R = H, Me | S, IR | [1243] |
| 1-[$C_6H_3$-*m*-CHO-*p*-OH] | S, H | [387] |

| Compound | Information | References |
|---|---|---|
| 1-[$C_6H_3$-*m*-R-*p*-R′] R = C(O)Me, CHO, $CH_2OH$; R′ = OMe, OH | S, H | [387] |
| 1-$CH_2CHO$ | S | [380,385,388] |
| 1-$CH_2CHO$-2-R R = H, Me | S | [380,390,391] |
| 1-$CH_2CHO$-2-Ph | S | [390] |
| 1-($CH_2$-O-*m*-$C_6H_4CHO$ | S | [1400] |
| 1-(*m*-$C_6H_4CHO$-2-$CH_2CH{=}CH_2$ | S | [392] |
| 1-(*m*-$C_6H_4CHO$-2-$CH_2CH(OH)CH_2OH$ | S | [392] |
| 1-$CH_2CPh{=}CFCHO$ R = Me, Ph, $CHMe_2$ | S | [1498] |
| *Ketones* | | |
| 1-CHBrC(O)Ph-2-Me | H | [395] |
| 1-$CH_2C(O)CH_2Br$-2-Ph | H | [395] |
| 1-$(CH_2)_n$C(O)Ph-2-Ph *n* = 1, 2 | S | [348] |
| 1-C(O)Ph-2-R R = Me, Ph | S, IR | [399] |
| 1,2-$[C(O)Ph]_2$-8,9,10,12-$Et_4$ | S | [172] |
| $PhCB_{10}H_{10}C$–C(O)-$CB_{10}H_{10}C$–Ph (FF) | S | [397] |
| 1-$CH_2C(O)Me$-2-$CH{=}CH_2$ | S, IR (actual spectrum) | [370] |
| 1-R-2-R′ R = C(O)Me, $CH_2C(O)Ph$; R′ = H, Me, Ph | S | [401] |
| 1-R-2-R′ R = $C(O)C_6H_4$-*p*-X X = Cl, Br, Me; R′ = H, Me, Ph | S | [401] |
| R-1,2-$CB_{10}H_{10}C$–CHPh–$CH_2C(O)$-1,2-$CB_{10}H_{10}C$–R R = Me, Ph (FF) | S | [402] |
| 1-$CH_2CH(CH_2C(O)CMe_3]_2$ | S, H, UV, IR | [99] |
| 1-$CH_2CH[CH_2C(O)R']_2$-2-R R = $CMe_3$, Ph, *p*-$C_6H_4O$ Me; R′ = Me, Ph | S, UV, IR | [403] |
| 1,2-*cyclo*-[—C(O)$C_6H_4$—] | S | [404] |
| 1,2-*cyclo*-[—$CH_2C(O)$—(*o*-$C_6H_4$)—] *cyclo*hexanone | S | [145] |
| $[1\text{-}(C_9H_6{=}O)\text{-}2\text{-}Ph]^{n-}$ *n* = 0, 1 indan-1-one | S, H(*n* = 0), IR | [405] |
| 9-$C_6H_4$-*p*-$OC_6H_4$-*p*-C(O)Ph | S, H, B, C, IR, S | [229] |
| 9-$C_6H_3$[*m*-C(O)Ph]-*p*-OPh | S, H, B, C, IR, S | [229] |
| 1,9/1,12-$[C_6H_4$-*p*-C(O)$C_6H_4$-*p*-OMe]$_2$ | S, H, B, C, IR, S | [229] |
| 9-C(O)Me | S | [406,407] |
| 9-$CH_2C_6H_4C(O)Ph$ | S | [173] |
| 1-$CH_2C(O)(C_5H_4)FeCp$ | S, H, B, IR | [1843] |
| 1-R-2-[C(O)CH=CHR′] R = Me, Ph, $CHMe_2$; R′ = Ph, *p*-$MeOC_6H_4$, *p*-$Me_2NC_6H_4$, 2-furyl, CH=CHPh α,β-unsaturated ketones | S | [412] |
| $[HO(O)C]_2C\{CH_2C{\equiv}CCH_2$-O-$CH[CH(CH_2$-$CB_{10}H_{10}CH)_2]_2\}_2$ octa(*o*-carboranyl)ether dicarboxylic acid (FF) | S, MS | [1416] |

*Continued*

| Compound | Information | References |
|---|---|---|
| *Carboxylic acids* | | |
| 1-C(O)OH | Complexes with α-cyclodextrin in aqueous solution; $K_a$ (association constant) | [481] |
| 1-C(O)OH encapsulation in CdTe-cysteamine capped quantum dots; anticancer pharmacophores | | [1632] |
| | Conjugation with CdTe quantum dots; labeling of anticancer pharmacaphores | [1570] |
| 1,2-$[C(O)OH]_2$ encapsulation in CdTe-cysteamine capped quantum dots; anticancer pharmacophores | | [1632] |
| 1-C(O)OH-2-COC(O)Me "asborin" aspirin analogue | Inhibition of aldo/keto reductase | [1567] |
| | Hydrolysis; COX acetylation) pharmacophore | [1568] |
| 1,2-$[C(O)OH]_2$-8,9,10,12-$Et_4$ | S | [172] |
| 1,2-$H_2C_2B_{10}H_6$-8,9-$[(HO)(O)C]_2$-10,12-$Et_2$ (FF) | S, H, B | [172] |
| 1,2-$[C(O)OH]_2 \cdot 0.5EtOH$ | X, B | [425] |
| 1-C(O)OH-2-R R = H, $CH_2NHC_6H_4$-*m*-$CF_3$, $C_6H_4$-*m*-F nonsteroidal anti-inflammatory drugs (NSAIDS) | Transthyretin (YYR), COX-1, and COX-2 (*cyclo*oxygenase) assays | [1364] |
| 1-C(O)OH-2-N(boc)NH(boc) boc = *tert*-butyloxycarbonyl | S, X, H, B, C, MS | [427] |
| 1-$CH_2$C(O)OH-2-R R = H, Me, Ph, CH═$CH_2$, $CH_2$Br, $CHMe_2$ | S | [432] |
| 1,2-$[CHPhC(O)OH]_2$ | S, H | [147] |
| 1-$CHMe_2$-9(12)-$(CH_2)_3$C(O)OH | S | [148] |
| $Na^+$ $[O(O)C(CH_2)_3]HC_2B_{10}Me_8H_2^-$ (FF) | S, H, B, C, MS | [194] |
| 1-$(CH_2)_n$C(O)OH *n* = 1,3 | S | [436] |
| 1-CH(OMe)C(O)OH-2-R R = Me, $CHMe_2$ | S, HMe, IR[$CHMe_2$] | [1499] |
| 1-[C(O)-*o*-$C_6H_4$C(O)OH]-2-R R = Me, Ph | S, IR | [399] |
| 1-C(O)$(CH_2)_2$C(O)OH-2-R R = Me, Ph | S, IR | [399] |
| 1-$CH_2$O—*p*-$C_6H_4$—C(O)OH | S, H, B, C, MS | [1315] |
| 1′,3′-$(HCB_{10}H_{10}C—CH_2-O)_2$—*p*-$C_6H_3$—C(O)OH (FF) | S, H, B, C, MS | [1315] |
| 1,2-[*p*-$C_6H_4$-C(O)OH]$_2$ | Dipole moments | [1459] |
| 1,2-[*p*-$CH_2C_6H_4C(O)OH]_2$ | S | [438] |
| 1-o-$C_6H_4$C(O)OH | S (from benzo*cyclo*pentanone) | [439] |
| 1-C(O)OH N- and P-containing salts | S, H, IR | [1338] |
| 1,9/1,12-[$C_6H_4$-*p*-C(O)OH]$_2$ | S, H, B, C, IR, S | [229] |
| $[HO(O)C]_2C\{CH_2C{\equiv}CCH_2$-O-CH[$CH(CH_2$-$CB_{10}H_{10}CH)_2]_2\}_2$ octa(*o*-carboranyl) ether dicarboxylic acid (FF) | S, MS | [1416] |
| 1-$(CH_2)_n$N[C(O)H]$C_6H_4$-*p*-C(O)ONa *n* = 1,3 folate analogues for BNCT | S, H, biological activity: toxicity, cellular uptake | [1586] |
| 1-$(CH_2)_n$O$C_6H_4$-*p*-C(O)ONa *n* = 1–3 | S, H, biological activity: toxicity, cellular uptake | [1586] |
| 1-$CH_2OC_6H_4$-*p*-C(O)NHCH[C(O)ONa]$(CH_2)_2$C(O)ONa folate analogues for BNCT | S, H, biological activity: toxicity, cellular uptake | [1586] |
| 1,2-(galactopyranose)2-9-$SCH_2$C(O)OH | S, H, B, C, IR, MS | [1618] |

| Compound | Information | References |
|---|---|---|
| HO(O)C($CH_2$)$_2$C(O)OC$H_2$-C($CH_2$S-9-$C_2B_{10}H_{11}$)$_3$ for incorporation into tumor-selective peptides FF | S, X, H, B, C, IR, MS | [1618] |
| 1-R-2-$C_6H_4$-*p*-OC$H_2$C(O)NH-$C_6H_3$R′R″ R, R″ = H, Me, Et, $CMe_3$, *n*-$C_4H_9$; R′ = C(O)OMe, C(O)OEt. C(O)OH, C(O)Ph, B(OH)$_2$ HIF-1α inhibitors | S | [1659] |
| 3-C(O)OH-1-R R = H, Me | S | [442] |
| 9-CHMe($CH_2$)$_2$C(O)OH | S | [148] |
| 9,12-[CHMe($CH_2$)$_2$C(O)OH]$_2$ | S | [148] |
| 9-$CH_2$-*p*-$C_6H_4$C(O)OH | S, B | [409] |
| ***Esters and acyl halides*** | | |
| 1-C(O)X X = Cl, OMe, $CH_2$OC(O)O, OSi$Me_3$ | S, p$K_a$ | [373] |
| 1-($CH_2$)$_n$C(O)Cl *n* = 1,3 | S | [436] |
| 1-$CH_2$C(O)Cl | $^{35}$Cl NQR | [1327] |
| 1-R-2-$CH_2$Cl R = C(O)Cl, C(O)OEt | $^{35}$Cl NQR | [1439] |
| *n*-OC(O)Me *n* = 3, 4, 9, 10 | S | [372] |
| 1-C(O)OEt | S | [422] |
| 1,2-$R_2$ R = $CH_2$C(O)OMe, $CH_2$C(O)OEt, C(O)Cl | S | [364] |
| 1-$CH_2CH_2$C(O)OMe-2-Me | S | [352] |
| 1-$CH_2CH_2$C(O)OMe | S, H, B | [446] |
| 1,2-[$CH_2CH_2$C(O)OR]$_2$ R = H, Me | S, H, B | [446] |
| 1-R-2-($CH_2$)$_3$OC(=O)C$Me_3$ R = H, Me, ($CH_2$)$_3$OC(=O)C$Me_3$ | S, H, B, C, IR, MS | [195] |
| 1-CHR′C(O)OMe-2-R R = H, Me; R′ = $CH_2$C=$CH_2$, $CH_2$C=CHPh | S, H, MS | [1430] |
| 1-R-2-$CH_2$CH=$CH_2$ R = C(O)OMe, *m*-$C_6H_4$CO)OMe, $CH_2$OC(O)Me, *p*-$C_6H_4$C(O)OMe | S | [392] |
| 1,2—{*cyclo*-C[C(O)OMe]=C[*cyclo*—$CH_2$—O—$CH_2$]C=C[C(O)OMe]—} | S, H, C, MS | [254] |
| 1-HC(O)NH—C[C(O)OEt]$_2$ | S, H, IR, MS | [189] |
| 1-*p*-$C_6H_4$—C(O)—*cyclo*-$NC_5H_9$R R = H, C(O)OEt | S, X[C(O)OEt], H, IR, MS | [230] |
| 1-*p*-$C_6H_4$—C(O)NH($CH_2$)$_2$-*cyclo*-$NC_5H_{10}$ | S, H | [230] |
| 1-C(O)NH($CH_2$)$_2$-*cyclo*-$NC_5H_{10}$ | S, H, IR, MS | [230] |
| 1-($CH_2$)$_n$O($H_2$)$_5$-*cyclo*-$NC_5H_5$($CH_2$OH)$_5$ *n* = 1–3 enantiomers *N*-substituted deoxynojirimycins glycoprocessing enzyme inhibitors | S, H, B, C, IR, MS | [1893] |
| 1-CH=N—CH[C(O)OMe]$CH_2CHMe_2$ | S, H, C, MS | [382] |
| 1-C($CF_3$)[NHOC(O)C$Me_3$]C(O)OMe-2-Me amino acid ester | S, X | [448] |
| 1-($CH_2$)$_n$OC(O)R R = Me, Ph; *n* = 1–3 | S | [127] |
| 1-R-2-R′ R=CHMeCH(COOEt)$_2$, CHPhCH(C(O)OEt]$_2$; R′ = Me, Ph, α-naphthyl | S | [1489] |
| 1-($CH_2$)$_4$OC(O)Ph | S | [127] |

*Continued*

| Compound | Information | References |
|---|---|---|
| 1-$CH_2OC(O)CF_3$ | S | [127] |
| [—$OCH_2$—$CB_{10}H_{10}C$—$CH_2$—O—C(O)—$(CH_2)_xC(O)$—]$_n$ polyesters (FF) | S | [449] |
| 1,2-$Et_2$-3-$(CH_2)_6OC(O)Me$ | S (from $B_{10}H_{13}R$ in ionic liquid), H, B, IR, MS | [450] |
| 1-$CH_2(O)OCR$ R = Et, $Me_2CH$, Ph, 1-1,2-$C_2B_{10}H_{11}$ (FF) | S | [1333] |
| 1,2-[$CH_2(O)OCR]_2$ R = Et, $Me_2CH$, Ph | S | [1333] |
| 1-R-2-$(CH_2)_nC(O)OEt$ R = H, Ph, $CH_2Ph$, $(CH_2)_2Ph$, $n$-$C_5H_{11}$, $C_6H_4NH_2$; $n$ = 0–3 | S | [436] |
| 1-Me-2-$CH_2C(O)CH_2C(O)OEt$ | S, IR | [1486] |
| 1-R-2-CHR′CH[C(O)OEt]$_2$ (R,R′ = Me, Ph) | S | [1372] |
| 1-C(O)O$(CH_2)_n$OOR R = $Me_3$, $CMe_2Et$; $n$ = 1,2 peroxy esters | S | [1406] |
| 1-C(O)OOR R = $CMe_3$, $CMe_2Et$ peroxy esters | S | [1405] |
| 1-C(O)O$OCMe_2C{\equiv}$CH-2-R R = H, $CHMe_2$ peroxy alkynes | S, heat capacity temperature dependence, $\Delta H_{combustion}$ | [1337] |
| $PhCH_2OC(O)(CH_2)_9OC(O)CMe\{CH_2OC(O)C$-Me-[$CH_2$-OC(O)$(CH_2)_2CB_{10}H_{10}CH]_2\}_2$ dendron (FF) | S, H, B, C, IR, MS | [429] |
| $(HCB_{10}H_{10}C–CH_2OCH_2)_3C$–C(O)OH pentaerythritol dendron building-block for BNCT (FF) | S, X, H, B, C, IR, MS | [453] |
| 1,2-$HCB_{10}H_{10}C$–C(O)O–$(CH_2)_n$–1,2-$CB_{10}H_{10}C$–R $n$ = 1,2; R = H, Me, $CHMe_2$, $CMe{=}CH_2$ esters (FF) | S, H, IR, UV | [454] |
| 1-Ph-4-$C_6H_2Me_3$ mesityl | S (insertion of Ph$C{\equiv}$CH into 6-mesityl-$B_{10}H_{13}$ with BMIMCl ionic liquid catalyst or *N*,*N*-dimethylaniline in toluene), X, H, B, C, IR, MS BMIMCl = 1-butyl-3-methyl-imidazolium chloride | [1634] |
| 1-$CH_2OC(O)$Me-4-Ph | S (insertion of HC$\equiv$C—$CH_2COC(O)$Me into 6-mesityl-$B_{10}H_{13}$ with BMIMCl ionic liquid catalyst or *N*,*N*-dimethylaniline in toluene), X, H, B, C, IR, MS BMIMCl = 1-butyl-3-methyl-imidazolium chloride | [1634] |
| 2-$CH_2OC(O)$Me-4-Ph | S (insertion of HC$\equiv$C—$CH_2COC(O)$Me into 6-mesityl-$B_{10}H_{13}$ with BMIMCl ionic liquid catalyst or *N*,*N*-dimethylaniline in toluene), H, B, C, IR, MS BMIMCl = 1-butyl-3-methyl-imidazolium chloride | [1634] |
| 1,2-[$CH_2OC(O)Me]_2$-4-Ph | S (insertion of $Me(O)COCH_2C{\equiv}C$—$CH_2COC(O)$Me into 6-mesityl-$B_{10}H_{13}$ with BMIMCl ionic liquid catalyst or *N*,*N*-dimethylaniline in toluene), H, B, C, IR, MS BMIMCl = 1-butyl-3-methyl-imidazolium chloride | [1634] |
| 1-R-2-$C_6H_4$-*p*-$OCH_2C(O)NH$-$C_6H_3$R′R″ R, R″ = H, Me, Et, $CMe_3$, *n*-$C_4H_9$; R′ = C(O)OMe, C(O)OEt. C(O)OH, C(O)Ph, $B(OH)_2$ HIF-1α inhibitors | S | [1659] |
| 1-R′-2-$(CH_2)_nOC(O)R$ $n$ = 1, 2; R′ = H, Me, $CHMe_2$, $CH_2{=}CMe$; R = *cyclo*-(C=N—O—CPh=C—), *cyclo*-[C=N—O—C($C_6H_4$Me)=C—], *cyclo*-(C=N—S—CCl=CCl—) | S, H, IR | [1667] |
| [$HCB_{10}H_{10}C–CH_2]_2C[C(O)OEt]_2$ (FF) | S | [125] |
| 1-Ph-2-C(O)O$OCMe_3$ peroxy ester | S | [128] |
| 1-$SiMe_2CMe_3$-2-$(CH_2)_3OC(O)CH{=}CH_2$ acrylate etch-resistant component for UV-nanoimprint lithography | S, H, C, MS | [1433] |

| Compound | Information | References |
|---|---|---|
| Poly[2-(hydroxyethyl)methacrylate]-OC(O)-$C_2B_9H_{11}$ silica nanoparticles for BNCT biocompatible polymers | S, H, B(solid state), TEM, dynamic light scattering | [1753] |
| Poly[2-(methacryloyloxy)ethyl succinate]-OC(O)-$C_2B_9H_{11}$ silica nanoparticles for BNCT biocompatible polymers | S, H, B(solid state), TEM, dynamic light scattering | [1753] |
| ***Ethers, epoxides, and peroxides*** | | |
| 1-$CH_2OC_6H_3$(OMe)-*o*-*cyclo*-CHS$(CH_2)_2$S | S, H, B, MS | [455] |
| 1-$CH_2OC_6H_4$-*p*-R R = *cyclo*-CHS$(CH_2)_2$S, *p*-$C_6H_4$OH, CH=NOH | S, H, B, MS | [455] |
| 1-$CH_2O$—$C_6H_4$-*p*-R R=dihydroisooxazole, isooxazole | S, X(isooxazole), H, B, MS | [455] |
| 1-R-2-R′ R, R′ = $CH_2OC_4H_9$, $CH_2OCH_2Ph$ | S | [456] |
| 1-$CH_2OCH_2CH$=$CH_2$ | S | [457] |
| 1,2-$(CH_2OCH_2CH$=$CH_2)_2$ | S | [457] |
| 1,2-*cyclo*-[—$SiMe_2$—O—$SiMe_2$—] | S, IR | [460] |
| 1-$CH_2$R R = OEt, OMe | S | [1495] |
| 1,2-$(CH_2OR)_2$ R = Et, 2,4-$C_6H_3Cl_2$ | S | [461] |
| 1,2-[*p*-$CH_2C_6H_4OMe]_2$ | S | [438] |
| 1-*p*-$C_6H_4OMe$ | S | [221,278] |
| 1-CLiMe(OMe)-2-alkyl | S | [1499] |
| 1-CH(OMe)C(O)OH-2-R R = Me, $CHMe_2$ | S, HMe, IR[$CHMe_2$] | [1499] |
| 1-$OCH_2OCH_2$Me-2-$CH_2CH$=$CH_2$ | S, H, B, C, IR, MS | [321] |
| 1-$CH_2OCH_2CH[CH_2$—O—$C_{17}H_{35}]_2$ | S, H, C, IR, MS | [462] |
| 1-(*p*-$C_6H_4$-$OC_6H_4$) | S | [1449] |
| 1-(*cyclo*-$CH_2$-O-CRR′-) R=CH=CHMe, Me, Ph; R′ = H, Me | S | [188] |
| 1,2-*cyclo*-[—$C(O)OCH_2$—] | S, IR | [363] |
| 1,2-*cyclo*-O[$(CH_2)_2S(CH_2)_2$-]$_2$ | S, X, H, B, C, IR | [463] |
| O[$CH_2$—$CB_{10}H_{10}C$–C(O)OH]$_2$ (FF) | S, IR | [363] |
| 1,2-[$C_6H_4$-*p*-OPh]$_2$ | S | [398] |
| 1-[$C_6H_4$-*p*-OPh] | S | [398] |
| 1,2-[*cyclo*-C(O)-*o*-$C_6H_4$-] | S | [129] |
| 1-R R=CHMe-O-$C_4H_9$, *cyclo*-$OC_5H_7$ | S(Ni-mediated carboryne coupling with alkenes), H | [244] |
| $B_{12}H_{12}$[$O(CH_2)_6CB_{10}H_{10}CR]_{12}$ R = H, Me closomer (FF) | S, H, B, C, MS, UV, E | [193] |
| $RCB_{10}H_{10}C$–$(CH_2)_4$O-$B_{12}H_{11}^{2-}$ R = H, Me (FF) water-soluble compounds for BNCT | S, H, B, C, IR | [464] |
| $MeOCH_2$—$CB_{10}H_{10}C$—$CB_{10}H_{10}CH$ (FF) | S | [129] |
| 1-$CH_2$—O—CH[$CH_2O(CH_2)_{15}Me]_2$ | S, H, B, C | [467] |
| 1-*cyclo*-$C_4H_3$(O), *cyclo*-$C_5H_4$(O), *cyclo*-$C_4H_3(O)_2$ | S(regioselective insertion of carborynes into ether C—H bonds), H, B, C, MS, IR, UV, MS | [1547] |

*Continued*

| Compound | Information | References |
|---|---|---|
| 1-CHMeOEt-3-R R = Ph, Br, Cl | S(regioselective insertion of carborynes into ether C—H bonds), H, B, C, MS, IR, UV, MS | [1547] |
| 1-$(CH_2)_4OCH_2Ph$ | S, H, C | [1557] |
| 12-$R_2$ R = $(CH_2)_4OCH_2Ph$, $(CH_2)_3C(O)O$(*N*-succinimide) | S, H, C, MS | [1557] |
| 1-$(CH_2)_3C(O)O$-(*N*-succinimide) cyclic RGD (Arg-Gly-Asp) peptide conjugates as $^{10}B$ carriers for BNCT | | [1557] |
| 1,3,5-[$RCB_{10}H_{10}C(CH_2)_3SiMe_2(CH_2)_3OC_6H_4]_3C_6H_3$ R = Me, Ph (FF) photoluminescent dendrimers | S, H, B, C, MS, UV, TBA(Me) | [1670] |
| 1,3,5-[$RCB_{10}H_{10}CCH_2C_6H_4(CH_2)_2SiMe_2(CH_2)_3OC_6H_4]_3C_6H_3$ R = Me, Ph (FF) photoluminescent dendrimers | S, H, B, C, MS, UV, TBA(Me) | [1670] |
| 1,3,5-{1,2,3-[$RCB_{10}H_{10}CCH_2C_6H_4(CH_2)_2SiMe_2(CH_2)_3O]_3C_6H_2$-5-$CH_2OC_6H_4\}_3C_6H_3$ R = Me, Ph (FF) photoluminescent dendrimers | S, H, B, C, MS, UV, TBA(Me) | [1670] |
| MeO—$[(CH_2)_2O]_{45}$—[C(O)CH($N_3C_2$—$CH_2$—$C_2B_{10}H_{11}$)-$(CH_2)_4O]_n$-$[C(O)(CH_2)_5O]_m$H block copolymers for covering Au nanoparticles functionalized with 1,2-$(HS)_2C_2B_{10}H_{10}$ for BNCT | S, TEM | [1722] |
| 9,12-[*p*-$C_6H_4O(CH_2CH_2O)_3Me]_2$ | S, H, B, C, MS | [240] |
| 9-$C_6H_4$-*p*-$OC_6H_4$-*p*-C(O)Ph | S, H, B, C, IR, S | [229] |
| 9-$C_6H_3$[*m*-C(O)Ph]-*p*-OPh | S, H, B, C, IR, S | [229] |
| 1,9/1,12-[$C_6H_4$-*p*-$C(O)C_6H_4$-*p*-$OMe]_2$ | S, H, B, C, IR, S | [229] |
| 9-*cyclo*-$CHOCH_2$ oxirane | S(Pd-catalyzed cross-coupling), H, B, C, IR, MS | [1724] |
| **Nitro and Nitroso Derivatives and Nitrates** | | |
| 1-(*o*/*m*/*p*-$C_6H_4NO_2$)-2-C(O)OH | S | [224] |
| 1,2-$(CH_2ONO_2)_2$ | S | [127] |
| 1-$CH_2OH$-2-$CH_2ONO_2$ | S | [127] |
| 1-*m*/*p*-$C_6H_4NO_2$ *n* = 3,4 | S | [471] |
| 1-$C_6H_4NO_2$ | S | [278] |
| 1-*o*-$C_6H_4NO_2$ | S, p$K_a$ | [227] |
| 1-*p*-$C_6H_4NO_2$ | Dipole moment | [103] |
| 1-$C_6H_4NO_2$-12-$C_5H_{11}$ | S, H, B, MS | [1767] |
| 1,2-(*m*-$C_6H_4NO_2)_2$ | S, X, NLO | [473] |
| 1-Ph-2-R R = $C_6H_4NO_2$ (3 isomers), $C_6H_3$-2,4-$(NO_2)_2$, $C_6H_4$-*p*-CN | S [aromatic nucleophilic substitution ($S_NAr$)] | [474] |
| 1-($C_6H_4$-*p*-$NO_2$)-2-($C_6H_4$-*p*-X) X = OMe, Cl, Br, Ph, C(O)OEt, $NO_2$ | S [aromatic nucleophilic substitution ($S_NAr$)] | [474] |
| 1-{*p*-$C_6H_4$-*cyclo*-[C–N(O)$CH_2CH_2$N(O)═]} nitronyl nitroxide radical | S, X, IR, ESR, MAG | [475] |
| 1,2-{*p*-$C_6H_4$-*cyclo*-[C–N(O)$CH_2CH_2$N(O)═]}$_2$ nitronyl nitroxide diradical | S, X, IR, UV, ESR, MAG | [476] |

| Compound | Information | References |
|---|---|---|
| 1,2-{*p*-$C_6H_4$-[*cyclo*-C═N(O)$CMe_2CMe_2$N(O)]}$_2$ nitronyl nitroxide radical; intramolecular interaction between two radical spins | S, X, IR, UV, ESR, MAG | [477] |
| $[CF_3)_2CHCHCO_2]_2$Mn(1,2-{*p*-$C_6H_4$-[*cyclo*-C═N(O)$CMe_2CMe_2$N(O)]})$_2$ $C_2B_{10}H_{10}$ nitronyl nitroxide $S=3/2$ ground state complex (FF) | S, X, MAG | [478] |
| 1-CMe(X)$CH_2NO_2$ X = $NO_2$, ONO, OH | S, H | [479] |
| 3-*o*-$C_6H_4NO_2$ | S | [443] |
| 1-R-2-R′-9-$ONO_2$ R = H, Me; R′ = H, Me | S, IR | [381] |
| 9-$CH_2$-*p*-$C_6H_4NO_2$ | S, B | [409] |
| *Amines and imines* | | |
| 1-$NH_2$-2-R R = H, Me, Ph | S | [482,483] |
| 1-N(boc)NH(boc)-2-R R = H, C(O)OH; boc = *tert*-butyloxycarbonyl | S, X, H, B, C, MS | [427] |
| 1-R-2-$NH_2$ R = Me, Ph | S | [484] |
| 1-$CH_2$R R = $NEt_2$, *cyclo*-N$(CH_2)_2O(CH_2)_2$ (morpholinyl), $C_7N_2H_6$ (benzimidazolyl) | S, H, B. IR | [1834] |
| 1-$CH_2CH_2NMe_2$-2-$CH_2CH$═$CH_2$ | S, H, B, C, IR | [320] |
| 1-$CH_2CH_2NMe_2CH_2CH$═$CH_2^+$ $Br^-$ | S, X, H, B, C, IR | [320] |
| 1-$CH_2CH_2NMe_2$-2-$CMe_2C_5H_4$ | S, X, H, B, C, IR | [320] |
| 1-R-2-($C_6H_{10}$-2′-$NH_2$) R = H, Ph, polystyryl | S, H, B, C, IR, TGA (polystyryl) | [1483] |
| 1-$C_6H_4(CO)_2NCH_2$-2-O$(CH_2)_2$R R = H, $CH_2$Ph | S, X($CH_2$Ph), H, B, C, IR, MS | [486] |
| 1-$CH_2NH_2$ | S | [151,487,583] |
| 1-$CH_2NEt_2$ | S | [151] |
| 1-Me-2-CH(*cyclo*-$NC_4H_8O$)(*cyclo*-$C_4H_3S$) | S, X, H, B, C, IR, MS | [228] |
| 1-Ph-2-CH($NEt_2$)(*cyclo*-$C_4H_2BrS$) | S, H, B, C, IR, MS | [228] |
| 1-Me-2-CHPh-NHCHMePh (enantiopure) | S, X, H, B, C, IR, MS | [228] |
| 1-$CH_2NEt_2$-2-SLi | S, IR | [487] |
| 1-$(CH_2)_n$$NH_2$ $n=1$, 2 | S, H, B, C, IR | [488] |
| [$(CH_2)_3$CN]$HC_2B_{10}Me_8H_2$ (FF) | S, X, H, B, C, MS | [190] |
| 1-$(CH_2)_2NEt_2$ | S | [123,445] |
| 1-R-2-$(CH_2)_n$$NH_3$Cl R = H, Me, $(CH_2)_3NH_3Cl$; $n=1,3$ aminoalkyl | S, H, B, C, IR, MS | [195] |
| 1,2-*cyclo*-[$(CH_2)_n$-NC(O)$C_6H_4C(OSiMe_2CMe_3)$] $n=2,3$ aminoalkyl | S, X($n=3$), H, B, C | [489] |
| 1-$(CH_2)_2N(CH_2Ph)_2$-2-R R = H, Me, Ph | S, X(H), H, IR | [490] |
| 1-CHMe$NEt_2$-9,12-$I_2$ | S(regioselective C—H bond insertion on *o*-carboryne with tertiary amines), H, B, C, MS | [1820] |
| [$H_2N(CH_2)_3$]$HC_2B_{10}Me_8H_2$ (FF) | S, H, B, C, MS | [194] |
| [$ClNH_3(CH_2)_n$]$HC_2B_{10}Me_8H_2$ $n=3$, 4 (FF) self-assembly into microrods via sonification) | S, H, B, C, MS | [194] |
| 1-$(CH_2)_n$-amino (aminoalkyl derivatives) | S, H, C, IR, MS | [491] |

*Continued*

| Compound | Information | References |
|---|---|---|
| 1-NRR′-2-R″ R = H, Me, Et; R′ = OH, OC(O)Me, Et, Me, C(O)H; R″ = H, Me, Ph | S | [492] |
| 1,2-($C_6H_4$-*p*-$NH_2$)$_2$ curing agent for epoxy resins | S, H, B, C, IR | [1870] |
| 1-*p*-$C_6H_4$-N($C_2H_4OH$)$_2$ | S | [494] |
| 1-{$C_6H_3$-*m*-N[($CH_2C(O)OH$]$_2$-*p*-OH} | S, H, C, IR | [231] |
| 1-{$C_6H_3$-*m*,*m*′-(N[($CH_2C(O)OH$]$_2$)$_2$-*p*-OH} | S, H, C, IR | [231] |
| $O_4(CH_2)_{12}N_2[CH_2C_6H_3$-*o*-OH-*m*-$C_2B_{10}H_{11}]_2$ crown ether amino alcohols (FF) | S, H, C, IR | [231] |
| 1-R-2-R′ R = H, $Me_2CH$; R′ = $CH_2NH_2$, $CH_2NMe_2$, $CH_2NEt_2$ | S | [495] |
| 1-$CH_2CH(NH_2)C(O)OH$ L and D enantiomers | S, H, C, IR, MS | [430] |
| 1-$CH_2CR(NHR')(CF_3)$ R = C(O)OH,C(O)OMe; R′ = $SO_2$Ph, C(O)CF3,C(O)$OCMe_3$ | S, X[C(O)OMe; $SO_2$Ph, C(O)$OCMe_3$], H, F, IR | [497] |
| 1-C($CF_3$)[C(O)OMe]NHC(=O)—O—*cyclo*-$C_6H_3Me(CHMe_2)$ *N*-protected carboranylalaninates | S, X, H, F, IR | [497] |
| 1-$CH_2C(O)NH(CH_2)_4CH(NH_2)C(O)OH$-3-R R = H, NHAc, Boc | S, H, MS | [1515] |
| 1-$CH_2C(O)NH(CH_2)_4CH(NH_2)$-C(O)OH·2$CF_3$C(O)OH | S, H, MS | [1515] |
| 1-NHC(O)$(CH_2)_2$CH-$(NH_2)$C(O)OH·2$CF_3$C(O)OH | S, H, MS | [1515] |
| 1-NHC(O)$OCMe_3$ | S, H, B, MS | [1865] |
| 1-$C_9H_6$NR-2-Ph R=$CH_2$Ph, Me | S, H, IR | [405] |
| 1-[$C_9H_6$-*cyclo*-$NC_4H_8O$]-2-$Ph^-$ morpholino | S, H, IR | [405] |
| 1-(R′-$NC_9R_2H_4$)$CH_2$ R = H, Me, OMe; R′ = $SO_2NH_2$, $SO_3H$, P(O)$(OH)_2$ tetrahydroisoquinolines for BNCT | S, H, C, IR | [499] |
| [R-$CB_{10}H_{10}$C–$(CH_2)_2$C(O)NH]$_2C_{14}H_6(O)_2$ R = H, Me, Ph; isomers anthraquinones (FF) | S, H, B, C, IR | [500] |
| [R-$CB_{10}H_{10}$C–$(CH_2)_2$C(O)NH]$_2C_{13}H_6$(O) R = H, Me, Ph; isomers fluorenones (FF) | S, H, B, C, IR | [500] |
| 1-B[$NMe_2$]$_2$ | S | [501] |
| 1-R-2-NHC(O)$OCMe_3$ R = C(O)OH, H | S, H, B, C | [424] |
| 1-R-3-$NH_2$ R = Me, Ph | S, H, B(2d) | [503] |
| 1-Me-3-NHC(O)R R = CHMe(naphthyl)OMe, *cyclo*-$C_4H_4$N-tosyl | S, H, B(2d) | [503] |
| 1,2-$R_2$-3-$NH_2$ R = H, Me | S | [347,504] |
| 1,2-$Me_2$-3-$NH_2$ | S, p$K_a$ | [347] |
| 1-R-3-NR′R″ R, R′ = Me, Et; R″ = Me, Et, C(O)H, C(O)Me | S | [505] |
| 1-Ph-2-$C_6H_4$-*m*/*p*-$NPh_2$ dependence of emission behavior on location of substituents | S, U(absorption, emission) | [1884] |
| 3-$NPh_2$ | S, IR | [506] |
| 9,12-[*p*-$C_6H_4NMe_2$]$_2$ | S, H, B, C, MS | [240] |
| 1-R-2-$CH_2C(O)OH$-3-R′ R = H, Me, Ph; R′ = NHC(O)Ph, NHC(O)Me, NHC(O)H, $NH_3^+$ | S, H, B, IR | [507] |

| Compound | Information | References |
|---|---|---|
| 1,4-$C_6H_4$(1,2-$C_2B_{10}H_{10}$-3-$NH_2$)$_2$ (FF) | S | [508] |
| $(CH_2)_2$(1,2-$C_2B_{10}H_{10}$-3-$NH_2$)$_2$ (FF) | S | [508] |
| 1,2-*cyclo*-[$Me_2Si$—$MeN(CO)_2N_2$—$OSiMe_2$] | S, H, C, Si, IR, MS | [315] |
| 1-$CH_2$-$C_4N_2Me(NH_2)_2$ conjugates with proteins in protein data bank (PDB) and HIV; for BNCT | | [1590] |
| 1-($Me_3NCH$)$C_2B_{10}H_{11}^+$ $I^-$ | S, X | [1598] |
| 1-$CH_2NH$—$C(=NH_2)NH_2^+$ $TFA^-$ guanidinyl derivative | S, X, H, B, C, MS, IR | [1622] |
| 1-$CH_2NH$—C(=Nboc)NHBoc Boc = $(Me_3C)_2C_2O_5$ | S, H, B, C, MS, IR | [1622] |
| 1-$CH_2NH$—$C(=NH_2)NH_2^+$ $NO_3^-$ | S, H, B, C, MS, IR | [1622] |
| 1-$CH_2NH$—$C(=NH_2))NHEt^+$ $TFA^-$ guanidinyl derivative | S, X, H, B, C, MS, IR | [1622] |
| 1-$CH_2N$=$CHC_6H_4R$ R = H, OH | S, X(H), H, B, C, IR | [1655] |
| 1-$S(CH_2)_n$C[C(O)OEt]$_2$NHC(O)Me $n$ = 4–6 amino acids | S, H, B, C, MS, IR | [1674] |
| 1-$S(CH_2)_n$CH[C(O)OH]$NH_2$·HCl $n$ = 4–6 | S, H, B, C, MS, IR | [1674] |
| 1,2-*cyclo*-B[$N(CHMe_2)_2$]—(1′,2′-$C_6H_4$)—B[$N(CHMe_2)_2$] | S, H, B, C, MS | [1681] |
| 1,2-*cyclo*-B($NMe_2$)—CHMe—B($NMe_2$) | S, H, B, C, MS | [1681] |
| 1,2-*cyclo*-B($NMe_2$)—B($NMe_2$)—B($NMe_2$) | S, X, H, B, C, MS | [1681] |
| 1-$H_2NSO_2NHCH_2$-2-R R = H, *n*-Ph ($n$ = 2, 9, 12) *in vitro* inhibition in carbonic anhydrase | | [1702] |
| 1-$CH_2NHSO_2NH_2$ sulfamide interaction with CAIX cancer-specific enzyme; inhibitor of carbonic anhydrase | S, X | [1833] |
| $[H_3NCH_2$-$C_2B_{10}H_{11}]^+$ $[Me_2C$=$NHCH_2$-$C_2B_{10}H_{11}]^+$ $[Mo_8O_{26}]^{2-}$ methylammonium polyoxometallate, and related salts | S, X, IR | [1863] |
| 1-$C_6H_4NH_2$-12-$C_5H_{11}$ | S, H, B, MS | [1767] |
| HN[SiRMe-$CH_2$-9-(1,2-$C_2B_{10}H_{11}$)]$_2$ R = Me, $NH_2$ (FF) | S, IR | [1883] |
| {*cyclo*-$H_3N_3Si_3(NH_2)_3[CH_2$-9-(1,2-$C_2B_{10}H_{11}$)]$_3$}$_n$ (FF) | S, IR | [1883] |
| 9-$CH_2SiMe(NHSiMe_3)_2$ | S, IR | [1883] |
| $Me_3SiNH${SiMe(9-$CH_2$-1,2-$C_2B_{10}H_{11}$)NH}$_x$-$SiMe_3$ (FF) | S, IR | [1883] |
| 1,2-*cyclo*-C($CMe_3$)—N[$C_6H_3(CHMe_2)_2$]—B[$Me_2C_3N_2(CHMe_2)_2$ | S, X, H, B | [1931] |
| 1,2-*cyclo*-C($CMe_3$)=N[$C_6H_3(CHMe_2)_2$]—B($OAc)_2$ carbene-stabilized iminocarborane | S, X, H, B | [1931] |
| ***Heterocyclic amines*** | | |
| 1-(2′-$NC_5H_4$) pyridyl | S, MS | [1319] |
| 1-Ph-2-(3′-pyridyl-6′-phenyl-1′,2′,4′-triazine) | S, X | [205] |

*Continued*

| Compound | Information | References |
|---|---|---|
| 1-(2′-$NC_5H_4$)-2-SR R = Et, $CHMe_2$ | S, X, H, B, C, IR | [269] |
| $C_5H_2XN$-2′,6′-($CH_2$S-1,2-$LC_2B_{10}H_{10}$)$_2$ X = H, Cl; L = H, Me (FF) | S, X(Me), H, B, C, IR | [270,271] |
| 1,2-*cyclo*-[*cyclo*-$C_5H_4N$-*arachno*-$B_{10}H_{10}$-*cyclo*-$NC_5H_4$-$(CH_2)_2$] | S, X, MS | [272] |
| | S, H, B, MS | [1319] |
| 2,2′-$N_2C_{10}H_6$[C(O)O$(CH_2)_3CB_{10}H_{10}$CR]$_2$ R = H, Me bipyridyl | S, H, B, C, IR | [510] |
| 2,6-($PhCB_{10}H_{10}CCH_2)_2$-*cyclo*-$NC_5H_3$ lutidine (FF) | S, X, H, B, C, IR, MS | [1314] |
| 1-$CH_2$(2′-$C_5H_5N$) supramolecular C–H···N hydrogen bonding vibrational frequencies | S, X, H, B, C, IR | [274] |
| 1-R-2-L R = terpyridine, terpyridyl-O$(CH_2)_3$, terpyridyl-O, terpyridyl-OH; L = H, $SiMe_2CMe_3$ | S, X[terpyridyl, H; terpyridyl-O$(CH_2)_3$,H], H, B, C, IR | [275] |
| 1,2-$C_2B_{10}H_{12}$·$C_{12}N_2H_8$ $C_{12}N_2H_8$ = 1,10-phenanthroline (FF) | S, X | [276] |
| 1-Me-2-$(CH_2)_n$-*cyclo*-$C_4H_3NH$ *n* = 0, 1, 2 pyrroles | S, H | [511] |
| | S, E(*n* = 1,2), electrochemical polymerization | [318] |
| 1-Me-2-$CH_2C_6H_4$-$C_4H_3$N-R R = H, Si$[CHMe_2]_3$ pyrroles | S, H, MS, UV | [512] |
| 1,2-*cyclo*-{$Me_2SiO$—(*o*-phenanthroline)—$OSiMe_2$} | S, H, C, Si, MS | [315] |
| 1-Me-2-*cyclo*-$C_4H_2$[C(O)OR]NH R = Et, $CMe_3$, $CH_2Ph$ pyrroles | S, H | [511] |
| *Cyclo*-$C_4H_2NH[CH_2$-$CB_{10}H_{10}$C–Me$]_2$ (FF) pyrrole | S, H | [511] |
| | S, E | [318] |
| *Cyclo*-$C_4H$[C(O)O$CMe_3$]NH [$(CH_2)_2CB_{10}H_{10}$CMe$]_2$ (FF) pyrrole | S, X | [318] |
| 1-$(CH_2)_2$[*cyclo*-CH=CR-NH-CH=C—]-2-Me R = H, C(O)O$CMe_3$ pyrroles | S, X[C(O)O$CMe_3$], H(R = H) | [298] |
| 1-$(CH_2)_n$$C_4H_2NH${C(O)O$CMe_3$}-2-Me pyrrole *n* = 1,2 | S, X (*n* = 2), H, MS | [513] |
| 1-$(CH_2)_n$$C_4H_3NH$-2-Me pyrrole *n* = 1,2 | S, H, MS, E | [513] |
| 1-$(CH_2)_2$-*cyclo*-$N_2C_3H_3$-$(CH_2)_nMe^+$ *n* = 4, 7–15 analogues of mycobacterium tuberculosis cell growth inhibitor SQ109 | S,H, MS, cell growth inhibition of M. tuberculosis (H37Rv and/or Erdman), Mycobacterium smegmatis, Bacillus subtilis, Escherichia coli, Saccharomyces cerevisiae, Trypanosoma brucei, human embryonic kidney, HEK293T, and hepatocellular carcinoma, HepG2) | [1858] |
| 1-$(CH_2)_2$-*cyclo*-$N_2C_3H_3$-$R^+$ R=$CH_2C_6H_4OPh$, $CH_2CH$=CMe$(CH_2)_2CH$=$CHMe_2$ analogues of mycobacterium tuberculosis cell growth inhibitor SQ109 | S,H, MS, cell growth inhibition of M. tuberculosis (H37Rv and/or Erdman), Mycobacterium smegmatis, Bacillus subtilis, Escherichia coli, Saccharomyces cerevisiae, Trypanosoma brucei, human embryonic kidney, HEK293T, and hepatocellular carcinoma, HepG2) | [1858] |
| Porphyrin$[MeCB_{10}H_{10}COCH_2]_4$ (FF) | S, H, MS | [511] |
| Dihydroxyethylporphyrin{CH[OC(O)-1-1,2-$C_2B_{10}H_{11}$]$CH_2$[O-C(O)-1-1,2-$C_2B_{10}H_{11}$]}$_2$ esters for BNCT (FF) | S, H, MS | [1366] |
| Porphyrin$[CH(CN)_2](C_6H_4$-*p*-1,2-$C_2B_{10}H_{11})_4$ for BNCT and PDT (photodynamic therapy) (FF) | S, UV | [515] |

| Compound | Information | References |
|---|---|---|
| (porphyrin)($C_6H_4$-9-$CH_2$-$C_2B_{10}H_{11}$)$_4$ (FF) | S, H, cytotoxicity | [516] |
| (porphyrin)$Ph_4$[$C_6H_4$-$CH_2$-$CB_{10}H_{10}$C–Me]$_4$ (FF) | S, X, H, MS, UV | [512] |
| Ni(porphyrin)[$C_6H_4$-$CH_2$-$CB_{10}H_{10}$C–Me]$_8$ (FF) | S, H, MS, UV | [512] |
| Porphyrin[S($CH_2$)$_6$-$CB_{10}H_{10}$C–$CH_2$C═$CH_2$]$_8$ sensitizers in liposomes for BNCT and other cancer therapies (FF) | S | [1418] |
| Porphyrin[S($CH_2$)$_6$-$C_2B_{10}H_{11}$]$_8$ deactivation following photoexcitation, due to flexibility of alkylthio chains | H(variable. T), transient absorption difference spectra | [1927] |
| Porphyrin[$C_6H_3$($CH_2$-$CB_{10}H_{10}$CMe)$_2$]$_n$ $n$=2,4 (FF) | S, H, MS, UV | [517] |
| 3-R-*cyclo*-$C_4H_2$(═O)$_2$N—$C_6H_4$-*p*-(porphyrin)$Ph_3$ R=O, NH N-malemido | S, H, B, MS | [1812] |
| 1-$CH_2$-*bicyclo*-$N_3C_4H_2$(═O)$_2$N—$C_6H_4$-*p*-(porphyrin)$Ph_3$ pyrrolidinotriazoline | S, H, B, MS | [1812] |
| 1-$CH_2$-*bicyclo*-$N_3C_4H_2$(═O)$_2$N—$C_6H_4$-*p*-C(O)NH-$C_6H_4$-*p*-(porphyrin)$Ph_3$ pyrrolidinotriazoline | S, H, B, MS | [1812] |
| Corrole(Cu)[*m*/*p*-$C_6H_4$-$CB_{10}H_{10}$CH]$_2$ (FF) | S, X(*m*-$C_6H_4$), UV | [518] |
| 1-[CH(OH)(2′-tetraphenylporphyrin)]M-9-R R=NCO, C(O)H, NHC(O)O$CMe_3$; M=2H, Cu, Zn for BNCT and PDT (photodynamic therapy) | S, H, B, IR, MS, UV | [519] |
| (porphyrin){$C_6F_4$-S[9-(1,2-$C_2B_{10}H_{11}$)]}$_4$ | S, H, B, F, IR, MS, UV | [1881] |
| 1-R-2-$CH_2$C(O)O-$C_6H_4$-O-$C_6H_3$(CN)$_2$ R=H, Me phthalonitriles | S, H, IR, MS | [1451] |
| phthalocyanines for BNCT | S, H, IR, MS, photooxidation of citronellol | [1451] |
| 1-(3′-thymidine) radioiodinated derivatives ($^{127}$I) | S, docking studies | [1775] |
| 1,2,4-triazin-5-yl derivatives | S, X | [1331] |
| 1′,3′,5′-$ClC_3N_3$(1,2-$CB_{10}H_{10}$CR)$_2$ R=H, Me s-triazine (FF) | S | [521] |
| 1′,3′,5′-$ClC_3N_3$(1,2-$CB_{10}H_{10}$CR)$_3$ R=H, Me, Ph s-triazine (FF) | S, X(Ph) | [521] |
| 1-$C_3N_3$[N($CH_2CH_2OR$)$_2CH_2$]$_2$ R=Me,H triazines | S, X, H, C, cytotoxicity; uptake in B-12 melanoma cells | [972] |
| $C_3N_3$[N($CH_2CH_2OR$)$_2$]$_2$(1,2-$C_2B_{10}H_{11}$)$_2$ R=Me,H | S, X, H, C, cytotoxicity; uptake in B-12 melanoma cells | [972] |
| 1-$C_3N_3$[N($CH_2CO_2CMe_3$)$_2$]$_2$ triazines | S, X, H, C, cytotoxicity; uptake in B-12 melanoma cells | [972] |
| $C_3N_3$[N($CH_2CO_2CMe_3$)$_2$]$_2$(1,2-$C_2B_{10}H_{11}$)$_2$ | S, X, H, C, cytotoxicity; uptake in B-12 melanoma cells | [972] |
| *Cyclo*-[—$Me_2$Si—$CB_{10}H_{10}$C—Si$Me_2$— NC═CHCH═CN—$Me_2$Si—$CB_{10}H_{10}$C— Si$Me_2$—NC═CHCH═CN—]$_2$ (FF) | S, X, H, C, Si, MS | [315] |
| 1-$CH_2C_5H_4N$ picolyl | S, H, IR | [522] |
| 1,2-(2′,4′-diamino-6-methylpyrimidine) antifolate | S, screening for anti-dihydrofolate reductase activity | [1417] |
| 1-SR-2-Si$Me_2CMe_3$ SR=*bicyclo*-$SNC_5H_4$, $S_2NC_7H_4$ | S, H, IR, COND | [525] |
| 9-(2′,5′-diazabicyclo[2′.2′.2′]oct-2-ene) derivatives | S, X, H, MS | [1419] |

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| Compound | Information | References |
|---|---|---|
| 1-[*cyclo*-B(NEt—$C_6H_4$—NEt)]-2-R R = H, Me, Ph, OMe, $SiMe_3$ C-diazaboryl derivatives as donor-acceptor systems | S, X, U(observed/emission) | [1623] |
| 1-[*cyclo*-BPh—$C_6H_4$—NPh]-2-R R = H, Me C-diazaboryl derivatives as donor-acceptor systems | S, X, U(observed/emission) | [1623] |
| 1,2-{*cyclo*-[B—N(R)—o-$C_6H_4$—N(R)—]}$_2$ R = Et, Ph diazaborolyl | S, X, H, B, C, MS, U(fluorescence) | [1684] |
| indomethacin-$C_2B_{10}H_{11}$ COX inhibition, enzyme selectivity (FF) | S, X, H, B, C, MS, IR | [1628] |
| 1-R-2-NHC(O)—[*cyclo*-$C_3R(C_6H_4$-*p*-Cl)$N_2$] —$C_6H_3Cl_2$ R, R′ = H, Me pyrazoles hydrophobic pharmacophores; analogues of inverse agonist Rimonabant receptors | S, H, B, C, MS | [1643] |
| 1-R R=N=CH—$C_6H_4$-*o*-OH, $NHCH_2C_6H_4$-*o*-OH, N=CH—$C_{14}H_9$ (anthracenyl), N=CH—$C_{12}H_7$NEt (carbazolyl), NH=CH—$C_5H_4N$ | S, X(N=CH—$C_6H_4$-*o*-OH, N=CH—$C_{12}H_7$NEt, NH=CH—$C_5H_4N$), H, B, C, IR, MS | [1908] |
| 9-*cyclo*-[C=N-N=CPh-O—] oxadiazole | S, H, B, IR | [1671] |
| *n*-$CH_2$—C*yclo*-[C=N-N=CPh—O—] *n* = 1,9 oxadiazole | S, H, B, IR | [1671] |
| 1,2-*cyclo*-M(*cyclo*-RNCR′NR)$_2$ R = *cyclo*-$C_6H_{13}$, $CHMe_2$; R′ = Me, Ph, *n*-$C_4H_9$; M = Zr, Ti, Hf insertion of unsaturated molecules | S, X, H, B, C | [1678] |
| Zn(phthalocyanine)(S-*n*-$C_6H_{13})_6$-S$(CH_2)_2$OC(O)-$(CH_2)_2C_2B_{10}H_{11}$ (FF) | S, H, B, UV, IR, MS, E | [1851] |
| Zn(phthalocyanine)[$OC_6H_4$-(*cyclo*-CH-O-$CH_2$) $C_2B_{10}H_{10}$) photocatalysis of oxidation of citronellol (FF) | S, H, UV, IR, MS | [1710] |
| Zn(phthalocyanine)[$C_5H_4$N-$(CH_2)_3CB_{10}H_{10}CMe]_3(OC_5H_4N)$ photocatalysis of oxidation of citronellol (FF) | S, H, UV, IR, MS | [1710] |
| $Cs^+{}_8$ {Zn(NCH)[S(CH)$(CB_{10}H_{10}CMe)$]}$^{8-}$ phthalocyananine incorporation in rat cancer cells water-soluble agent for BNCT | S, H, B, C, UV, IR, fluorescence emission | [1880] |
| {—[$C_7H_5$—$(CH_2)_5$—$C_6H_4$—*p*-$NC_{12}H_8]_x$—[$C_7H_5$— $(CH_2)_5$—$CB_{10}H_{10}$C—R]$_y$—}$_n$ R = Ph, Me polynorbornene-carbazole-carborane copolymers (FF) | S, H, B, C, E, UV, photoluminescence, TGA, DSC, gel permeation chromatography | [1719] |
| (3S,4S; 3R,4R; 3R,4S; 3S,4R)-1-$CH_2$NH-*tricyclo*-$C_{13}H_4Me_2O_3$(OH) pyranonaphthoquinone | S, X(3R,4S), H. B, C, MS, IDO1 inhibition | |
| IDO1 = indoleamine-2,3-dioxygenase-1 | 1770 | |
| 1,2-*bicyclo*-$OC_6H_4$-N$(CH_2C_6H_4$-*p*-$CF_3)$CHPh | S, X, H, C | [1906] |
| 1,2-*bicyclo*-OCMe-$C_4H_3$Me-C=N-CHPh | S, X, H, C | [1906] |
| 1-(2′-$C_8H_5N_2$) 1′-quinoxalinyl | S, H, B, C, IR, MS | [1915] |
| 1-(2′-$C_4H_3N_2$) 1′-pyrimidinyl | S, H, B, C, IR, MS | [1915] |
| 1-(2′-$C_{12}H_7N_2$) 1′,10′-phenanthrolinyl | S, H, B, C, IR, MS | [1915] |
| 1-[$C_6H_4$—C≡C—$C_6H_4$—DPP]-2-[$C_6H_4$—C≡C—$C_6H_4$-BODIPY] DPP = diketopyrrolopyrrole BODIPY = extended borondipyrrolemethane Through-space electronic energy transfer across proximal molecular dyads | S, UV(absorption, fluorescence | [1683] |

| Compound | Information | References |
|---|---|---|
| 1,2-[$C_6H_4$-*p*-C($C_4EtMe_2N$)═C($C_4EtMe_2N$-$BF_2$)]$_2$ BODIPY (boron dipyrromethen) dyads for low-energy photosensitization | S, H, B, C, F, IR, MS, UV(fluorescence), E | [1847] |
| 1-[C≡C—$C_6H_4$-*p*-C($C_4EtMe_2N$)═C($C_4EtMe_2N$-$BF_2$)]-2-[$C_6H_4$-*p*-C($C_4EtMe_2N$)═C($C_4EtMe_2N$-$BF_2$) BODIPY (boron dipyrromethen) dyads for low-energy photosensitization | S, X, H, B, C, IR, MS, UV(fluorescence), E | [1847] |
| 1-HS-2-(8′-BODIPY) BODIPY = $C_9H_2Me_4N_2BF_2$ | S, permeability across hCMEC/D3 cell monolayers | [1904] |
| 1-Me-2-$C_6H_4$-(8′-BODIPY) | S, permeability across hCMEC/D3 cell monolayers | [1904] |
| $Me_4$(BODIPY)-2′,6′-($C_6H_4$-*p*-$CH_2CB_{10}H_{10}CMe)_2$-8′-$C_6H_4$-*p*-C(O)OH (FF) | S, H, C, MS, UV, fluorescence, permeability across hCMEC/D3 cell monolayers | [1904] |
| 1-H-2-S(8′-BODIPY) | S, H, C, MS, UV, fluorescence, permeability across hCMEC/D3 cell monolayers | [1904] |
| *Amides and imides* | | |
| 1-C(O)$NEt_2$ | S | [123] |
| 1-C(O)$NH_2$-2-R R = Me, Ph | S | [128,526] |
| 1,2-[NHC(O)OMe]$_2$ | S | [364] |
| 1,2-[$CH_2$C(O)$ONH_2$]$_2$ | S | [364] |
| 1-R-2-R′ R = C(O)$NH_2$, C(O)$NEt_2$; R′ = Me, Ph | S | [128] |
| 1-$CH_2$C(O)$NEt_2$ | S | [123,445] |
| 1-$CH_2$C(O)$NMe_2$-2-R R = H, Me | S | [182] |
| 1-C(O)NHPh | S | [399] |
| 1-*p*-$C_6H_4CH_2$C(NHCHO)[C(O)OEt]$_2$ | S, H, IR, MS | [189] |
| 1,2-{$CH_2$—C*yclo*[NC(O)$C_6H_4$C(O)-]}$_2$ phthalimidomethyl | S, X, H, B, C, IR | [528] |
| 1-DDQC (DDQC = amidoquinoline group) (2 rotamers) | S, X, H(NOESY), B, C | [1328] |
| 1-$C_6H_4$-*p*-$OCH_2$C(O)NH-$C_6H_4$-*m*-/*p*-$CH_2C$≡CH | Probes of HIF-1α inhibitor *o*-carboranyl phenoxyacetanilide (Chapter 16, ref. 262) | [1519] |
| 1-CHR*OMe R = H, Ph chiral | S, X, H, B, C, IR, MS | [529] |
| 1-(*cyclo*-C═N—CHR*$CH_2$O—) R═$CHMe_2$, $CMe_3$ oxazolinyl, chiral | S, H, B, C, IR, MS | [529] |
| 1-$CHMe_2$-9-$CH_2$-*cyclo*[CHC(R)═N—N═C(R)$CH_2$] R═$CH_2$-bis(3′,5′-dimethylpyrazolyl)-4,5-pyridazine | S([4 + 2] cycloaddition), H | [1516] |
| 9-$CH_2$-*cyclo*[CHC(R)═N—N═C(R)$CH_2$] R═$CH_2$-bis(3′,5′-dimethylpyrazolyl)-4,5-dihydropyridazine | S([4 + 2] cycloaddition), H | [1516] |
| 1-CHR*OMe-2-$SnMe_2$Br (O→Sn) R = H, Ph | S, X(H, Br), H, B, C, IR, MS | [529] |
| 1-Me-3-NHMeC(O)R | S | [134] |
| 1-R-3-C(O)$NH_2$ R = H, Me | S, IR | [183] |
| 1-$OC_6H_3$(OR)CH═N$(CH_2)_2NC_6H_3$Me R = Me, Et Schiff bases | S, H, I | [267] |
| 1-phthalimide($NCH_2$) | S[from $B_{10}H_{12}(MeCN)_2$ and RC≡CH with homogeneous Ag catalyst, high yield] | [1760] |

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| Compound | Information | References |
|---|---|---|
| 1-C(O)NCH$_2$(*cyclo*-C$_4$H$_4$NR) amido analogues of benzamides as D2 receptor ligands | S, H, B, C, MS | [1553] |
| 1-(CH$_2$)$_2$C(O)NH(CH$_2$)$_4$CH[C(O)OH]NH-C(O)OCH$_2$-C$_{13}$H$_9$ (FF) fluorenyl incorporation of HCB$_{10}$H$_{10}$C(CH$_2$)$_2$C(O)NH into peptides for BNCT | S, H, C, Si, IR, MS | [1554] |
| 1,3-*cyclo*-[MCp*NR═C(NHR)]-1,2-$C_2B_{10}H_9$-μ(C, M)-Se R═CHMe$_2$, *cyclo*-C$_6$H$_{13}$ M = Ir, Ru (FF) | S, X(Ir, CHMe$_2$, *n*-C$_6$H$_{13}$; Ru, *cyclo*-C$_6$H$_{13}$), H, B, C, IR | [1652] |
| 1-C$_6$H$_4$—O—CH$_2$C(O)NHC$_6$H$_4$—C(O)C$_6$H$_4$-*o*/*m*-R═OCH$_2$C≡CH, OH | S, H, C, IR, MS, HIF-1α inhibition, fluorescence imaging | [1654] |
| 1-S(CH$_2$)$_3$NH(CO)C$_6$H$_4$CH$_2$OH hydroxymethylbenzoyl | S, H, B, C | [1700] |
| 1-CH$_2$NC(O)R-2-R′ R = Ph, *p*-C$_6$H$_4$Me, *p*-C$_6$H$_4$-OMe, C$_5$H$_4$N; R′ = H, Me | S[Pd(0)-catalyzed aminocarbonylaton of aryl halides], H, B, C, IR, MS | [1713] |
| 1-*p*-C$_6$H$_4$—OCH$_2$C(O)NH—C$_6$H$_3$R(OH) R = C(O)OMe, B(OH)$_2$ phenoxyacetanilides | S, H, inhibition of HIF-1 transcriptional activity | [1714] |
| 1-*p*-C$_6$H$_4$—OCH$_2$-*cyclo*-CONC$_6$H$_3$—C(O)R R = OMe, OH benzoxazoles | S, H, inhibition of HIF-1 transcriptional activity | [1714] |
| 1-NH-C(O)-C$_6$H$_3$ClOMe P2X$_7$ receptor antagonist; central nervous system antidepressant | S, X, H, inhibition of human P2X$_7$R pore formation | [1734] |
| 1-C(S)NHC$_6$H$_4$-*p*-Et | S, X, H, B, IR, MS | [1746] |
| RN[(CH$_2$)$_3$NHC(O)(CH$_2$)$_2$C(O)OCH$_2$C-(CH$_2$OCH$_2$-C$_2$B$_{10}$H$_{11}$)$_3$]$_2$ trifunctional dendritic wedge R = group containing cyanine dye and a nonpeptidic integrin, or cyanine dye only (control) for BNCT | S, H, B, IR, MS, UV, cellular uptake in live mice | [1811] |
| 3-NHC(O)CH$_2$NHEt$_2$ lidocaine analogues local anesthetics | S, H, B, IR, MS, analgesic activity | [1831] |
| ***Isocyanates*** | | |
| 1-NCO-3-R R = H, Me | | [505] |
| 1-(CH$_2$)$_n$NCOR-2-R R = H, Me, Ph, CH$_2$═CMe; *n* = 0,1 | S | [533] |
| 1,2-(CH$_2$NCO)$_2$ | S | [534] |
| 1-*p*-C$_6$H$_4$-NCO | S | [535] |
| 1,2-(*p*-C$_6$H$_4$-NCO)$_2$ | S | [535] |
| 1-(CH$_2$)$_3$N(CO)$_2$C$_6$H$_4$ | S, X | [537] |
| ***Azides*** | | |
| 1-N$_3$-2-R R = Me, Me$_2$SiCMe$_3$ | S, H, C, IR | [538] |
| 1-CH$_2$-(*cyclo*-N$_3$CHR) R = (CH$_2$)$_n$Me (*n* = 4,5), Ph, SiMe$_3$, CMe$_2$OH, CH$_2$OH, CH$_2$OAc triazoles | S, H, B | [1528] |
| 1-C(O)N$_3$-2-R R = H, Me, Ph | S | [482] |
| 1-Me-2-(CH$_2$)$_3$N$_3$ | S, H, B, C, IR, MS | [1624] |
| 8,9,10,12-[(CH$_2$)$_3$N$_3$]$_4$ | S, X(Cl), H, B, C, IR, MS | [1898] |
| 9,12-[(CH$_2$)$_3$N$_3$]$_2$ | S, H, B, C, IR, MS | [1898] |
| **Azo and Hydrazo Derivatives** | | |
| 1-Ph-2-(NHNH-C$_6$H$_4$-*p*-Me) | S, X, H, B, C | [540] |

| Compound | Information | References |
|---|---|---|
| $RR'N_2C_3H_3^+$ $C_2B_{10}H_{11}^-$ R = Me, Et; R′ = Et, *n*-$C_4H_9$ imidazolium; ionic liquid (FF) | S, H, B, C, COND | [541] |
| ***Nitriles and isonitriles*** | | |
| 1-CN-2-R R = Me, Ph | S | [386,542–544] |
| 1-$CH_2$CN-2-R R = H, Me | S | [182,543] |
| 1-$CH_2$CN-2-Ph | S | [543] |
| 1-$CH_2$CN-2-R R = CH = $CH_2$, $CH_2CH_2$CN | S | [545] |
| 1,2-$(CH_2CH_2CN)_2$ | S | [546] |
| 1-$CH_2CH_2$CN-2-R R = H, Me, Ph, $CH_2$ = CMe | S | [546] |
| 1-$CH_2$-O-*m*-$C_6H_4$CN | S, X | [1473] |
| $MeCB_{10}H_{10}C$–CN = N-$CB_{10}H_{10}$CMe (FF) | S | [483] |
| 3-R R = NC, CN | S | [505,548] |
| 3-R R = $CH_2NHC(O)C_6H_4$-*o*-$CH_2OH$, $CH_2NH_3^+$, $CH_2NHC(O)H$, $CH_2NC$ | S, H, B, C, IR, MS | [502] |
| ***Amidinates*** | | |
| 1-C(NHCMe$_2$) = NCMe$_2$-2-Li(Me$_2$O$_2$C$_2$H$_4$) (N → Li) | S, X, H, B, C | [1531] |
| *Trans*-[1,2-*cyclo*-C(NH-CHMe$_2$) = N(CHMe$_2$) $C_2B_{10}H_{10}]_2Fe^{III}Cl$ 2 Fe—C, 2 Fe—N | S, X, IR | [1797] |
| 1-C[N(LiR$_2$)(CHMe$_2$)] = N(CHMe$_2$)-2-LiR$_2$ R$_2$ = DME, (THF)$_2$ N → Li | S, X(THF), H, B, C, Li, IR | [1742] |
| 1-C[N(SiMe$_3$)(CHMe$_2$)] = N(CHMe$_2$)-2-SiMe$_3$ | S, X, H, B, C, Si, IR | [1742] |
| 1-C[N(CHMe$_2$)] = N(CHMe$_2$)$^-$ | | |
| 2-Sn = SnN$_4$(CHMe$_2$)$_4$[μ-CH(CH$_2$)$_3$Me]$_2$ | S, X, H, B, C, IR | [1742] |
| 1-C[N(CHMe$_2$)] = N(CHMe$_2$)-2-PPh N → P | S, X, H, B, C, P, IR | [1742] |
| 1,2-*cyclo*-C(N-$C_6H_{11}$) = N($C_6H_{11}$)—$ER_2$ E = Si, Ge R = Cl, Me, Ph | S, X(Si,Ph), H, B, C, P, IR | [1742] |
| 1,2-*cyclo*-C(N-$C_6H_{11}$) = N($C_6H_{11}$)—$MCp_2$ | S, X(Ti, Zr), H, B, C, P, IR | [1742] |
| 1-C(NRH) = NR R = 2′,6′-(CHMe$_2$)$C_6H_3$ | S, X, H, B, IR, MS | [1842] |
| ***Ureas*** | | |
| 1,2-[($C_6H_4$)-*m*/*p*-NMeC(O)NMe($C_6H_4$)-*p*-R]$_2$ R = H, $C_2B_{10}H_{11}$, $PhC_2B_{10}H_{10}$ (FF) | S, X(R = H), H | [549] |
| C(O)[NR-$C_6H_4$-3,5-(1,2-$C_2B_{10}H_{11})_2]_2$ R = H, Me phenylureas (FF) | S, X, H | [550] |
| 1-HO-2-C(O)NH$(CH_2)_4$-ureido derivatives | S, H, B, C, IR, MS, inhibition of prostate specific antigen (PSMA), biodistribution, tumor uptake | [1739] |
| Urea-based glutamate carboxypeptidase II inhibitors | | [1924] |
| **Phosphorus Derivatives** | | |
| 1-(MePh$_2$P)$^+$I$^-$ selective targeting of mitochondria for BNCT | S, H, B, C, P, MS | [554] |
| 1-P(*n*-$C_6H_{13})_2$-2-Ph | S | [555] |

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| Compound | Information | References |
|---|---|---|
| 1-PEtN($SiMe_3$)$_2$-2-Me | S, X | [1520] |
| 1,2-$(FP)_2(C_2B_{10}H_{10})_2$ (FF) | S, H, P, F, IR, MS | [556] |
| 1-R-2-P($NEt_2$)$_2$ R = H, Me, Ph | S | [557] |
| 1,2-[P(OMe)($NR_2$)]$_2$ chiral R = Et, $CHMe_2$ | S, X, H, B, C, P, IR, MS | [558] |
| 1-R-2-PCl($NEt_2$) R = H, Me, Ph | S | [557] |
| 1-$PPh_2$-2-R R = H, P[NMe$_2$]$_2$, PF[NMe$_2$]$_2$, $PF_2$ | S, H, P, F, IR, MS | [559] |
| 1,2-($PPh_2$)$_2$-9-X X = H, Cl | S | [560] |
| 1,2-[(*p*-$MeC_6H_4CHMe_2$)$_2$P | S, X, H, C, P | [562] |
| 1,2-($Ph_2P$)$_2$-8,9,10,12-$Et_4$ | S | [172] |
| 1-R-2-S(=S)P(OR′)$_2$ R = Me,Ph,1-cyclohexenyl, dimethylpyranyl; R′ = Me, Et, $CHMe_2$ thiophosphates, thiophosphonates | S | [563] |
| 1,2-RR′ R = PhClP = S, R′ = PPhCl,H,P; R = PPhCl, R′ = H, Ph; RR′ = PhP(=S)-S-P(=S)Ph | S, X(ClP = S, Ph), H, B, C, P, IR | [552] |
| 1-$CH_2$P[$NEt_2$]$_2$-2-Me | S | [564] |
| 1-$PPh_2$I-2-Me (I–I intermolecular interaction in solid state and solution) | S, X, P(variable temp) | [568] |
| 1-$PPh_2$-2-$CH_2NMe_2$ | S, X, H, B, C, P, IR | [572] |
| 1-$PPh_2$-2-SR R = SEt, S($CHMe_2$), S(*n*-$C_4H_9$), $SCH_2Ph$ | S, X[S($CHMe_2$)], H, B, IR | [573] |
| 1-P(*n*-$C_6H_{13}$)$_2$-2-Ph | S | [575] |
| 1-P($CMe_3$)$_2$-2-R R = Me, Ph Pd-catalyzed cross-coupling | S, H, B, C, P | [576] |
| 1-P(*cyclo*-$C_6H_{12}$)$_2$ Pd-catalyzed cross-coupling | S, H, B, C, P | [576] |
| 1-$CH_2$P(*cyclo*-$C_6H_{12}$)$_2$ Pd-catalyzed cross-coupling | S, H, B, C, P | [576] |
| 9-$CH_2PPh_2$ Pd-catalyzed cross-coupling | S, H, B, C, P | [576] |
| 1-PHPh | S, H, B, C, P, IR, MS | [577] |
| 1,2-*cyclo*-[—P(=S)Ph-S-P(=S)Ph—] | S, X, H, B, C, P, IR, MS | [577] |
| 1,2-*cyclo*-(—$CH_2$—PR—$CH_2$—) R = Me, Ph phospholane | S, X(Ph) | [579] |
| 1,2-*cyclo*-(—PhP—NH—PPh—) | S | [50] |
| 1,2-*cyclo*-(—ClP—$CB_{10}H_{10}$—PCl—) biscarborane | S, IR (actual) | [50] |
| 1-P($CHMe_2$)$_2$-2-Me | S, X, H, B, P, IR | [580] |
| ($MeCB_{10}H_{10}C$)$_2$PPh (FF) | S, H, B. P, IR | [567] |
| | X | [569] |
| 1-$CH_2PR_2$ R = Me, $CMe_3$ | S, X | [582] |
| ($C_{13}H_9$)[N($CHMe_2$)]$_2$P—$C_2$ $B_{10}H_{11}$ $C_{13}H_9$ = fluorenyl | S, X, H, B, C, P, IR | [1464] |
| ($C_{13}H_9$)[N($CHMe_2$)]$_2$P(O)—$C_2B_{10}H_{11}$ | | |
| $C_{13}H_9$ = fluorenyl (FF) | S, X, H, B, C, P, IR | [1464] |

| Compound | Information | References |
|---|---|---|
| 1-{$C_6H_3$-3′,5′-[$C_6H_2$-2″,4″,6″-$(CHMe_2)_3$]$_2$}-2-P $(CHMe_2)_2$ terphenyl | S, H, IR | [1841] |
| 1-$CH_2PPh_2$ | S, X | [583] |
| 1-$PR_2$-2-$SiHMe_2$ R = Me, OEt, Ph | S, H, C, P | [584] |
| 1,2-$(R_2P)CB_{10}H_{10}C$–[$Me(Me_2Si)_2Si$]$_2$-$CB_{10}H_{10}C$–$PR_2$ R = Me, OEt, Ph (FF) | S, H, C, P | [584] |
| 1,2-[$(CHMe_2)_2P(O)$]$_2C_2B_{10}H_{10}$·$B(OH)_3$ | S, X | [1876] |
| 1-P(O)$(OEt)_2$-2-Me | S | [585] |
| *Rac*/*meso*-1,2-[P(O)(OEt)Cl]$_2$ | S, H, B, C, P, MS | [1436] |
| 1-PMe(OEt)-2-R R = H, Me, $CH_2$=CMe, Ph | S | [586] |
| 1-(O=$PPH_2$)-2-$PPh_2$ | S, H, C, IR | [587] |
| 1-$CH_2P(OEt)_2$ | S | [588] |
| 1-PMe(OEt)$R^{\cdot}$ R = $OCMe_3$, Me phosphoranyl radicals | ESR | [589] |
| 1-P$(OEt)_2$-2-Me | S | [590] |
| 1,2-P(OR(OR′) R, R′ = *cyclo*-$C_6H_9Me_2(CHMe_2)$, *cyclo*-$C_6H_4$-*p*-$CMe_3$, adamantyl chiral phosphanyl derivatives | S, X(*o*-$C_6H_9Me_2(CHMe_2)$, *cyclo*-$C_6H_4$-*p*-CMe), H, B, C, P, IR, MS | [591] |
| 1,2-$(PPh_2)_2$-B-$Br_n$ ($n$ = 1, 2, 3) | S | [133] |
| 1,2-$(PPhCl)_2$-B-$Br_2$ | S | [133] |
| 1,2-*cyclo*-[$CH_2OP(O)OCH_2CF_3OCH_2$] 1-(1,3,2-dioxaphosphepane) | X | [594] |
| 1-Ph-2-(*cyclo*-PCl=N—$PCl_2$=N—$PCl_2$=N—) cyclotriphosphazene | S, X, P, MS | [595] |
| 1,2-*cyclo*-[$N_3P_3(O_2C_{12}H_8)_2$](μ-$OCH_2)_2$ cyclotriphosphazene | S, H, C, P, IR, MS | [596] |
| 1,2-*cyclo*-[$N_3P_3Cl_4$](μ-$OCH_2)_2$ cyclotriphosphazene | S, H, C, P, IR, MS | [596] |
| 1,2-$Me_2$-9-O-*bicyclo*-$PC_5H_9N_2Ph$ diamidophosphite | S, B, C, P | [1392] |
| $(MeCB_{10}H_{10}C)_2P(O)(OCl)$ (FF) | S | [557] |
| $OP(CB_{10}H_{10}C—R)_3$ R = H, Me, Ph (FF) | S | [557] |
| 1-R-2-P$(OCl)_2$ R = H, Me, Ph | S | [557] |
| 1-R-2-PH(O)OH R = H, Ph phosphinic acid | S | [557] |
| $(RCB_{10}H_{10}C)_2POEt$ R = Me, $CH_2$=CMe, Ph (FF) | S | [599] |
| $(RCB_{10}H_{10}C)_2P(O)X$ X = Cl, Br; R = Me, $CH_2$=CMe, Ph (FF) | S | [599] |
| 1-[$CH_2P(MeC_2B_{10}H_{10})_2$]-2-P$(MeC_2B_{10}H_{10})CH_2$-$C_2B_{10}H_{11}$ (FF) | S, X, MS | [600] |
| 1,2-*cyclo*-[—PhP—$CB_{10}H_{10}C$—$CB_{10}H_{10}C$—] (FF) | S | [601] |
| 1,2-*cyclo*-[—CH(O) Me—$CB_{10}H_{10}C$—PPh—$CB_{10}H_{10}C$—] (FF) | S | [602] |
| 1,2-*cyclo*-P$(NMe_2)$—C[P($NMe_2$—C≡C—Ph]= CPh phosphanyl | S, X, H, B, P | [1828] |
| 1,2-[$P(NR_2)C≡CR′]_2$ R = Me, Et R′ = Ph, $CMe_3$, SiMe | S, P, E, MS | [1828] |

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| Compound | Information | References |
|---|---|---|
| 1,2-*cyclo*-P[$(Me_2CH)N(CH_2)_2N(CHMe_2)$—AuX—P[$(Me_2CH)N(CH_2)_2N(CHMe_2)$] X = CO, $CPh_2$ carbene | S, X, C, P, IR | [1829] |
| 1-PCl($C_5H_3$—*o*-$CHRNMe_2$)FeCp R = H, Me | S, X(pure enantiomer), H, B, C, P, IR, MS | [603] |
| 1,2-[PCl($C_5H_3$—*o*-$CH_2NMe_2$)FeCp]$_2$ | S, X(pure enantiomer), H, B, C, P, IR, MS | [603] |
| 1-P[$N(CHMe_2)_2$](O)$C_9H_6$ indenyl | S, X, H, B, C, P, IR, MS | [604] |
| 1-P[$N(CHMe_2)_2$]($C_9H_5$Li)-2-Li$(OEt_2)_{1.5}$ indenyl | S, X, H, B, C, P, IR | [605] |
| 1-P[$N(CHMe_2)_2$]$(C_9H_6)^-$ indenyl | S, X, H, B, C, P, IR | [605] |
| 1-$CH_2OP(O)RR'$ R, R′ = Cl, $OCH_2CF_3$, OPh | S, P | [606] |
| 1-$(CH_2)_3$OH-2-$(CH_2)_3$OTBDMS phosphates | S, H, B, C, IR | [607] |
| $(C_{10}H_6)_2[OP(\mu\text{-}O)_2C_2B_{10}H_{10}]_2$ ($(C_{10}H_6)_2$ = BINOL chiral catalyst for Pd-catalyzed asymmetric allylic amination) (FF) | S, H, B, P | [1393] |
| (*bicyclo*-$C_6O_2$)$[OP(\mu\text{-}O)_2C_2B_{10}H_{10}]_2$ chiral catalyst for Pd-catalyzed asymmetric allylic amination (FF) | S, H, B, P | [1393] |
| Nucleoside mono- and diphosphites and phosphonates (carborane attached at 5′ position of sugar) for BNCT | S | [1460] |
| 1-S[*cyclo*-$PO_2(C_{20}H_{12})_2$] chiral thiophosphite | S, H, B, P | [323] |
| 1-R-2-S(=S)$P(OR')_2$ R = Me,Ph,1-cyclohexenyl, dimethylpyranyl; R′ = Me, Et, $CHMe_2$ thiophosphates, thiophosphonates | S | [563] |
| $(HCB_{10}H_9CH\text{-}9\text{-}S)_2P(=O)Me$ methyldithiophosphonate (FF) | S, H, P, IR | [609] |
| 1,2-*cyclo*-[$PPh_2$—$NiCl_2$—$Ph_2P$] | S, X, H. B, IR | [1548,1574] |
| | C, P | [1574] |
| 1-$PPh_2$ = S-2-SH | S, H, B, C, P, IR | [1596] |
| 1,2-*cyclo*-$Ph_2P$=S-MCp*Cl M = Ir, Rh M = Ir, norbornene polymerization catalyst | S, X(Ir), H, B, C, P, IR | [1596] |
| 1,3,2-*bicyclo*-$Ph_2P$=S—IrCp*S— S→C(2) | S, X, H, B, C, P, IR | [1596] |
| 1,2-*cyclo*-$Ph_2P$=S—RhCp*S | S, X, H, B, C, P, IR | [1596] |
| 1-P(=S)$(CHMe_2)_2$-2-R R = H, $CHMe_2$ | S, H, B, C, P, IR | [1574] |
| Ni[$CB_{10}H_{10}$-$PPh_2$=S—]$_2$ 2 Ni—S | S, X, H, P, IR | [1591] |
| Ni[S-$CB_{10}H_{10}$-$PPh_2$=S-]$_2$ 4 Ni-S | S, X, H, P, IR, EXAFS | [1591] |
| 1-P(=Se)$(CHMe_2)_2$ | | |
| 1-P(=E)$Ph_2$-2-R R = Me, Ph E = S, Se | S, H, B, C, P, IR | [1574] |
| *Rac*-1,2-*cyclo*-$P_2R_2$ R = $CMe_3$, $N(CHMe_2)_2$ 1,2-diphosphetanes | S, X, H, C, P | [1578] |
| 1,2-$(PIR)_2$ R = $CMe_3$, $N(CHMe_2)_2$ | S, X, P | [1578] |
| 1-P(H)$CMe_3$ | S, X, H, B, C, P | [1638] |
| *Rac*/*meso*-1,2-[P(H)$CMe_3$]$_2$ | S, H, B, C, P | [1638] |
| 1,2-*cyclo*-P($CMe_3$)—$CH_2$-NPh—$CH_2$—P($CMe_3$) | S, X, H, B, C, P | [1638] |
| 3-$NHPO_2(C_{20}H_{12})$ amidophosphite $C_{20}H_{12}$ = binaphthalenyl | S, H, B. P | [1579] |

| Compound | Information | References |
|---|---|---|
| $(C_8H_{12})$ $Rh[3-NHPO_2(C_{20}H_{12})-1,2-C_2B_{10}H_{11}]_2^+$ $BF_4^-$ amidophosphite $C_{20}H_{12}$ = binaphthalenyl; catalyst for asymmetric hydrogenation of α- and β-dehydroamino acids (FF) | S, P | [1579] |
| 1-$P(CMe_3)_2$ | S, X, H, B, C, P, MS | [1607] |
| $(Me_3Si)_2N—Sn—P(CB_{10}H_{10}CH)_2$ | S, X, H, P | [1620] |
| 1-$PPh_2$(=S)-2-$SCH_2$-$C_6H_2(OH)R_2$ R = Me, $CMe_3$ | S, X($CMe_3$), H, C, P, IR | [1680] |
| 1-$PPh_2$(=S)-2-*cyclo*-$SCH_2C_6H_2R_2(O)$ $[CrCl_2(OC_4H_8)]_2$ Cr—S Cr—O R = Me, $CMe_3$ catalyzes $C_2H_4$ polymerization in presence of MAO | S, IR | [1680] |
| 1,2-*cyclo*-OP(X)O X = Cl, Br, I dioxaphospholane | S, H, B, P | [1730] |
| 1-($OPO_2$-$C_2B_{10}H_{10}$)-2-OH dioxaphospholane | S, H, B, P | [1730] |
| 1,2-*cyclo*-OPRO R=$CHMe_2$, *n*-$C_4H_9$, $CH_2$-$C_3H_3Me_2$, Ph, $NEt_2$, OEt dioxaphospholane | S, H, B, C, P | [1730] |
| *Cyclo*-$H_{10}B_{10}C_2(\mu\text{-OPRO})_2C_2B_{10}H_{10}$ R=$CHMe_2$, *n*-$C_4H_9$, $CH_2$-$C_3H_3Me_2$, Ph, $NEt_2$, OEt | S, X($CH_2$-$C_3H_3Me_2$), H, B, C, P | [1730] |
| 1-OP(O)(OH)(*n*-$C_4H_9$)-2-OH dioxaphospholane | S, X, H, B, C, P | [1730] |
| 1,2-*cyclo*-$SeP(CHMe_2)(BH_3)Se$ | S, H, B, C, P, Se | [1814] |
| 1,2-*cyclo*-$SePH(CHMe_2)BH_2Se$ | S, X, H, B, C, P, Se | [1814] |
| 1,2-*cyclo*-$SeB(SMe_2)HSe$ | S, X, H, B, C, P, Se | [1814] |
| 1,2-*cyclo*-$SeP(BH_3)HSe$ | S, X, H, B, C, P, Se | [1814] |
| 1,2-*cyclo*-SeRhCp*Cl-$P(CHMe_2)ClSe$ | S, X, H, B, C, P, Se | [1814] |
| 1,2-*cyclo*-SeRhCp*$[PCl_2(CHMe_2)]Se$ | S, X, H, B, C, P, Se | [1814] |
| 1,2-*cyclo*-(S—R—S) R=$SiMe_2$, $P(CMe_3)$, P(S)$(CMe_3)$, P(Se)$(CMe_3)$ | S, X[P(S)$(CMe_3)$], H, B, C, P, Si, MS | [1744] |
| $(1,2\text{-}S_2C_2B_{10}H_{10})_2[\mu\text{-}S—P(CMe_3)—S]_2$ (FF) | S, X, H, B, C, P, MS | [1744] |
| $(1,2\text{-}C_2B_{10}H_{10})_2(\mu\text{-}S—PR—S)_2$ R=$CHMe_2$, $CH_2C_6H_3Me_2$, *n*-$C_6H_{11}$, Ph (FF) | S, H, B, C, P, MS | [1744] |
| $1,2\text{-}[SP(CMe_3)Cl]_2$ | S, H, B, C, P, MS | [1744] |
| 1,2-*cyclo*-$[S—P(CH_2PCl_2)—S]$ | S, H, B, C, P, MS | [1744] |
| $CH_2[P(\mu\text{-}S)_2C_2B_{10}H_{10}]_2$ (FF) | S, H, B, C, P, MS | [1744] |
| $(1,2\text{-}C_2B_{10}H_{10})_2[\mu\text{-}SPCl—CH_2—PClS]_2$ (FF) | S, X, H, B, C, P, MS | [1744] |
| 1,2-*cyclo*-$[S—P(CH_2)_2Cl_2—S]$ | S, H, B, C, P, MS | [1744] |
| 1′,2′-$CH_2CH_2[P(\mu\text{-}S)_2C_2B_{10}H_{10}]_2$ (FF) | S, H, B, C, P, MS | [1744] |
| $[\mu\text{-}S\text{-}PR\text{-}S]_2(1,2\text{-}C_2B_{10}H_{10})_2$ R=$(CH_2)_2P(\mu\text{-}S)_2C_2B_{10}H_{10}$ (FF) | S, H, B, C, P, MS | [1744] |
| $CH_2CH_2[P(\mu\text{-}S)_2C_2B_{10}H_{10})]_4$ (FF) | S, H, B, C, P, MS | [1744] |
| 1-$CH_2C(CF_3)[P(O)(OEt)_2]NHC(O)OCH_2Ph$ aminophosphonic acid | S, X, H, P, F | [1756] |
| 1,2-*cyclo*-$P_3R_2R'$ R=$CMe_3$, Ph, *cyclo*-$C_6H_{11}$; R′=Ph, *cyclo*-$C_6H_{11}$ triphospholanes | S, X($CMe_3$, Ph; Ph, Ph; $C_6H_{11}$, $C_6H_{11}$; Ph, $C_6H_{11}$), H, B, C, P, MS | [1757] |

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| Compound | Information | References |
|---|---|---|
| 1,2-*cyclo*-($Ph_2P$—M—$PPh_2$) M = Pd, Pt | S, H, P | [1758] |
| 1,2-(μ-$Ph_2P$)$_2$M(μ-S)$_2$($C_2B_{10}H_{10}$) M = Pd, Pt | S, H, P | [1758] |
| $H_{10}B_{10}C_2$(μ-S)$_2$M(–M′$PPh_3$)-7,8-(μ-$PPh_2$)$_2$-7,8-*nido*-$C_2B_9H_{10}$ M = Pd, Pt, Ni; M′ = Cu, Ag, Au heterobimetallic $d^8$–$d^{10}$ interactions | S, X(Pd, Au; Pt, Au; Pd, Ag; Pd, Cu; Ni, Au), H, P, MS, diffuse reflectance UV, emission | [1758] |
| 1-Me-2-$PPh_2$AuX X = Cl, $SC_4H_8^+$, $PPh_3^+$ For X = Cl, pyrolysis and deposit on Si→Au crystals microcrystalline materials | S, H, P, F, IR | [1763] |
| Me—$CB_{10}H_{10}C$—$PPh_2$—M[*nido*-7,8-(μ-$PPh_2$)$_2C_2B_9H_{10}$] M = Ag, Au | S, X (Ag), H, P, IR, UV(luminescence emission) | [1763] |
| 1-Me-2-$PPh_2$Au(μ-$PPh_2$)$_2C_2B_{10}H_{10}^+$ $OTf^-$ | S, H, P, F, IR | [1763] |
| 1,2-[$AuPh_2P$—$CB_{10}H_{10}C$—Me)$_2$ | S, H, P, IR | [1763] |
| 1,12-($AuPPh_2$-1,2-$CB_{10}H_{10}CMe)_2$-1,12-$C_2B_{10}H_{10}$ pyrolysis and deposit on Si→Au crystals microcrystalline materials | S, H, P, IR, UV(luminescence emission) | [1763] |
| 1-P(=S)$Ph_2$-2-$SCH_2C_6H_2(CMe_3)_2$-$OZrCl_2Cp$ ethylene polymerization co-catalyst with MAO | S, X, H, B, C, P | [1787] |
| 1,2-[$(CHMe_2)_2$P-Ag-($N_2C_{11}OH_6$)-P($CHMe_2)_2$] phosphanes diazafluorene-9-one | S, X, H, P, emission/excitation luminescence | [1794] |
| 9-$OPO_2(C_{10}H_6)_2$ phosphite ligands for Rh-catalyzed asymmetric hydrogenation of dimethyl itaconite | S, H, B, P | [615] |
| 9-OP(O-$C_6H_3$-2′,6′-$Me_2)_2$ phosphite Suzuki-Miyaura Pd-catalyzed cross-coupling with aryl bromides | S, H, B | [1544] |
| 9-$SPPh_2$–X X = $W(CO)_5$, $CpMn(CO)_2$ | S, H, P, IR | [612] |
| 9-SP(O)$(OEt)_2$ thiophosphate | S | [610] |
| 9-SP$(OEt)_2$ thiophosphite | S | [613] |
| | S, P | [614] |
| 9-$(CH_2)_3PMe_3^+$-12-$(CH_2)_3Br^-$ | S, H, B, C, MS | [611] |
| 9,12-[$(CH_2)_3PMe_3^+Br^-]_2$ | S, H, B, C, MS | [611] |
| **Sulfur Derivatives** | | |
| 1,2-$(SH)_2$ increases the surface potential of modified Ag film more than 9,12-$(SH)_2$ isomer | | [1545] |
| SH and $(SH)_2$ derivatives, self-assembly on Au surfaces | | [1558] |
| 9-SH | S, X, thermal isomerization | [1903] |
| 1,2-$(SR)_2$ (SR = *bicyclo*-$S_2NC_7H_4$, $S_2CNEt_2$) | S, H, IR, COND | [525] |
| 1-S-*cyclo*-$NC_5H_4$ | S, X, H, IR, COND | [525] |
| 1-SH-2-(2′-$NC_5H_4$) | S, X, H, B, C, IR | [618] |
| 1-SH-2-$CHPhC_5H_4$ | S, H, B, C, IR | [619] |
| 1,2-$[(CH_2)_2SLi]_2$ | S, H, B, C, IR | [463] |
| 1-SMe-2-R R = H, Me, Ph | S | [616] |
| 1-S-2-$MeC_2B_{10}H_{10}^-$ $PMePh_3^+$ (FF) | X | [1376] |
| 1-S-2-$PhC_2B_{10}H_{10}^-$ $C_{10}H_6(NMe_2)_2H^+$ (FF) | S, X, B | [623] |

| Compound | Information | References |
|---|---|---|
| 1,2-$[S(O)Ph]_2$ | S, IR | [624] |
| 1-R-2-$(CH_2)_n$CH(SPh)$CH_2$Cl R = H, Me; $n$ = 1, 2 | S, X(Me; $n$ = 1) | [318] |
| 1,2-SR-2-Me R = H, Me | S, H, B, IR | [626] |
| 1,2-$(SH)_2$ -8,9,10,12-$Et_4$ | S | [172] |
| 1-$CH_2SCH_2Me$ | C, C–H coupling, C hybridization | [45] |
| 1-$(CH_2)_2$SH-2-Me | X | [631] |
| μ-[—$SCH_2(CH_2OCH_2)_2CH_2S$—]-1,2-$C_2B_{10}H_{10}$ (FF) | S, X, H, C, IR | [634] |
| 1-$(CH_2)_n$S-Pt(terpyridyl)$^+$ $OSO_2CF_3^-$ $n$ = 0–3 | S, H, B, C, MS, cytotoxicity | [633] |
| 1-$CH_2O$-$C_6H_3$(OMe)-*o*-*cyclo*-CHS$(CH_2)_2$S | S, H, B, MS | [455] |
| 1,2-$(SCl)_2$ | S | [635] |
| 1,2-$(\mu\text{-}S)_2$BR R = *n*-$C_4H_9$, Et, Ph, Cl, $NMe_2$ | S, B($C_4H_9$) | [636] |
| $B\left[(\mu-S)_2C_2B_{10}H_{10}\right]_2^{2-}$ | S, B | [636] |
| 1,2-$(C_4H_3S)_2$ thiophene precursor to conducting polymers with high electrochemical and thermal resistance | S, E, UV, TGA | [637] |
| $SC_4H_3$-$C_6H_4(CB_{10}H_{10}CMe)_2$ thiophene (FF) | S, UV, electropolymerization | [379] |
| *Cis*/*trans*-1-CH=CH-$C_4HBr_2S$ thiophene | S, H, B, C, MS | [1808] |
| 1-SBr-2-R R = H, Me, Ph | S, H, B | [639] |
| $B_{12}H_{10}$-1′,7′-$(SMeCH_2$-1,2-$C_2B_{10}H_{11})_2$ (FF) | S, H, B, C, MS | [640] |
| $B_{12}H_{10}$-1′-$SMe_2$-7′-($SMeCH_2$-1,2-$C_2B_{10}H_{11}$) (FF) | S, H, B, C, MS | [640] |
| (1,2-$C_2B_{10}H_{11}$-9-)$_2S_2$ disulfide (FF) | S | [641] |
| (1,2-RR′$C_2B_{10}H_9$-9-)$_2S_2$ R, R′ = H, Me disulfide (FF) | S | [642] |
| [1-R-2-$CH_2$-CH($CH_2$X)S-]$_2$ (S-S) R = Ph, Me, $CHMe_2$; X = Cl, Br, I disulfides | S | [643] |
| $[MeO(CH_2)_2C_5H_4]_6Ti_6(\mu_3-O)_8^{2+}$ (1,2-$C_2B_{10}H_{10}$) (μ-$S_2)_2$($nido-7,8-C_2B_9H_{10})_2^{2-}$ (FF) | S, X, H, B, C, IR | [433] |
| (RC$B_{10}H_{10}$C)-S-(*nido*-7,8-$RC_2B_9H_{10})^-$ R = H, Me (FF) | S, X(Me), H, B, C, IR, MS | [639] |
| $S_2(CB_{10}H_{10}CR)_2^-$ R = H, Me, Ph (FF) | S, H, B, C, IR, MS | [639] |
| 1,2-*cyclo*-[—SC(R)=CH—S—] R = Ph, ($C_5H_4$)FeCp vinyl sulfides | S, X[($C_5H_4$)FeCp], H, B, C, IR, MS | [645] |
| | E, real-time electronic sensing, cytotoxiciy | [1541] |
| 1,2,3,4-[S—CH=CH—C(O)OMe]$_2$ 3 isomers vinyl sulfides | S, X, H, B, C, IR, MS | [645] |
| 1,2-*cyclo*-{—$SC_4$[C(O)OMe]$_4$—} vinyl sulfides | S, H, B, C, IR, MS | [645] |
| 1,2-*cyclo*-(SCoCpS)-3-C($CO_2$Me)=CH($CO_2$Me) | S, X, H, B, C, IR, MS | [646] |
| 1,2-*cyclo*-{SC(CO)[($C_5H_4$)FeCp]=CHS} | S, X, H, B, C, IR, MS, E, real-time electronic sensing, cytotoxiciy | [1541] |
| {1-$CH_2$SCH[C(O)OMe]-$C_2B_{10}H_{11}$}$_2$ (FF) | S, X, H, B, C, IR | [648] |
| 1-$CH_2O_3$SMe-2-R R = H, Me | S | [649] |
| 1-$(CH_2)_2O_3S$—$C_6H_4$Me | S, H, IR, MS | [146] |

*Continued*

| Compound | Information | References |
|---|---|---|
| 1-$CH_2SO_2H$-2-R methylsulfinic acid | S, p$K_a$ | [650] |
| [R-$CB_{10}H_{10}C$–$C_6H_4$]$_2SO_2$ R = H, Me, Ph; isomers (FF) sulfones | S, H, B, C, IR | [500] |
| 1,2-$(CH_2O_3SMe)_2$ sulfonyloxy | S | [1355] |
| 1-CPhH($OSO_3C_6H_4Me$)-2-$C_6H_4$R R = H, $CF_3$, Me, OMe, $NMe_2$ 1-benzyl *p*-toluenesulfonates (tosylates) | S, rate constants, electronic effects of substituents | [651] |
| 1-C(Ots)$C_6H_4$X X = H, $CF_3$, F, OMe OPh, $Me_2$; tosylates | S, solvolysis; mechanism of hydrolysis; Hammett plots; electron-donating effects of substituents | [652,653] |
| $C_5H_2$XN-2′,6′-($CH_2$S-1,2-L$C_2B_{10}H_{10})_2$ X = H, Cl; L = H, Me (FF) | S, X(Me), H, B, C, IR | [270,271] |
| $C_4H_2$S-2,5-($CH_2$S-1,2-L$C_2B_{10}H_{10})_2$ L = H, Me (FF) | S, H, B, C, IR | [271] |
| 1-$CH_2$-$OSO_2CF_3$ triflate | S, H, B | [654] |
| 1,2-$(TfOCH_2)_2$ | S, H, B, IR | [1639] |
| 1-CH($OSO_2$Me)R-2-R′ R = Ph, R′ = Me; R = py, R′ = Me, Ph | S, H, B, C, IR, MS | [1521] |
| 1-CH(py)$NHCH_2$Ph-2-Me R = Ph, R′ = Me; R = py, R′ = Me,Ph | S, H, B, C, IR, MS | [1521] |
| 1-$(CH_2)_n$C($SO_2$Ph)═$CH_2$-2-Me *n* = 1,2 | S, H, MS | [513] |
| 1,2-R′$C_2B_{10}H_9$-9-S—$CH_2CH_2$—P(═X)RR′ R = Me, Ph, EtO; R′ = EtO, *p*-$NO_2C_6H_4O$, Ph, 1,2-$C_2B_{10}H_{11}$; X = O, S esters, thioesters (FF) | S | [1421] |
| 1,2-*bicyclo*-CpCo(FcC═CH-CH═CFc)$S_2$ Fc═$CpFeC_5H_4$ | S, X, H, B, C, IR, MS | [1595] |
| 1-P(═S)($CHMe_2)_2$-2-R R = H, $CHMe_2$ | S, H, B, C, P, IR | [1574] |
| Ni[S-$CB_{10}H_{10}$-$PPh_2$═S-]$_2$ 4 Ni-S | S, X, H, P, IR, EXAFS | [1591] |
| 1-C(═S)NHPh | S, X, H, B, IR | [1837] |
| 1,2-*cyclo*-$Ph_2$P═S-MCp*Cl M = Ir, Rh M = Ir, norbornene polymerization catalyst | S, X(Ir), H, B, C, P, IR | [1596] |
| 1,3,2-*bicyclo*-$Ph_2$P═S—IrCp*S— S→C(2) | S, X, H, B, C, P, IR | [1596] |
| 1,2-cyclo-$Ph_2$P═S—RhCp*S | S, X, H, B, C, P, IR | [1596] |
| LM(E-$CB_{10}H_{10}$CPh)$_2$ L = $Me_2P(CH_2)_nPMe_2$, *n* = 1–3; M = Pd, Pt; E = S, Se (FF) | S, X(*n* = 1, Pt, S, Se), H, P, Se, Pt | [1602] |
| 1,2-*cyclo*-SMLS L = $Me_2P(CH_2)_nPMe_2$, *n* = 1–3; M = Pd, Pt | S, H, P, Pt | [1602] |
| 1,2-*cyclo*-SM($PR_3)_2$S $R_3$ = $Et_3$, $Ph_3$, $MePh_2$, $Me_2Ph$, ; M = Pd, Pt | S, X(Pt, $Me_2Ph$, $MePh_2$), H, P, Pt | [1602] |
| 1,2-(galactopyranose)$_2$-9-$SCH_2$C(O)OH | S, H, B, C, IR, MS | [1618] |
| 1-$CH_2$-*tricyclo*-$C_7O_5HMe_4$ di-O-isopropylidine-deoxygalactopyranosyl buiding block for peptide conjugation | S, X, H, B, C, IR, MS | [1901] |
| HO(O)C($CH_2)_2$C(O)O$CH_2$-C($CH_2$S-9-$C_2B_{10}H_{11})_3$ for incorporation into tumor-selective peptides FF | S, X, H, B, C, IR, MS | [1618] |
| 1,2-*cyclo*-$C_8H_2R_2S_2$ R = Br, $C_4H_3S$, $(C_4H_3S)_2$ (substituted dithiophenes) | S, H, B, C, IR, MS | [1637] |
| 1,2-[*cyclo*-SCo($C_5H_4$Me)S]-3,6-[CH═CHC(O)OMe]$_2$ | S, H, B, C, IR, MS | [1642] |

| Compound | Information | References |
|---|---|---|
| 1,2-*cyclo*-SCH═C[C(O)OMe]*CH═C[C(O)OMe]-Co($C_5H_4$Me)S}-3-CH═CHC(O)OMe S→Co | S, X, H, B, C, IR, MS | [1642] |
| 1,2,3-{*bicyclo*-SCo(L)C[C(O)OMe](S)$CH_2$} L=$C_5H_4$Me, $C_5HMe_4$ S→Co | S, X, H, B, C, IR, MS | [1642] |
| 1,2-{*cyclo*-SCo($C_5Me_4H$)C[C(O)OMe]═CH-C[C(O)OMe]═CHS} S→Co | S, X, H, B, C, IR, MS | [1642] |
| 1-SCH═CHC(O)OMe-2-SCoL$S_2$C-(μCR) L=Cp, $C_5H_4$Me, Cp* R═$CHMe_2$, $NC_4H_8$ | S, H, X(Cp,$CHMe_2$), B, C, IR, MS | [1642] |
| 1-SCo[$S_2$C-$CHMe_3$]$_2$-2-SCH═C[C(O)OMe] CoCp$S_2$C—$CHMe_2$ | S, X, H, B, C, IR, MS | [1642] |
| 1,2-*cyclo*-($Me_3Sn$)$_2C_8S_2H_2$ 2 C→C dithiophene | S, H, polymerization | [1721,1727] |
| 1-($C_6H_4$-*o*-Br)-2-$C_4SH_2$Br thiophene | S, X, H, B, MS | [1911] |
| 1,2-*cyclo*-$C_6H_4$-$C_4SH_2$ thiophene | S, X, H, B, C, MS | [1911] |
| 1,2-*cyclo*-($Me_2$S—S—$SiMe_2$) | S, X, H, B, C, Si | [1626] |
| 1,2-$(HS)_2C_2B_{10}H_{10}$ self-assembled monolayers on Cu surfaces (FF) | | [1627] |
| *n*-SH *n*=3, 8, 9 *n*=3, 9: self-assembly on Au surface | S(Pd-catayzed I exchange), B, H, C, XPS(Au surface | [1668] |
| 1,2-*cyclo*-[CpFe($C_5H_4$)$C_2$]$_2S_2C_2B_{10}H_{10}$ C—B(3) (FF) | S[insertion of HC≡C—$C_5H_4$FeCp into CpCo ($S_2C_2B_{10}H_{10}$)], X | [1644] |
| ($MeC_6H_4CHMe_2$)Ru$S_2$Ru[(μ-S)$_2C_2B_{10}H_{10}$]$_2$(μ-CH═CR R=*cyclo*-$C_6H_{12}$, C(O)Ph, and related derivs (FF) | S, X, H, B, C, IR, MS | [1653] |
| 1-S($CH_2$)$_n$C[C(O)OEt]$_2$NHC(O)Me *n*=4–6 | S, H, B, C, MS, IR | [1674] |
| 1-S($CH_2$)$_n$CH[C(O)OH]$NH_2$·HCl *n*=4–6 | S, H, B, C, MS, IR | [1674] |
| 1-$PPh_2$(═S)-2-S$CH_2$-$C_6H_2$(OH)$R_2$ R=Me, $CMe_3$ | S, X($CMe_3$), H, C, P, IR | [1680] |
| 1-$PPh_2$(═S)-2-*cyclo*-S$CH_2C_6H_2R_2$(O)[$CrCl_2(OC_4H_8)]_2$ Cr—S Cr—O R=Me, $CMe_3$ catalyzes $C_2H_4$ polymerization in presence of MAO | S, IR | [1680] |
| 1,2-[S$CH_2$—$C_6H_2$(OH)($CMe_3$)$_2$]$_2$ | S, X, H, C, IR | [1689] |
| 1-$H_2NSO_2NHCH_2$-2-R R=H, *n*-Ph (*n*=2, 9, 12) | In vitro inhibition in carbonic anhydrase | [1702] |
| 1,2-*cyclo*-SeP(R)(S)PhSe R═$CHMe_2$, OEt | S, X(OEt), H, B, C, P, Se | [1711] |
| 1-R-2-[$C_5H_3N$—*p*-$C_8H_5S$] R=Me, *n*-$C_4H_9$ pyridyl, benzothienyl | S, H, B, C | [1710] |
| 9-SAc | S(Pd-catalyzed cross-coupling), H, B, C, IR, MS | [1724] |
| 1-SR-2-S$CH_2$CHMeC(O)O[$CH_2CH_2O$]$_n$ R=H, rhodamine B polyethylene glycol conjugate polymer | S, H, UV, fluorescence, laser light scattering, confocal laser scanning microscopy, TEM, in vivo cellular uptake | [1733] |
| 1,2-*cyclo*-SRu($MeC_6H_4CHMe_2$)($PPh_3$)S | Solid state $^1$H, $^{11}$B, $^{13}$C, $^{31}$P MAS (magic angle spinning) NMR | [1738] |
| (1,2-$S_2C_2B_{10}H_{10}$)$_2$[μ-S—P($CMe_3$)—S]$_2$ (FF) | S, X, H, B, C, P, MS | [1744] |
| (1,2-$C_2B_{10}H_{10}$)$_2$(μ-S—PR—S)$_2$ R═$CHMe_2$, $CH_2C_6H_3Me_2$, *n*-$C_6H_{11}$, Ph (FF) | S, H, B, C, P, MS | [1744] |

*Continued*

| Compound | Information | References |
|---|---|---|
| 1,2-$[SP(CMe_3)Cl]_2$ | S, H, B, C, P, MS | [1744] |
| 1,2-*cyclo*-[S—$P(CH_2PCl_2)$—S] | S, H, B, C, P, MS | [1744] |
| $CH_2[P(\mu\text{-}S)_2C_2B_{10}H_{10}]_2$ (FF) | S, H, B, C, P, MS | [1744] |
| $(1,2\text{-}C_2B_{10}H_{10})_2[\mu\text{-}SPCl—CH_2—PClS]_2$ (FF) | S, X, H, B, C, P, MS | [1744] |
| $(1,2\text{-}C_2B_{10}H_{10})_2(\mu\text{-}S—PR—S)_2$ R═$CH_2P(\mu\text{-}S)_2C_2B_{10}H_{10}$ (FF) | S, H, B, C, P, MS | [1744] |
| $[\mu\text{-}S\text{-}PR\text{-}S]_2(1,2\text{-}C_2B_{10}H_{10})_2$ R=$(CH_2)_2P(\mu\text{-}S)_2C_2B_{10}H_{10}$ (FF) | S, H, B, C, P, MS | [1744] |
| $H_{10}B_{10}C_2(\mu\text{-}S)_2M(\text{–}M'PPh_3)$-7,8-$(\mu\text{-}PPh_2)_2$-7,8-*nido*-$C_2B_9H_{10}$ M=Pd, Pt, Ni; M′=Cu, Ag, Au heterobimetallic $d^8$–$d^{10}$ interactions | S, X(Pd, Au; Pt, Au; Pd, Ag; Pd, Cu; Ni, Au), H, P, MS, diffuse reflectance UV, emission | [1758] |
| 1-P(═S)$Ph_2$-2-$SCH_2C_6H_2(CMe_3)_2$-$OZrCl_2Cp$ ethylene polymerization co-catalyst with MAO | S, X, H, B, C, P | [1787] |
| 9,12-$(SR)_2$ R=H, Me | S | [659] |
| 9,12-$(HS)_2C_2B_{10}H_{10}$ self-assembled monolayers on Cu surfaces (FF) | | [1627] |
| 9,12-$(SH)_2$ effective protective coating for Ag surfaces | | [1823] |
| 9,12-(—S-$CMe_2$—S—) isopropylidenedithio | X | [661] |
| 9,12-*cyclo*-[—S—CRR′—S—] R=H, Me; R′=Ph, Me heteroacetals | S | [659] |
| 9/12-SH-1-Me | S, H, B, $pK_a$ | [617] |
| $B_2Cl_2\left[(\mu-S)_2C_2B_{10}H_{10}\right]_3^{2-}$ (FF) | S, X, H, B | [662] |
| 9,12-$[p\text{-}C_6H_4S(O)Me]_2$ | S, H, B, C, MS | [240] |
| 9-$SP(OEt)_2$ thiophosphite | S | [613] |
| | S, P | [614] |
| 1-R-2-S(═S)$P(OR')_2$ R=Me,Ph,1-cyclohexenyl, dimethylpyranyl; R′=Me, Et, $CHMe_2$ thiophosphates, thiophosphonates | S | [563] |
| 9-$SPPh_2$ $Me^+$ $I^-$ thiophosphinite | S, H, P, IR | [612] |
| 9-$SPPh_2$–X X=$W(CO)_5$, $CpMn(CO)_2$ | S, H, P, IR | [612] |
| 9-$SP(O)(OEt)_2$ thiophosphate | S | [610] |
| 9-SP(O)(OEt)Et ethylphosphonate | S | [610] |
| $(HCB_{10}H_9CH\text{-}9\text{-}S)_2P(═O)Me$ methyldithiophosphonate (FF) | S, H, P, IR | [609] |
| 9-$HO(O)C\text{-}CH_2$-S receptor-mediated neuropeptide analogues for BNCT | S, H, B, C, IR, MS, cellular uptake | [1832] |
| $(HCB_{10}H_9CH\text{-}9\text{-}S)_2P(O)OEt$ dithiophosphate (FF) | S, H, P, IR | [609,610] |
| $(HCB_{10}H_9CH\text{-}9\text{-}S)_2P(S)OEt$ trithiophosphate (FF) | S, H, P, IR | [609,610] |
| 1,2-*cyclo*-[—$SCH_2S$—]-8,9,10,12-$Et_4$ | S, H | [172] |
| 1,2-*cyclo*-[—$SCH_2CH_2S$—]-8,9,10,12-$Et_4$ | S, H | [172] |
| 1,2-*cyclo*-[–$SRh_2(C_8H_{12})_2S$–] | S, X, H, B, C, IR | [663] |
| 1,2-*cyclo*-[–$SRh_2(CO)_4S$–] | S, X(S), H, B, C, IR | [663] |
| 1,2-*cyclo*-[–S–$M_2(C_8H_{12})_2$-S–] M=Rh, Ir | S, X(Rh), H, C, IR, E | [664] |

| Compound | Information | References |
|---|---|---|
| 1,2-*cyclo*-[Cp*(CO)Ir$S_2$] | S, X | [666] |
| {1,2-*cyclo*-[Cp*Ir(CO)$S_2$]$C_2B_{10}H_{10}$}[W(CO)$_5$] (FF) | S, X | [666] |
| 1,2-*cyclo*-[—S(CoCp)($C_4Ph_2$)S—] | S, X, H, B, C, MS | [667] |
| 1,2-*cyclo*-[—S(CoCp)$H_2$CPhS—] | S, X, H, B, C, MS | [667] |
| 1,2-*cyclo*-{HB[$C_3HMe_2$]$N_2$}Mo(O)—μ(O)$_2$Mo(O)$S_2$]-$C_2B_{10}H_{10}^-$ (FF) | S, X | [668] |
| [1,2-{*cyclo*-SRu[$MeC_6H_4CHMe_2$]S}-$C_2B_{10}H_{10}$]$_2$Mo(CO)$_2$[1,2-{*cyclo*-SRu(CO)$_3$S}$C_2B_{10}H_{10}$] (FF) | S, X, H, B, C, IR | [669] |
| $N_3C_3$[($C_5H_4N$)RhCp*(*cyclo*-$S_2C_2B_{10}H_{10}$)]$_3$ ($N_3C_3$ = triazine) (FF) | S, X, H, B, IR | [670] |
| $N_2OC_2$ [($C_5H_4N$)RhCp*(*cyclo*-$S_2C_2B_{10}H_{10}$)]$_2$ ($N_2OC_2$ = oxadiazole) (FF) | S, X, H, B, IR | [670] |
| L[($C_5H_4N$)MCp*(*cyclo*-$S_2C_2B_{10}H_{10}$)]$_2$ M = Rh, Ir; L = pyrazine, 1,2-di(4-pyridylethylene, 4,4′-dipyridine, diisonicotinic acid 1,4-phenylene diester (FF) | S, X(Rh,pyrazine; Ir,dipyridylethylene; Ir, diisonicotinic acid phenylene diester), H, B, IR | [670] |
| [—C≡C–$C_6H_2$($CHMe_2$)$_2$-NCRhCp*(μ-S)$_2$-1,2-$C_2B_{10}H_{10}$]$_2$ (FF) | S, X, H, C, IR, MS | [671] |
| Cp*M(*cyclo*-$S_2C_2B_{10}H_{10}$)-$NC_5H_4$-*n*═N–$C_5H_4N$–MCp*(*cyclo*-$S_2C_2B_{10}H_{10}$) | | |
| M = Rh, Ir (FF) | S, X(Rh), H, B, IR | [670] |
| [(1,2-*cyclo*-$S_2$)$C_2B_{10}H_{10}$]Mo(μ-CO)$_2$[(1,2-*cyclo*-SRhCp*S)$C_2B_{10}H_{10}$] (FF) | S, X, H, B, C, IR | [672] |
| [(1,2-*cyclo*-$S_2$)$C_2B_{10}H_{10}$]W(μ-CO)$_2$({1,2-*cyclo*-SRh{$C_5H_3$[$C(Me)_3$]$_2$}S}$C_2B_{10}H_{10}$) (FF) | S, X, H, B, C, IR | [672] |
| ($N_2C_4H_4$){1,2-[*cyclo*-SM[$MeC_6H_4CH$-$Me_2$]S]$C_2B_{10}H_{10}$}$_2$ M = Ru, Co (FF) | S, X, H, B, IR | [673] |
| ($N_2C_4H_4$)$_2$[1,2-[*cyclo*-Cp*Co$S_2$($C_2B_{10}H_{10}$)]]$_2$ (FF) | S, X, H, B, IR | [673] |
| **Fluoro Derivatives** | | |
| 1-F-2-Ph | X (icosahedral cage distortions caused by π-bonded substituents), H, B | [343] |
| 1-CF═CFC(O)OH-2-Me | S | [1496] |
| 3-F | IR (80–300 K; band structure; order-disorder transitions) | [1427] |
| 1,2-$Me_2$-3-F | S, F | [674] |
| 1-Me-3-F | p$K_a$ | [237] |
| 1-Me-2-R-3-F R = C(O)OH, SH, $SiMe_3$ | S | [347] |
| 1-R-2-R′-8,9,10,12-$F_4$ R, R′ = H, Me, Ph, $CH_2Ph$, C(Ph)═CHPh | S[Pd(II) catalysis with $F^+$ reagent], X($Me_2$), H, B, C, F, MS | [1686] |
| 1,2-*cyclo*-R R = $(CH_2)_3$, $(CH_2)_4$, $CH_2CH$═$CHCH_2$, $C_4H_4$, $CH_2$-O-$C_6H_4CH_2$, $C_4Et_4$, $(CH_2)_2C_6H_4$, $CH_2CHMe$-*o*-$C_6H_4$ | S[Pd(II) catalysis with $F^+$ reagent], X[$(CH_2)_3$, $CH_2C_6H_4CH_2$, $C_4Et_4$, $(CH_2)_2C_6H_4$], H, B, C, F, MS | [1686] |
| 1,2,12-$Me_3$-8,9,10-$F_3$ | S[Pd(II) catalysis with $F^+$ reagent], X, H, B, C, F, MS | [1686] |
| 1,2,9,12-$Me_4$-8,10-$F_2$ | S[Pd(II) catalysis with $F^+$ reagent], X, H, B, C, F, MS | [1686] |
| 1-[CH(OH)-*p*-$C_6H_4$OMe]-*n*-R *n* = 9,12 R = $^{18}F$, $^{19}F$ | S, H, B, C, F | [1715] |
| 1-R-9-F R = H, Me | S | [676] |

*Continued*

| Compound | Information | References |
|---|---|---|
| 8,9,10,12-$F_4$ | X (crystal packing; H···F versus H···H interactions) | [677] |
| | S | [678] |
| R—$CB_{10}H_9$•C—CF═$CFCF_3$ R = Me, Ph boron-centered radicals (FF) | S, ESR | [680] |
| R—$CB_{10}H_{10}$C—CF•—$CF(CF_3)$—$B_{10}H_9C_2$(R)CF═CF-$CF_3$ R = F, Me carbon-centered radicals (FF) | S, ESR | [680] |
| **Chloro Derivatives** | | |
| 1-Cl | S | [681] |
| | H (C–H shift, coupling constants) | [17] |
| | Dipole moment | [1342] |
| 1-Cl-2-Ph | S | [682] |
| | $^{35}$Cl NQR | [287] |
| 1-Cl-2-Me | S | [683] |
| 1-Cl-2-R R = H, Me, Ph | S | [684] |
| 1-Cl-2-R R = H, Cl, Me, Ph | S, IR (actual spectrum) | [685] |
| 3-Cl | S | [346,347] |
| 1-Me-3-Cl | S | [346,505] |
| 1-R-8-Cl R = H, Me, Ph | S | [216,686,687] |
| 1-R-*n*-Cl *n* = 9,12; R = H, Me, Ph | S | [216] |
| 1-Me-2-R-*n*-Cl R = H, Me; *n* = 3, 9, 12 | H | [711] |
| 9-Cl | S | [73,688–691] |
| | B (comparison with 1,7- and 1,12-$C_2B_{10}H_{12}$ derivatives) | [692] |
| | H | [693] |
| | E (reduction) | [71–73] |
| | IR (C–H; H-bonding with solvents) | [55] |
| | IR (actual spectrum, C–H intensity) | [51] |
| | IR (actual spectrum) | [689] |
| | $^{35}$Cl NQR, polarity of B–Cl bond | [694] |
| | Dipole moment | [100], |
| | He photoelectron spectra | [695] |
| $H_2C_2B_{10}Me_8$-9-X-12-Y (X,Y = H, I, Cl) (FF) | S, X(H, I) | [268] |
| 9-Cl-12-I | S, MS | [696] |
| 10-Cl | $^{35}$Cl NQR | [287] |
| | H (C–H shift, coupling constants) | [17] |
| 1-Br-*n*-Cl *n* = 10, 12 | S | [683] |
| $RHC_2B_{10}Cl_nH_{10-n}$ R = H, Me, Ph; *n* = 1, 2, 3 (FF) | S (electrophilic halogenation) | [197] |
| 1-R-3-Cl R = H, Me | S | [347] |
| 1,2-$Cl_2$ | S | [681,697] |
| 9,10-$Cl_2$ | p$K_a$, metallation equilibrium constants | [90] |
| | S, IR (actual spectrum) | [689] |
| | H | [693] |

| Compound | Information | References |
|---|---|---|
| 9,12-$Cl_2$ | S | [691] |
| | IR (actual spectrum, C–H intensity) | [51] |
| | S, E (reduction) | [73] |
| | Dipole moment | [100], |
| 10,12-$Cl_2$ | H, B, IR (substituent effects) | [22] |
| | B | [29] |
| | E | [209] |
| | H (C–H shift, coupling constants) | [17] |
| | E ($pK_a$) | [210] |
| 1-Me-9,12-$Cl_2$ | IR (C–H intensity) | [51] |
| 1-CH═$CH_2$-9,12-$Cl_2$ | IR (C–H intensity) | [51] |
| 1-$CH_2$Cl-9,12-$X_2$ X = Cl, Br | $^{35}$Cl NQR (substituent electron transfer effect) | [698] |
| 1-R-10,12-$Cl_2$ R = Cl, $CH_2$Cl, CH═$CH_2$ | $^{35}$Cl NQR | [287] |
| 1-$CH_2$Cl-10,12-$Cl_2$/1-$CH_2$Cl-9,10,12-$Cl_3$ | E (reduction; comparison with 1,7- and 1,12-$C_2B_{10}H_{12}$ derivatives) | [185] |
| $H_2C_2B_{10}Cl_4H_6$ (FF) | S (radical halogenation) | [197] |
| 1-$CH_2$Cl-9,10,11,12-$Cl_4$ | E (reduction; comparison with 1,7- and 1,12-$C_2B_{10}H_{12}$ derivatives) | [185] |
| 1-R-9,10,11,12-$Cl_4$ R = H, Me, $CH_2$Cl | $^{35}$Cl NQR | [287] |
| 1-Me-2,9,10,11,12-$Cl_5$ | S | [683] |
| ($CH_2$Cl)$HC_2B_{10}H_5Cl_5$ (FF) | S (radical halogenation) | [197] |
| $MeHC_2B_{10}H_3Cl_7$ (FF) | S (radical halogenation) | [197] |
| 4,5,7,8,9,10,11,12-$Cl_8$ | X | [32,699] |
| $H_2C_2B_{10}H_2Cl_8$ (FF) | $^{35}$Cl NQR | [287] |
| $PhHC_2B_{10}H_2Cl_8$ (FF) | S (radical halogenation) | [197] |
| $H_2C_2B_{10}Cl_8Br_2$ (FF) | S, IR(actual spectrum) | [700] |
| $D_2C_2B_{10}Cl_{10}$ (FF) | S, IR(actual spectrum) | [700] |
| $RHC_2B_{10}Cl_{10}$·L R = H, Me, Et; L = $Me_2SO$, $Me_2NCHO$, $NEt_3$, THF | S, IR(actual spectrum) | [700] |
| $MeEtC_2B_{10}Cl_{10}$ (FF) | S, IR(actual spectrum) | [701] |
| $EtHC_2B_{10}Cl_{10}$ (FF) | S, IR(actual spectrum) | [701] |
| ($CH_2$CH═$CH_2$)$HC_2B_{10}Cl_{10}$ (FF) | S, IR | [701] |
| ($PhCH_2$)$RC_2B_{10}Cl_{10}$ R = H, $PHCH_2$ (FF) | S, IR | [701] |
| $H_2C_2B_{10}Cl_{10}$ (FF) | S (ClF) | [679] |
| (*m*-$C_6H_4F$)$HC_2B_{10}Cl_{10}$ (FF) | S, F | [283] |
| $PhHC_2B_{10}Cl_{10}$ (FF) | S (radical halogenation) | [197] |
| 1-R-$HC_2B_{10}Cl_{10}$·X R = Me, Et; X = $Et_3N$, $Me_3N$, pyridine (FF) | IR (C–H—N bonds) | [705] |
| **Bromo Derivatives** | | |
| 1-Br | S | [684] |
| | Dipole moment | [1342] |

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| Compound | Information | References |
|---|---|---|
| 1-Br-*n*-Cl *n*=10, 12 | S | [683] |
| 1-Br-2-Ph | S | [682] |
| 1-Br-2-R R=Me, Ph | S, IR (actual spectrum) | [685] |
| | S | [684] |
| | E (reduction) | [71] |
| B-Br | S (radical halogenation) | [197] |
| (+)-4-Br optical isomer | S, OR | [710] |
| 1-Me-2-R-*n*-Br R=H, Me; *n*=3, 9, 12 | H | [711] |
| 1-R-8-Br R=H, Me, Ph | S | [687] |
| 1-Ph-*n*-Br *n*=2, 12 | S, E (reduction) | [73] |
| *n*-Br *n*=8,9 | IR (actual spectrum) | [51] |
| 9-Br | S | [688, 689,728] |
| | S, E (reduction) | [73] |
| | IR (actual spectrum, C–H intensity) | [51] |
| | Dipole moment | [100], |
| 9-Br-12-Cl | S | [216] |
| *n*-Br *n*=3, 4, 8, 9 | S, IR, MS | [714] |
| 1,2-$Ph_2$-9-Br | S | [216] |
| 10-Br | H (C–H shift, coupling constants) | [17] |
| 12-Br | S | [715] |
| $Me_2C_2B_{10}Br_nH_{10-n}$ (FF) *n*=1, 2 | S | [133] |
| 9,10-$Br_2$ | S, IR (actual spectrum) | [689] |
| 9,12-$Br_2$ | S | [691] |
| | X | [717] |
| | dipole moment | [100,1139] |
| 10,12-$Br_2$ | S | [715] |
| | H (C–H shift, coupling constants) | [17] |
| | B | [29] |
| 1-R-8,*n*-$Br_2$ *n*=9,12; R=H, Me, Ph | S | [687] |
| 1-Me-8,9-$Br_2$ | IR (actual spectrum, C–H intensity) | [51] |
| 1-Me-8,*n*-$Br_2$ *n*=9,12 | S | [686] |
| 1-Me-8,9,12-$Br_3$ | S | [686] |
| 1,2-$Me_2$-8,9,10,12-$Br_4$ | X | [719] |
| **Iodo Derivatives** | | |
| 1-I | Dipole moment | [1342] |
| 1-I-2-R R=Me, Ph | S | [684] |
| 1-I-2-Ph | S | [682] |
| 1-Ph-*n*-I *n*=2, 12 | S, E (reduction) | [73] |
| 1-R-12-I R=CH=$CH_2$, Ph | S(large scale) | [1767] |

| Compound | Information | References |
|---|---|---|
| 3,8-$I_2$ | S, X, H, B, C, MS | [1606] |
| 1-C(O)OEt-8-I | S, X, H, B, C, MS | [1606] |
| 8,9,10,12-$I_4$ additive to radioopaque cement for vertebroplasty | S, IR(solid state), SCM, X-ray contrast spectroscopy | [1593] |
| 9-I | S, H, B, C | [1715] |
| 1-R-2-3-I R = *n*-$C_4H_9$, $SiMe_3$, OEt, $C_2H_4NMe_2$ | S, H, B, C, MS | |
| 3-$^{125}$I | S (radiolabeling via Pd-catalyzed isotopic exchange) | [721] |
| 3-I-6-Me | S, X, H, B, C, IR, MS | [140] |
| 1-Ph-3-$^{125}$I | S (radiolabeling via Pd-catalyzed isotopic exchange) | [721] |
| 1,2-$Ph_2$-3-$^{125}$I | S (radiolabeling via Pd-catalyzed isotopic exchange) | [721] |
| 1-R-8-I R = H, Me, Ph | S | [216,687] |
| 1-R-*n*-I *n* = 9,12; R = H, Me, Ph | S | [216] |
| 1-Me-2-R-*n*-I R = H, Me; *n* = 3, 9, 12 | H | [711] |
| 1,2-$I_2$ | S | [697] |
| 3,6,8,9,10,12-$I_6$ | S, H, B, IR, MS | [140] |
| 9-I | S, H, B, C, IR | [726] |
| | S | [691,715,727] |
| | Dipole moment | [100], |
| 1-Me-9/12-I | S, H, B, C, MS | [1902] |
| 9-I-12-Et | S, H, B | [174] |
| 9-$^{125}$I | S (radiolabeling via Pd-catalyzed isotopic exchange) | [721] |
| 2-R-12-X R = Ph, *p*-$C_6H_4Me$, C(O)OEt, $(CH_2)_5OTs$ X = $^{125}$I, $^{131}$I | S | [1877] |
| 1-Ph-9-I | X | [731] |
| RR′$C_2B_{10}H_9$-9-$I^{-\bullet}$ radical anions R, R′ = H, Me (FF) | MS (electron resonance capture mass spectra) | [115] |
| 9-$IR_2$ R = Cl, $O_2CCF_3$ | S | [732] |
| 9-$IPh^+$ $X^-$ X = I, $BF_4$ | S | [732] |
| 9-$IPh^+$ $X^-$ X = $BF_4$, Cl, I | $^{127}$I NQR quadrupole coupling | [734] |
| 10-I | $^{127}$I NQR | [735] |
| | H (C–H shift, coupling constants) | [17] |
| 1,2-$Ph_2$-9,12-$I_2$ | S, X, H, B, IR | [220] |
| 9,12-$I_2$ | S | [73,168,691,727] |
| | Dipole moment | [100,1440] |
| | ED | |
| 1-R-9,12-$I_2$ R = Me, Ph | S, X(Me), H, B, C, MS | [1902] |
| 1-I-2-R R = Me, Ph | E (reduction) | [71] |
| 3,6,9/3,9,12-$I_3$ | S(regioselective, via electrophilic iodination and deboronation/reconstruction of carborane cage), H, B, MS | [722] |

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| Compound | Information | References |
|---|---|---|
| 1-Me-8,9,10,12-$I_4$ | X (C—H···I—B intermolecular interactions; designed crystal lattices) | [730] |
| 1-R-8,9,10,12-$I_4$ R = H, Me, Ph | S(direct reaction with $I_2$ without solvent), X(H, Ph) | [737] |
| 1-Ph$C_6H_4$-8,9,10,12-$I_4$ | S, X, H, B, C, MS | [1902] |
| **Exo-Polyhedral Main-Group Metal and Metalloid Element Derivatives** | | |
| *Lithium* | | |
| {1-$Me_2Si[C_5Me_4]$-2-Li(THF)$C_2B_{10}H_{10}$}$_2Li^-\cdot$Li(THF)$_4\cdot THF^+$ (FF) | S, X, H, B, C, IR | [741] |
| *Magnesium and calcium* | | |
| 1-R-2-MgI R = H, Me Grignards | S | [125,745] |
| 1-R-2-MM = Li, K, Na, Ca | S | [188] |
| *Boron, aluminum, gallium, and indium* | | |
| 1-$BO_3$[N=CMe-CMe=N$(NH_2)$]$_3Fe^{II}$ semiclathrochelate | S, B, MS | [746] |
| 1-oxime-hydrazonate clathrochelate $Fe^{II}$ complexes | S, H, B, C, MS, Mössbauer | [746] |
| 1-*nido*-$BC_4Et_4BI$ | S, X, H, B, C, MS | [747] |
| 1-B[N$(CHMe_2)$Cl] | S, X, H, B, C, MS | [1712] |
| 1,2-[B$(NR_2)$Cl]$_2$ R=$CHMe_2$, Et | S, X, H, B, C, MS | [1712] |
| 1-$CHMe_2$-2-$BX_2$ X = Cl, OMe, chloropinacolatoborane, $C_6F_5$, $C_6H_{13}$, CH=CHPh | S, X(Cl, OMe, $C_6F_5$), H, B, C, IR, MS | [1882] |
| O[B$(OC_6F_5)$B—$CB_{10}H_{10}$—$CHMe_2]_2$ (FF) | S, X, H, B, C, IR, MS | [1882] |
| 1,2-*cyclo*-$MX_2PMe_2CH_2$ M = Al, Ga, In; X = Cl, Br | S, H, C, P, Al | [752] |
| X$M[Me_2PCH_2$-$C_2B_{10}H_{10}]_2$ (M—P) M = Al, Ga, In; X = Cl, Br (FF) | S, X(Ga, In), H, C, P, Al | [752] |
| 1,2-*cyclo*-$X_2GaPMe_2CH_2$ X = Cl, Me | S, X(Me), H, C, P | [752] |
| Me$Ga[Me_2PCH_2$-$C_2B_{10}H_{10}]_2$ (M—P) (FF) | S, H, C, P | [752] |
| 1-Ph-2-$AlEt_2\cdot Me_2NCH_2CH_2NMe_2$ M = Ga, In | S | [753] |
| 1-GaMeCl-2-Ph | S | [753] |
| 1-Ph-2-$MMe_2\cdot Me_2NCH_2CH_2NMe_2$ M = Al, Ga | S | [753] |
| 1-$Me_2NCH_2$-$C_2B_{10}H_{11}\cdot GaCl_3$ (FF) | S, X, H, B, C, IR, MS | [754] |
| 1-$(C_5H_5N)GaCl_2NMe_2CH_2$ | S, X, H, B, C, IR, MS | [754] |
| [1-$Me_2NCH_2$-$C_2B_{10}H_{10}]_2GaCl\cdot OH_2$ (FF) | S, X, H, B, C, IR, MS | [754] |
| *Thallium* | | |
| 1-R-2-R′-9-Tl$(SCN)_2$ R, R′ = H, Me | S | [755] |
| 1,2-$Me_2$-9-Tl$[OC(O)CF_3]_2$ | S | [756] |
| 1-TlCl$C_4H_9$Cl-2-R R = H, Ph | S | [758] |
| 1,2-RR′-B-Tl$[OC(O)CF_3]$ R, R′ = H, Me, Ph | S | [759] |
| *n*-TlCl *n* = 1, 9 | Raman | [760] |
| B-$TlX_2$ X = Cl, Br | S, IR, Raman | [761] |
| 9-Tl$[OC(O)CF_3]_2$ | S | [756,762,763] |

| Compound | Information | References |
|---|---|---|
| 9-Tl[OC(O)$CF_3$]-1-(1,2-Ph$C_2B_{10}H_{10}$)] (FF) | S | [756] |
| Tl$Cl(1\text{-}C_2B_{10}H_{11})_2$ (FF) | S, IR, Raman | [761] |
| $Tl[OC(O)O]_2^{2+}[1,2-Me_2C_2B_{10}H_9]_2^{2-}$ (FF) | S | [1322] |
| Br$Tl(CH_2—CB_{10}H_{10}CH)_2$ (FF) | S | [742] |
| ***Silicon*** | | |
| 1,2-*cyclo*-[—$Me_2$Si-CPh=CH($SiMe_2$)$_2$—] | S, X, H, C, P, Si, IR | [768] |
| 1-$SiMe_2SiMe_2$OEt | S, H, B, C | [767] |
| 1-$SiMe_2$H-2-$SiMe_2$OEt | S, H, B, C | [767] |
| 1,2-$(SiMe_2H)_2$ | S | [770] |
| 1-$SiMe_3$-2-Me | S, H, IR, MS | [771] |
| 1-SiPh[$SiMe_3$]$_2$ | S, H, IR, MS | [771] |
| 1-$SiR_3$ R = Me, Ph | S | [364] |
| 1-Si($CMe_3$)$Me_2$-9,12-$R_2$ R = H, Me | S, H, B, C, MS | [266] |
| {1-$Me_2$Si[$C_5Me_4$]-2-Li(THF)$C_2B_{10}H_{10}$}$_2$$Li^-$·Li$(THF)_4$·$THF^+$ (FF) | S, X, H, B, C, IR | [741] |
| $Me_2$($CMe_3$)Si—$CB_{10}H_8$(9,12-$R_2$)C—$(CH_2)_3$—$CB_{10}H_8$(9,12-$R_2$)C—Si($CMe_3$)$Me_2$ R = H, Me (FF) | S, H, B, C, MS | [266] |
| 1-[$SiMe_2CMe_3$]-9,12-$(C_6H_4R)_2$ R = H, OMe | S, H, B, C, MS | [240] |
| {1-[$SiMe_2CMe_3$]-$C_2B_{10}H_8$-9,12-$(C_6H_4R)_2$-2-}$_2$R′ R = H, OMe; R′ = $(CH_2)_n$, $n$ = 1–4, $(C_6H_4)_2$, $C_5H_3Me_2$ (FF) | S, H, B, C, MS | [240] |
| 1-$SiMe_2CMe_3$-2-R R = H, $n$-$C_4H_9$, $CH_2Ph$, $CH_2CH$=$CH_2$, $CH_2CH_2CH$=$CH_2$, $(CH_2)_3OH$, *o*-tolyl-1-1,2-$C_2B_{10}H_{11}$, CH[$CH_2Ph$]–$CH_2$-1-1,2-$C_2B_{10}H_{11}$, $(CH_2)_3C_2B_{10}H_{11}$ (FF) | S, H, B, C, IR, MS | [149] |
| μ-TosN$(CH_2CH_2)_2$-(1,2-R$C_2B_{10}H_{10}$)$_2$ R = H, $SiMe_2CMe_3$ (FF) | S, H, B, C, IR, MS | [775] |
| 1-$SiMe_2CMe_3$ | S | [776] |
| 1-$SiMe_2CMe_3$-2-Ph | S, X | [777] |
| 1-$Me_2$SiH-2-$PR_2$ R = Me, OEt, Ph | S, H, C, P | [584] |
| 1-$SiMe_2$[5′-2,3-$(Me_3Si)_2C_2B_4H_5$]-2-R) R = Me, Ph | S, H, B, C, IR | [1506] |
| 1-$SiMe_2$(σ-$C_5H_5$) | S, H, B, IR | [778,779] |
| 1-$SiMe_2$NHR-2-R′ R = H, 2,6-$(Me_2CH)_2C_6H_3$; R′ = Ph, $CMe_3$ | S, H, X[H, $(Me_2CH)_2C_6H_3$], B, C, IR | [780] |
| [1-$Me_2$(σ-$C_5H_4$)Si—$C_2B_{10}H_{11}$]$NdCl_2$·3THF (FF) | S, X | [779] |
| [1-$Me_2$(σ-$C_5H_4$)Si—$C_2B_{10}H_{10}$]NdCl·2THF (FF) | S, X | [779] |
| [1-$Me_2$(σ-$C_5H_4$)Si—$C_2B_{10}H_{10}$]$_2$$Nd^-$ $Li(THF)_4^+$ (FF) | S, X | [779] |
| 1,2-($R_2$P)-$CB_{10}H_{10}$C–($Me_2Si$)$_2$-$CB_{10}H_{10}$C–$PR_2$ R = Me, OEt, Ph (FF) | S, H, C, P | [584] |
| 1-$(CH_2)_n$$SiMe_3$ $n$ = 0,1 | S | [782] |

*Continued*

| Compound | Information | References |
|---|---|---|
| 1-$CH_2SiMe_3$ | S | [364,783] |
| 1-Me-2-$(CH_2)_2C{\equiv}C{-}SiMe_2CMe_2CHMe_2$ | S (lithium iodide catalyzed alkylation) | [139] |
| 1,2-$[(CH_2)_2SiCl_3]_2$ | S, H, B, C, Si | [319] |
| 1-$CH_2SiPh_2Cl$ | S | [364] |
| {1-$[Me_3SiO]_2SiCH_2$-1,2-$C_2B_{10}H_{10}\}_2O$ (FF) | X | [784] |
| 1-$CH{=}CH_2$-2-$SiMe(OMe)_2$ | S | [317] |
| 1,2-$[Me_2SiOSiMe_2(OBu)]_2$ | S | [770] |
| 1-R-2-$Si(CH{=}CH_2)_3$ R = $Si(CH{=}CH_2)_3$, Me, Ph dendrons | S, X, H, B, C, Si | [786] |
| 1-$(CH_2)_3SiMe_2Cl$-2-R R = Me, Ph | S, H, B, C, Si, IR, MS | [294] |
| 1-$(CH_2)_3SiMe_2CH{=}CH_2$-2-R R = Me, Ph | S, H, B, C, Si, IR, MS | [294] |
| $Si[(CH_2)_2SiMe_2(CH_2)_3{-}CB_{10}H_{10}CR]_4$ R = Me, Ph dendrimers (FF) | S, H, B, C, Si, IR, MS | [294] |
| 1-$C{\equiv}CSiMe_3$-2-$Si(CMe_3)Me_2$ | S, H, B, C, IR, MS | [159] |
| 1-{$[SiMe_2O]_2Si(CH_2)_3$}-2-Me | S, H | [787] |
| 1-R-2-$CH_2SiMe_2OMe$ R = H, $CH_2SiMe_2OMe$ | S | [788] |
| 1-R-2-R′ R = $CH_2SiMe_n(OEt)_{3-n}$ $n$ = 0–2, $CH_2SiMe_2(OMe)$; R′ = H, Ph | S | [789] |
| 1,2-$[CH_2SiMe_2(OMe)]_2$ | S | [789] |
| $p$-$C_6H_4\{[(MeO)SiMe_2CH_2{-}CB_{10}H_{10}C]$-1-$\}_2$ (FF) | S | [789] |
| 1-$(CH_2)_3SiMeCl_2$-2-R R = Me, Ph | S, H, B, C, IR, MS | [791] |
| Vinyl-terminated carboranyl siloxane | Structural relaxation dispersion | [1804] |
| *Cyclo*-[$-SiMe_2-CB_{10}H_{10}C-X-CB_{10}H_{10}C-$] (X = PPh, $SnMe_2$, $GeMe_2$, AsMe) (FF) | S | [792] |
| 1-$SiHEt_2$-2-$SiPhEt_2$ | S, H, C, Si, MS | [794] |
| 1,2-*cyclo*-($-Et_2SiCR'{=}CRSiEt_2-$) R, R′ = H, Ph, C(O)OMe, $n$-$C_4H_9$ | S, H (H, Ph), C, Si, MS | [794] |
| 1,2-*cyclo*[$-CH(CH{=}CHPh)-O-SiEt_2-O-CH(CH{=}CHPh)-$] | S, X, H, C, Si, MS | [794] |
| 1,2-*cyclo*-[$-CH_2$-O-$SiMe_2$-O-$CH_2-$] | S | [783] |
| *Cyclo*-[$-CH_2-CB_{10}H_{10}C-SiR_2-CB_{10}H_{10}C-$] R = Me, Et (FF) | S | [795] |
| *Cyclo*-[$-SiMe_2$-$CB_{10}H_{10}C-(CH_2)_2-CB_{10}H_{10}C-$] (FF) | S | [601] |
| 1,2-*cyclo*-($SiMe_2-CHR-O-SiMe_2$) R = $CHMe_2$, $(CH_2)_4Me$, Ph, $CMe_3$, norbornene, $p$-$C_6H_4$-CN | S, X($p$-$C_6H_4$-CN), H, C, Si, IR, MS | [797] |
| 1,2-*cyclo*-[$Me_2Si-RC{=}CR'-SiMe_2$] R, R′ = Ph, H, Et, Me, C(O)OMe | S, X(Ph), MS | [315] |
| 1,2-*cyclo*-{$Me_2SiO-PhC{=}CPh-OSiMe_2$} | S, H, C, Si, MS | [315] |
| *Cyclo*-[$-Me_2Si-CB_{10}H_{10}C-SiMe_2-NC{=}CHCH{=}CN-Me_2Si-CB_{10}H_{10}C-SiMe_2-NC{=}CHCH{=}CN-]_2$ (FF) | S, X, H, C, Si, MS | [315] |
| 1-$SiMe_2OH$-2-$SiMe_2CHPhCH_2C(O)Me$ | S, X, H, C, Si, IR, MS | [797] |
| [1-Me-1,2-$C_2B_{10}H_{10}]_2$[*cyclo*-$SiMe(CH_2)_3$] (FF) | S | [1458] |

| Compound | Information | References |
|---|---|---|
| $Cl_2Si(PhC_2B_{10}H_{10})_2$ (FF) | IR (detailed assignments) | [1320] |
| $Me_2Si(CB_{10}H_{10}CLi)_2$ (FF) | S | [798] |
| $C_{13}H_6Br_2$-9,9′-[$(CH_2)_3$-$CB_{10}H_{10}C$-$SiMe_2CMe_3$]$_2$ $C_{13}H_6Br_2$ = dibromofluorene (FF) | S, H, C, MS | [799] |
| 1,2-[2′-(7′-bromo-9′,9″-dihexylfluorenyl)]$_2$ | S, H, C, IR, DSC, fluorescence | [800] |
| {1,2-[2′-(9′,9″-dihexylfluorenyl)$C_2B_{10}H_{10}$]$_2$}$_2$ dimer (FF) | S, H, C, IR, DSC, fluorescence | [800] |
| 1-$SiMe_2C_9H_5(CH_2)_2OMe$·Li$(OEt)_2$-2-R R = H, Li$(OEt)_2$ indenyl | S, H, B, C, IR | [801] |
| 1,2-[$SiMe_2(C_9H_7$} ($C_9H_7$ = indenyl) | S, H, B, C, IR, MS | [802] |
| $Sm[(\eta^5-C_9H_6-SiMe_2-C_2B_{10}H_{10})]_2^-$ (FF) | S, X, H, B, C, IR | [802] |
| $(THF)_3Yb[(\eta^5$-$C_9H_6$-$SiMe_2)C_2B_{10}H_{10}]$ (FF) | S, X, H, B, C, IR | [802] |
| $(THF)_2Yb(C_5H_4$-$SiMe_2$-$C_2B_{10}H_{11})_2$ (FF) | S, X, H, B, C, IR | [1477] |
| 1-$SiMe_2C_9H_5(CH_2)_2NMe_2$·$LiOEt_2$-2-R R = H, $LiOEt_2$ | S, H, B, C, IR | [803] |
| —[$Si(CH_2)_3$-$CB_{10}H_{10}C$–$(CH_2)_3$-Si(-L-)$_3$]*n*- L = O, NCN hybrid polymers; gels (FF) | S, C, IR, x-ray powder diffraction, TEM | [319] |
| B-$CH_2CH_2SiMe_3$, B,B′-$(CH_2CH_2SiMe_3)_2$ | MS (detailed) | [1317] |
| *n*-$CH_2CH_2SiCl_3$ *n* = 1, B | MS (fragmentation patterns) | [715] |
| B-$CH_2CH_2SiR_3$ R = Cl, Me | S | [462] |
| B,B′-$(CH_2CH_2SiR_3)_2$ R = Cl, Me | S | [462] |
| B-$CH_2SiCl_3$, B-$CH_2CH_2SiR_3$, B,B′-$(CH_2CH_2SiR_3)_2$ R = Me, Cl | IR (detailed analysis); inductive effect | [805] |
| 1,2-$(SnMe_3)_2$-B,B′-$(CH_2CH_2SiR_3)_2$ | IR (detailed analysis); inductive effect | [805] |
| —[$CB_{10}H_{10}C$—*m*-$C_6H_4$—C≡C-SiMeR]$_x$—[C≡C—*m*-$C_6H_4$-C≡C—SiMeR]$_y$—polymers with side groups on main chain R = H, Me,CH=$CH_2$ | S, H, C, IR, TGA, DSC, viscosity | [1613] |
| 1,2-$R_2$ R = $SiMe_3$, $SiMe_2Cl$ | S, X, H, B, C, Si | [1626] |
| 1,2-*cyclo*-($Me_2S$—$SiMe_2$) | S, X, H, B, C, Si | [1626] |
| 1,2-*cyclo*-($Me_2S$—O—$SiMe_2$) | S, X, H, B, C, Si | [1626] |
| 1-SiH[$(CHMe_2)_2N_2CPh]_2$ 6-coordinate silicon complex | S, H, B, C, Si, N | [1819] |
| ***Germanium*** | | |
| 1-$HgGeEt_3$-2-R R = H, Me, $CH_2Cl$, Ph | S | [807] |
| 1-$(CH_2)_n GeMe_3$ *n* = 0,1 | S | [782] |
| 1-$CH_2GeMe_3$ | C (detailed assignments) | [43] |
| 1-$GeEt_3$-2-R R = H, $CHMe_2$, Ph | | [1448] |
| μ(1,2)-{MeO-$C_6H_4$-$CH_2CH[GeMe_2]_2$} | S, X, H, C | [990] |
| $Cl_2Ge(PhC_2B_{10}H_{10})_2$ (FF) | IR (detailed assignments) | [1320] |
| $Me_2Ge(C_2B_{10}H_{11})_2$ (FF) | X | [810] |
| *Cyclo*-$[GeMe_2]_2(C_2B_{10}H_{10})_2$ (FF) | S, X, H, C, MS | [809] |

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| Compound | Information | References |
|---|---|---|
| $Ge[1,2\text{-}(CH_2)_2C_2B_{10}H_{10}]_2$ (FF) | S | [743] |
| *Cyclo*-[—$CH_2$-$CB_{10}H_{10}C$–$GeR_2$-$CB_{10}H_{10}C$—] R = Me, Et (FF) | S | [795] |
| *Cyclo*-[—$GeMe_2$—$CB_{10}H_{10}C$—$(CH_2)_2$—$CB_{10}H_{10}C$—] (FF) | S | [601] |
| *Cyclo*-[—PhP—$CB_{10}H_{10}C$—$GeMe_2$—$CB_{10}H_{10}C$—] (FF) | X | [811] |
| *Cyclo*-[—$GeMe_2$—$CB_{10}H_{10}C$—X—$CB_{10}H_{10}C$—] (X = PPh, $SnMe_2$, $GeMe_2$, AsMe) (FF) | S | [792] |
| *Cyclo*-[—CH(O)Me—$CB_{10}H_{10}C$—$GeMe_2$—$CB_{10}H_{10}C$—] (FF) | S | [602] |
| ***Tin*** | | |
| 1-R-2-R′ R = H, $SnEt_3$, CH=$CH_2$, CMe=$CH_2$, Sn(*n*-$C_4H_9)_3$, $SnMe_3$; R′ = $SnMe_3$, $SnEt_3$, (*n*-$C_4H_9)_3$ | S, IR | [813] |
| 1-$SnR_3$ R = Et, *n*-$C_4H_9$ | S | [815] |
| 1-(*n*-$C_3H_7)_3$Sn | S | [575] |
| 1-$SnPh_3$-2-Ph | S | [555,575,684,772] |
| 1-$SnMe_3$-2-(2′-$NC_5H_4$) | S, X, H, B, C, Sn, IR | [618] |
| 1,2-$[SnMe_2X]_2$ X = H, Br | S, H, C, MS | [809] |
| 1,2-[μ-$SnMe_2]_3$ | S, X, H, C, Sn, MS | [809] |
| 1-$(CH_2)_n SnMe_3$ *n* = 0,1 | S | [782] |
| 1-$CH_2SnMe_3$ | X | [817] |
| | C (detailed assignments) | [43] |
| 1-CHR—$CH_2$—SnR′$_3$ R = H, Me; R′ = Et, *n*-$C_4H_9$, Ph | S | [818] |
| RSn($CH_2$-CHR′-1,2-$C_2B_{10}H_{11})_2$ R = H, Me; R′ = Et, *n*-$C_4H_9$, Ph (FF) | S | [818] |
| *Cyclo*-[—CHMe$CH_2$—Sn(*n*-$C_4H_9)_2$—$CH_2CH_2$—] | S | [818] |
| 1-(cyclo-C=N-CHR*CH2-O—)-2-$SnMe_2X$ (N → Sn) R=$CHMe_2$, $CMe_3$; X = Cl, Br oxazolinyl, chiral | S, X($CHMe_2$, Br), H, B, C, IR, MS | [529] |
| 1-CHR*OMe-2-$SnMe_2Br$ (O → Sn) R = H, Ph | S, X(H, Br), H, B, C, IR, MS | [529] |
| (*n*-$C_4H_9)_2$Sn($PhC_2B_{10}H_{10})_2$ (FF) | S | [819] |
| $Ph_3Sn(C_2B_{10}H_{11})$ (FF) | S | [819] |
| XSn($PhC_2B_{10}H_{10})_2$ X = O, $Br_2$ (FF) | S | [819] |
| Sn{$CB_{10}H_{10}C$—C($NHCMe_2$)=$NCMe_2$}$_2$ (2N → Sn) (FF) | S, X, H, B, C | [1531] |
| $[Me_2NCH_2CB_{10}H_{10}C]_2Sn_2Me_4$ (FF) | S, X, H, B, C, Sn, IR, MS | [820] |
| $ClSn(PhC_2B_{10}H_{10})_3$ (FF) | S | [575] |
| $Br_2Sn(PhC_2B_{10}H_{10})_2$ (FF) | S | [575] |
| $Me_2Sn[9\text{-}1,2\text{-}Me_2C_2B_{10}H_9]_2$ (FF) | S, X | [821] |
| $Cl_2Sn[9\text{-}1,2\text{-}Me_2C_2B_{10}H_9]_2$ R = H, Me (FF) | S | [822] |
| *Cyclo*-[—$CH_2$—$CB_{10}H_{10}C$—$SnR_2$—$CB_{10}H_{10}C$—] R = Me, Et (FF) | S | [795] |

| Compound | Information | References |
|---|---|---|
| *Cyclo*-[—$MMe_2$—$CB_{10}H_{10}C$—$SnMe_2$—$CB_{10}H_{10}C$—] M = Si, Ge (FF) | S | [792] |
| *Cyclo*-[—(MeO)—C—$CB_{10}H_{10}C$—$SnMe_2$—$CB_{10}H_{10}C$—] (FF) | S | [602] |
| 1-[$(CH_2)_nC(O)O^-$ $SnMe_3^+$]-2-R $n$ = 0, 1; R = Me, Ph | Mössbauer, p$K_a$, E (half-neutralization potential) | [423] |
| $(Me_3Si)_2N$—Sn—$P(CB_{10}H_{10}CH)_2$ | S, X, H, P | [1620] |
| 1-Me-2-$SnMe_2$-$C_6H_3(OCH_2CMe_3)_2$ | S, X, H, B, C, Sn | [1708] |
| $[(Ph_2P)(Me_2Sn)C_2B_{10}H_{10}]_2Pd$ (FF) | S, X, H, C, P, Sn | [824] |
| μ-$(Ph_3PClPd)$-$(Ph_2P)[Me_2Sn]C_2B_{10}H_{10}$ (FF) | S, X, H, C, P | [824] |
| 9-Sn{CH[$MeC(O)O]_2$}$_2$Me | S | [826,827] |
| 9-HgSn{CH[$MeC(O)O]_2$}$_2$Me | S | [826] |
| 9-[HgSn{CH[$MeC(O)O]_2$}$_2$-9-(1,2-$C_2B_{10}H_{11}$)] (FF) | S | [827] |
| ***Arsenic*** | | |
| 1-R-2-$CHMe_2$ R = $As(NEt_2)_2$, $AsCl_2$, AsO | S | [830] |
| 1-$CH_2AsMe_2$ | S | [742] |
| 1,2-*cyclo*-[—MeAs—$CB_{10}H_{10}C$—AsMe—] (FF) | S | [50] |
| *Cyclo*-[—$CH_2$—$CB_{10}H_{10}C$—AsR—$CB_{10}H_{10}C$—] R = Me, Et (FF) | S | [795] |
| *Cyclo*-[—MeAs—$CB_{10}H_{10}C$—$CB_{10}H_{10}C$—] (FF) | S | [601] |
| *Cyclo*-[—X—$CB_{10}H_{10}C$—$CB_{10}H_{10}C$—] X = PhP, MeAs (FF) | S | [601] |
| *Cyclo*-[—MeAs—$CB_{10}H_{10}C$—$(CH_2)_2$—$CB_{10}H_{10}C$—] (FF) | S | [601] |
| *Cyclo*-[—CH(O)Me—$CB_{10}H_{10}C$—AsMe—$CB_{10}H_{10}C$—] (FF) | S | [602] |
| ***Antimony*** | | |
| $Sb(PhC_2B_{10}H_{10})_3$ (FF) | S | [575] |
| 1-C(O)$OSbPh_4$-2-R R = H, C(O)$OSbPh_4$ | S, X, H, IR | [1921] |
| ***Selenium*** | | |
| 1-$Se(CH_2)_2SP(O)R'_2$ R′ = $OC_2H$, Ph | S, P | [837] |
| | S, MS | [842] |
| *Cyclo*-$[Se_2(C_2B_{10}H_{10})_2]_2 \cdot C_6D_6$ (FF) | S, H, B, C, Se | [843] |
| | X | [843,1352] |
| 1,2-*cyclo*-{SeCH[$(C_5H_4)$FeCp]=CHSe} | S, X, H, B, C, IR, MS | [646] |
| 1,2-*cyclo*-[SeC($CO_2$Me)=C($CO_2$Me)CoCpSe] | S, H, B, C, IR, MS | [646] |
| 1,2-*cyclo*-(—Se—$CPh_2$—Se—) | S, X, H, B, C, Se | [844] |
| 1,2-*cyclo*-(—$Se_2$—$SiPh_2$—) | S, H, B, C, Si, Se | [844] |
| 1,2-*cyclo*-{Se[$Pt(PPh_3)_2$]$SnR_2$Se} R = Me, Ph | S, H, B, C, Se, Sn, Pt | [844] |
| 1,2-*cyclo*-[$SePt(PPh_3)_2$Se] | S, H, B, C, Se, Pt | [844] |

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| Compound | Information | References |
|---|---|---|
| 1,2-*cyclo*-(SePPhSe) | S, X, H, B, C, P, Se | [845] |
| 1,2-[*cyclo*-PhP(═Se)—Se—P(═Se)Ph] | X | [1353] |
| 1-SeP(═Se)PhOH | S, X, H, B, C, P, Se | [845] |
| $(Ph_3P)_2Pt(\mu\text{-}Se)_2C_2B_{10}H_{10}$ (FF) | S, Se, Pt, H, B, C | [843] |
| 1-Me-2-SeAu($PPh_3$) (FF) | S, X, H, B, C, P, IR | [838] |
| $Se_2(1\text{-}RC_2B_{10}H_{10})_2$ R = H, Me, *n*-$C_3H_7$, Ph, $Me_2CH$ (FF) | S | [846] |
| $B_2\left[(\mu-Se)_2C_2B_{10}H_{10}\right]_3^{2-}$ (FF) | S, X, MS | [662] |
| *1,2-cyclo*-[Se-Co{$C_5H_3[CMe_3]_2$}-Se] | S, X, H, IR | [847] |
| 1,2-*cyclo*-[—Se-BH(py)-Se—] | S, H, B | [1522] |
| 1,2-*cyclo*-[—Se-BX-Se—] X = Cl, Br | S, H, B | [1522] |
| 1,2-*cyclo*-[—Se-BX($SeMe_2$)$_n$-Se—] X = Cl, Br | S, H, B | [1522] |
| 1,2-*cyclo*-[—Se-BR-Se—] X = bicycloheptyl, $(CH_2)_2SiMe_2Ph$, α-vinylpyridyl | S, H, B | [1522] |
| 1,2-*cyclo*-[—Se-$SnMe_2$-Se—] | S, H, B | [1522] |
| 1,2-*cyclo*-[—Se-Pt($PPh_3$)$_2$-Se—] | S, H, B | [1522] |
| 1,2-*cyclo*-[—Se-AlHR-Se—] R = $SMe_2$, $NHMe_2$ | S, H, B | [1522] |
| 1,2-*cyclo*-[$SeRh_2(C_8H_{12})_2Se$] | S, X, H, B, C, IR | [663] |
| 1,2-*cyclo*-{$HB[C_3HMe_2]N_2$]Mo(O)$Se_2$] | S, X, IR | [668] |
| [1,2-{*cyclo*-SRu[$MeC_6H_4CHMe_2$]S}$C_2B_{10}H_{10}$]$_2$Mo(CO)$_2$[1,2-{*cyclo*-SRu(CO)$_3$S}$C_2B_{10}H_{10}$] (FF) | S, X, H, B, C, IR | [669] |
| [(1,2-*cyclo*-Se-RhCp*-Se)$C_2B_{10}H_{10}$]$_2$Mo(μ-CO)$_2$ E = S, Se (FF) | S, X, H, B, C, IR | [672] |
| M{[μ-Se(*n*-$C_4H_9$)Cp*Rh](μ-Se)$_2C_2B_{10}H_{10}$}$_2$ M = Ni, Pd (FF) | S, X, H, B, C, IR | [850] |
| 1-$SeC_{10}H_6$R-2-R′ R = H, R′ = Me, Ph; R = SePh, R′ = Me naphthyl selenides | S, X(R = H), H, B, C, Se, IR, MS, E(R′ = Me) | [1571] |
| *Spirocyclo*-$\left[B(1,2-Se_2C_2B_{10}H_{10})\right]_2^-$ (FF) | S, X, H, B, C, Se | [1575] |
| 1-P(═Se)($CHMe_2$)$_2$ 1-P(═E)$Ph_2$-2-R R = Me, Ph E = S, Se | S, H, B, C, P, IR | [1574] |
| 1,2-*cyclo* –SeCoCpC[$CH_2$ → B(3)]-[C(O)($C_5H_4$)FeCp]Se | S, X, H, B, C, IR, MS | [1582] |
| 1,2-*cyclo* –SeC[$CH_2$ → B(3)][C(O)-($C_5H_4$)FeCp]Se | S, X, H, B, C, IR, MS | [1582] |
| LM(Se—$CB_{10}H_{10}CPh)_2$ L = $Me_2P(CH_2)_nPMe_2$, *n* = 1–3; M = Pd, Pt (FF) | S, X(*n* = 1, Pt), H, P, Se, Pt | [1602] |
| 1,2-*cyclo*-SePXSe—X = Cl, Br, I | S, H, B, C, P, Se | [1619] |
| 1,2-(Se-*cyclo*-$PSe_2$-$C_2B_{10}H_{10}$)$_2$ (FF) | S, H, B, C, P, Se | [1619] |
| 1,2-*cyclo*-SeC($CMe_3$)═CH—BCl—Se— | S, H, B, C, Se | [1640] |
| 1,2-cyclo-SeCEt═CEt—BX—Se— X = Cl, Br, I, Ph | S, H, B, C, Se | [1640] |
| 1,2-*cyclo*-SeCPh═CEt—BCl—Se— | S, H, B, C, Se | [1640] |
| 1,2-*cyclo*-SeCPh═CEt—BCl—CEt═CPh—Se— | S, H, B, C, Se | [1640] |
| [1,2-*cyclo*-SeCR═CEt—B—CEt═CR—Se—]$_2$ B—O R = Et, Ph | S, H, B, C, Se | [1640] |

| Compound | Information | References |
|---|---|---|
| 1,2-*cyclo*-SeCR═CEt—B(OH)—CEt═CR—Se—R = Et, Ph | S, H, B, C, Se | [1640] |
| 1,3-*cyclo*-[MCp*NR═C(NHR)]-1,2-$C_2B_{10}H_9$-μ(C, M)-Se R = $CHMe_2$, *cyclo*-$C_6H_{13}$ M = Ir, Ru (FF) | S, X(Ir, $CHMe_2$, *n*-$C_6H_{13}$; Ru, *cyclo*-$C_6H_{13}$), H, B, C, IR | [1652] |
| $CpCo(\mu\text{-}Se)_2C_2B_{10}H_9$-3-$CH_2C(O)C_4H_3O$ (FF) | S, X, H, B, C, IR, MS | [1705] |
| 1,2-*cyclo*-SeP(R)(Se)PhSe R = $CHMe_2$, OEt | S, X(OEt), H, B, C, P, Se | [1711] |
| 1,2-*cyclo*-$Se_2P(Se)PhSe_2$ (2 isomers) | S, X, H, B, C, P, Se | [1711] |
| 1,2-*cyclo*-$Se_2P(Se)(CHMe_2)Se_2$ | S, X, H, B, C, P, Se | [1711] |
| 1,2-*cyclo*-S—P(Se)($CMe_3$)—S | S, H, B, C, P, Si, MS | [1744] |
| 1,2-cyclo-$SeRu_2(MeC_6H_4CHMe_2)$ | S, X, H, B, C, IR, MS | [1771] |
| 1,2-cyclo-SeRu(Me $C_6H_4CHMe_2$){RC═C-[C(O)-OMe]}Se Se→Ru | S, X(H), H, B, C, IR, MS | [1771] |
| 1,2-*cyclo*-$Se_2P(═Se)CH_2C_6H_3Me_2$ | S, H, B, C, P, Se | [1751] |
| $(CH_2)_n[P(\mu\text{-}S)_2C_2B_{10}H_{10}]_2$ (FF) | S, X(*n* = 1), H, B, C, P, Se | [1751] |
| $(H_{10}B_{10}C_2)[\mu\text{-}SeP(R)Se]_2(C_2B_{10}H_{10})$ R═$CHMe_2$, *cyclo*-$C_6H_{11}$, $CMe_3$ (FF) | S, X($CMe_3$), H, B, C, P, Se | |
| 9-$SeP(OEt)_2$ selenophosphite | S | [613] |
| 9,12-*cyclo*-[-Se-CRR′-Se-] R = H, Me; R′ = Ph, Me | S | [659] |
| 9-SeP(X)$(OR)_2$ X = O, S, Se; R = Et, $C_4H_9$ | S, P | [837] |
| ***Tellurium*** | | |
| 9-$TeX_3$ X = Cl, Br | S | [852] |
| $HCB_{10}H_{10}C$—Te—Te—$CB_{10}H_{10}CH$ (FF) | S, X, MS | [853] |
| *Cyclo*-[—$CB_{10}H_{10}C$—Te—Te—$CB_{10}H_{10}C$—$SnMe_2$—] (FF) | S, X, C, Sn, Te, MS | [853] |
| 1,2-*cyclo*-{HB[$HMe_2C_3N_2$}$_3$Mo(O)$Te_2$] | S, IR | [668] |
| $(\mu\text{-}Te_2)_2(C_2B_{10}H_{11})_2$ (FF) | S, H, B,Te | [1663] |
| 1,2-*cyclo*-($SiMe_2$-Te-$SiMe_2$) | S, X, H, B, C, Te, MS | [1663] |
| 1,2-cyclo-TeP(R)P(R) R═$CHMe_2$, $CMe_3$, Ph | S, H, B, C, P, Te | [1751] |
| 1,2-*cyclo*-P($CHMe_2$)TeP($CHMe_2$) | S, H, B, C, P, Te | [1751] |
| $(H_{10}B_{10}C_2)[\mu\text{-}P(R)TeP][\mu\text{-}TeP(R)](C_2B_{10}H_{10})$ R═$CHMe_2$, $CMe_3$ (FF) | S, H, B, C, P, Te | [1751] |
| **Exo-Polyhedral Transition Metal Derivatives** | | |
| ***Yttrium and lanthanide elements*** | | |
| 1,2-$C_2B_{10}H_{11}$-$SiMe_2$-($\eta^5$-$C_9H_6$)Yb(THF)[($\eta^5$-$C_9H_6$)$SiMe_2$-$C_2B_{10}H_{10}$]$^-$ (FF) | S, X, H, B, C, IR | [802] |
| Gd (tetracarboranylmethoxyphenyl)porphyrin complexes NMR imaging contrast agents) | S | [1428] |
| $Gd^{3+}$*cyclo*-[$NCH_2(CO_2)CH_2CH_2]_4$NH$(CH_2)_6$—*cyclo*-$N_3CH$═C—$CH_2OCH_2CH_2$—$CB_{10}H_{10}C$—$CH_2OCH_2$—C*yclo*-C═$CHN_3$—$C_{16}H_{33}$ (FF) conversion to LPL adducts lipophilic NRI-Gd-BNCT agent | S, H, C, IR, MS, MRI imaging | [1657] |

*Continued*

| Compound | Information | References |
|---|---|---|
| $Gd^{3+}(CH_2)_8N_4[CH_2C(O)O]_3CH_2C(O)NH$-$(CH_2)_6NHC(O)CH_2$—$CB_{10}H_{10}C$—$NHC(O)$-$(CH_2)_2$-cholesterol incorporation in liposome for BNCT and MRI application | S, H, C, IR, MS | [1747] |
| $PhCB_{10}H_{10}C$—$MCl_2\cdot(THF)_6$ M = Tm, Sm, Yb (FF) | S | [855] |
| $M(CB_{10}H_{10}CR)_nCl_{3-n}$ R = Me, Ph; M = La, Tm, Yb; $n$ = 1–3 (FF) | S | [856] |
| $PhCB_{10}H_{10}C$—$MCl_2\cdot LiCB_{10}H_{10}CPh$ Ln = Tm, Yb (FF) | S | [856] |
| $[1\text{-}Me_2(\sigma\text{-}C_5H_4)Si\text{-}C_2B_{10}H_{11}]NdCl_2\cdot 3THF$ (FF) | S, X | [779] |
| $(THF)La[(C_9H_6)CB_{10}H_{10}C—]\}_2^-$ indenyl | S, X, H, B, C, IR | [858] |
| $M[Me_2Si(C_9H_6)C_2B_{10}H_{11}]Cl_2(THF)_3$ $C_9H_6$ = indenyl; M = Er, Nd (FF) | S, H, B, C, IR | [859] |
| $M[(C_5H_4)CMe_2\text{-}C_2B_{10}H_{11}]_2$ M = Sm, Yb (FF) | S, H, B, C, IR | [1330] |
| $Li(solv)_n^+\{1\text{-}B[N(i\text{-}C_3H_7)_2]_2M(C_9H_7)\}^-$ indenyl (solv = dme, THF; M = Sm, Yb, Y, Nd) | S, X (Sm, Yb), H, B, C, IR | [860] |
| $1\text{-}P[N(i\text{-}C_3H_7)_2](C_9H_6)\text{-}2\text{-}Yb[(OMe)C_2H_4(OMe)]$ indenyl | S, X, H, B, C, P, IR | [605] |
| $\{[1-SiMe_2C_9H_5(CH_2)_2OMe-2-Ln-C_2B_{10}H_{10}]_2(\mu-Cl)_3(THF)\}_2^{2-}Li^+(THF)Li^+(THF)_4$ (Ln = Y, Yb) (FF) indenyl | S, X, H, B, C, IR | [801] |
| $1\text{-}SiMe_2C_9H_5(CH_2)_2NMe_2\cdot Li[OEt_2]\text{-}2\text{-}YbCl_2^-$ (N-Yb) | S, X, H, B, C, IR | [803] |
| $1\text{-}C_9H_6$6-2-Y(THF)-*cyclo*-$[N(CMe_3)\text{-}CH(CH_2\text{-}C_6H_4\text{-}o\text{-}NMe_2)\text{-}N(CMe_3)]$ Y-($\eta^5$-$C_9H_6$-indenyl) | S, X, H, B, C, IR | [1839] |
| $1\text{-}C_9H_6\text{-}2\text{-}Dy(THF)_2$-*cyclo*-$[S\text{-}CH(CH_2\text{-}C_6H_4\text{-}o\text{-}NMe_2)\text{-}N(C_6H_3Me_2)]$ Dy-($\eta^5$-$C_9H_6$-indenyl) | S, X, H, B, C, IR | [1839] |
| $1\text{-}C_9H_6\text{-}2\text{-}Ln(THF)2\text{-}cyclo\text{-}(NMe_2\text{-}o\text{-}C_6H_4\text{-}CH_2)\text{-}N(SiMe_3)]$ Ln = Y, Gd, Dy Ln-($\eta^5$-$C_9H_6$-indenyl) | S, X(Y), H, B, C, IR | [1839] |
| $1\text{-}C_9H_6\text{-}2\text{-}C(=NR)\text{-}NR\text{-}Y[cyclo\text{-}N(SiMe_3)\text{-}CH(CH_2\text{-}C_6H_4\text{-}o\text{-}NMe_2)\text{-}N(SiMe_3)]$ R = $C_6H_{13}$, $CHMe_2$ Y-($\eta^5$-$C_9H_6$-indenyl) | S, X($C_6H_{13}$), H, B, C, IR | [1839] |
| $1\text{-}C_9H_6\text{-}2\text{-}C(=CPh_2)\text{-}O\text{-}Y[cyclo\text{-}N(SiMe_3)\text{-}CH(CH_2\text{-}C_6H_4\text{-}o\text{-}NMe_2)\text{-}N(SiMe_3)]$ Y-($\eta^5$-$C_9H_6$-indenyl) | S, X, H, B, C, IR | [1839] |
| $1\text{-}C_9H_6\text{-}2\text{-}C(C_5H_4N)_2\text{-}O\text{-}Y(THF)[cyclo\text{-}N(SiMe_3)\text{-}CH(CH_2\text{-}C_6H_4\text{-}o\text{-}NMe_2)\text{-}N(SiMe_3)]$ Y-($\eta^5$-$C_9H_6$-indenyl) | S, X, H, B, C, IR | [1839] |
| 1-DOTA[$M^{III}$] M = Dy, Gd DOTA = 1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraacetic acid MRI blood pool contrast agents | S, H, B, C, MS, binding to human serum albumin (HSA) | [1896] |
| ***Titanium, zirconium, and hafnium*** | | |
| *cyclo*-1,2-$[TiCl_2(OC_6H_4CH{=}NCH_2]$ Ti—N catalyst for copolymerization of $C_2H_4$ and methylundecanoate | S, H, B, C, IR | [1655] |
| $(Me_2CHO)_2Ti\{1,2\text{-}[(Me_3C)(OH)C_6H_2\text{-}SCH_2]_2$ $C_2B_{10}H_{10}$ catalyst for $C_2H_4$ polymerization and copolymerization with 1-hexene (FF) | S, X, H, C, IR | [1689] |

| Compound | Information | References |
|---|---|---|
| $Cl_2Hf$\{1,2-[$(Me_3C)(OH)C_6H_2$—$SCH_2]_2C_2B_{10}H_{10}$\} 2Hf—O, 2Hf—S catalyst for $C_2H_4$ polymerization and copolymerization with 1-hexene) (FF) | S, EXAFS, H, C, IR | [1689] |
| $(thf)_2Cl_2Zr$\{1,2-[$(Me_3C)(OH)C_6H_2$-$SCH_2]_2$ $C_2B_{10}H_{10}$\} 2Zr—O catalyst for $C_2H_4$ polymerization and copolymerization with 1-hexene (FF) | S, EXAFS, H, C, IR | [1689] |
| 1,2-*cyclo*-$Cp_2M(CH_2)_2$ M = Ti, Zr | S | [743] |
| 1-$CHPhC_5H_4$-2-$STi[NMe_2]_2$ | S, X, H, B, C, IR | [619] |
| 1,2-*cyclo*-1,2-[$Cp_2RZrCEt$=CEt] R = N≡CPh, C=N—$C_6Me_2H$ | S, X, H, C | [307] |
| {1,2-*cyclo*-[$Me_2C$—$C_5H_4$—Zr[(MeN$(CH_2)_3NMe]\}_2$[μ-PhN(O)CHNMe$(CH_2)_2$NMeCH(O)NPh]$)_2$ | S, X, H, B, C, IR | [862] |
| {1,2-*cyclo*-[$Me_2C$—$C_5H_4$—Zr[(MeN$(CH_2)_3NMe]\}_2$[μ-N=CPh—NMe$(CH_2)_3$NMe—CPh=N]$_2$ | S, X, H, B, C, IR | [862] |
| 1,2-*cyclo*-[$Cp_2Zr$-Cl-Li$(OEt_2)_2$] | S, H, B, C, IR | [863] |
| 1,2-*cyclo*-{$CMe_2C_5H_4$—Ti=N(Ar)$(NC_5H_5)$] Ar = 2,6-$C_6H_3Me_2$, 2,6-$(CHMe_2)_2C_6H_3$ | S, X[$C_6H_3Me_2$], H, B, C, IR | [1462] |
| 1,2-*cyclo*-$Me_2C(C_5H_4)Ti[NMe_2]R$ R=$CH_2Ph$, $CH_2SiMe_3$, Me | S, X($CH_2Ph$), H, B, C, IR | [1465] |
| 1,2-*cyclo*-{$P^V$[$N[CHMe_2]_2$)(=$C_9H_6$)-O-$ML(NR_2)_2$\} M = Ti, Zr, Hf; R = Me, Et; L = $HNMe_2$, THF $C_9H_6$ = indenyl | S, X, H, B, C, P, IR | [604] |
| ($C_{13}H_8$) = P{*cyclo*-O—P[N$(CHMe_2)]_2$—$CB_{10}H_{10}C$—}-$Zr(NMe_2)_2$(THF) $C_{13}H_8$ = fluorenyl (FF) | S, X, H, B, C, P, IR | [1464] |
| 1-R-2-$CMe_2(C_5H_4)MCl_2Cp^*$ R = H, Me; M = Ti, Zr, Hf | S, X, H, B, C | [865] |
| 1,2-*cyclo*-{$Cl_2M(C_9H_6)B[N(i\text{-}C_3H_7)_2]_2)$\} M = Ti, Zr, Hf | S, H, B, C, IR | [866] |
| 1,2-*cyclo*-[$SiMe_2C_5Me_4$]$TiCl_2$ | S, X, H, B, C | [867] |
| 1,2-*cyclo*-{[$(Me_2CH)_2N$-P]-$(C_9H_6)M(NR_2)_2$\} M = Ti, Zr, Hf; R = Me, Et catalyst for polymerization of $C_2H_4$ and ε-captolactone (Zr, Me) | S, X, H, B, C, P | [868] |
| $Cp_2Ti(CH_2CB_{10}H_{10}CH)_2$ (FF) | S | [593] |
| Zr[$C_5H_4$-$CMe_2C_2B_{10}H_{10}$-1-Zr]$_2$ (FF) | S, X, H, B, C, IR | [869] |
| {1,2-*cyclo*-$CMe_2(C_5H_4)Zr[NMe_2]$-$C_2B_{10}H_{10}\}_2$(PhC=C=C=CPh) (FF) | S, X, H, B, IR | [1471] |
| [1-$Me_2Si(C_9H_6)$-2-Zr(OMe)(μ-OMe)$C_2B_{10}H_{10}]_2$ (FF) | S, X, H, B, C, IR, MS | [870] |
| 1-$Me_2E(C_9H_6)$-2-$Zr[S_2CNMe_2]_2$ E = C, Si | S, X, H, B, C, IR, MS | [870] |
| $\eta^5$-σ-$Me_2E(C_9H_6)(C_2B_{10}H_{10})ZrCl(\eta^3\text{-}C_2B_{10}H_{10})^-$ (FF) 1,2-dehydro-*o*-carborane complex | S, X, H, B, C, IR | [1463] |
| 1-$ZrCp_2C_5H_3BrN$ N→Zr | S, X, H, B, C | [1599] |

*Continued*

| Compound | Information | References |
|---|---|---|
| 1-$ZrCp_2C_5H_2Me_2N$ N→Zr | S, X, H, B, C | [1599] |
| 1-$ZrCp_2C_9H_6N$ N→Zr | S, X, H, B, C | [1599] |
| 1,2-*cyclo*-$ZrCp_2N(C_6H_4)_2(\mu\text{-}CH)$ | S, X, H, B, C | [1599] |
| 1,2-*cyclo*-$ZrCp_2C_5H_3(C{\equiv}C{-}n\text{-}C_4H_9)N$ (N→Zr) 3 isomers | S, X, H, B, C | [1599] |
| 1,2-*cyclo*-$ZrCp_2C(C_5H_4N){=}CR$ N→Zr R = *n*-$C_4H_9$, Ph | S, X, H, B, C | [1599] |
| 1,2-*cyclo*-$ZrCp_2CH_2CR$ R = $SiMe_3$, $PPh_2$, H, $C_5H_4N$, *n*-$C_4H_9$, $CH_2PPh_2$ | S, X($SiMe_3$, $PPh_2$, H, $CH_2PPh_2$), H, B, C, IR, MS | [1614] |
| 1,2-*cyclo*-$ZrCp_2CH_2CH(CH_2C{\equiv}CPh)$ | S, H, B, C, IR, MS | [1614] |
| 1,2-*cyclo*-$ZrCp_2CH(CH_2C{=}CH_2){=}CPh$ | S, H, B, C, IR, MS | [1614] |
| ***Tantalum*** | | |
| 1,2-*cyclo*-$TaMe_2$(*cyclo*-$CH_2C(=NR)C_5H_4CMe_2$] *R* = *cyclo*-$C_6H_{12}$, $CHMe_2$ | S, X, H, B, C | [1597] |
| 1,2-[*cyclo*-$TaMe_2(THF)C_5H_4CMe_2]C_2B_{10}H_{10}$ (FF) | S, H, B, C, F | [1597] |
| ***Chromium, molybdenum, and tungsten*** | | |
| 1-$(CO)_3CrPh(CH_2)_n$-2-R *n* = 1, 2; R = H, Ph, $CH_2Ph$ | S | [1396] |
| 1-$PhCr(CO)_3$-2-R R = Me, Ph | S | [874] |
| $(\mu\text{-}I)_2[Cr{-}CB_{10}H_{10}C{-}C(NHCMe_2){=}NCMe_2]_2$ 2N→Cr | S, X, H, B, C | [1531] |
| 1-$PPh_2(=S)$-2-*cyclo*-$SCH_2C_6H_2R_2(O)$ $[CrCl_2(OC_4H_8)]_2$ Cr—S Cr—O R = Me, $CMe_3$ catalyzes $C_2H_4$ polymerization in presence of MAO | S, IR | [1680] |
| 1,2-*cyclo*-$[CH_2PPh_2M(CO)_2PPh_2]$ M = Cr, Mo, W | S | [1492] |
| 1-$(CO)_5M{=}C(OMe)$-2-R M = Cr, W; R = Me, Ph | S, H, B, IR, MS | [875] |
| 1-R-2-R′ R=$CH_2PhCr(CO)_3$, $PhCr(CO)_3$]; R′ = H, Ph, $CH_2Ph$ | MS (fragmentation study) | [1457] |
| 1,2-*cyclo*-(—$CH_2$—P[$M(CO)_6$]R-$CH_2$—) R = Me, Ph; M = Cr, Mo, W phospholane | S | [579] |
| 1,2-*cyclo*-(—$CH_2$—As[$M(CO)_6$]R-$CH_2$—) R = Me, Ph; M = Cr, Mo, W arsolane | S | [579] |
| 1-($\eta^6$-$C_7H_7$)$Cr(CO)_3$-2-R R = H, Me, Ph | S, X(Ph), H | [1367] |
| I(NO)$CpMo(\mu\text{-}S)_2C_2B_{10}H_{10}^-$ (FF) | S, X, H, COND, IR, MS | [882] |
| 1,2-*cyclo*-[—$Ph_2P$—$M(CO)_3$—$CMeOMe\text{-}PPh_2$—] M = Cr, Mo, W | S, H, B, IR, MS | [876] |
| 1,2-*cyclo*-[(HO)($Me_3C$)P—$Cr(CO)_4$—P(OH)-($CMe_3$)] | S, X, H, B, C, P, MS | [877] |
| 1-MeO-C[=$M(CO)_5$]-2-R M = Cr, W; R = Me, Ph | S, X(W, Ph), H, B, C, IR, MS | [880] |
| $\mu\text{-}(Cu_2MoS_4)\{1,2\text{-}(Ph_3P)_2C_2B_{10}H_{10}\}_2$ (FF) | S, X, H, C, IR, UV | [1340] |
| 1,2-*cyclo*-[-$Ph_2P$-$M(CO)_4$-$SMeCH_2$⁻] M = Mo, W | S | [1491] |
| 1-[-*cyclo*-$(CO)_2(CF_3)MCp(CO)_2$]-2-Me M = Mo, W | S, ESR | [1453] |
| $[MeCB_{10}H_{10}C{-}(CO)_2(CF_3)]_2M$ M = Mo, W (FF) | S, ESR | [1453] |
| $[C_5H_3[CMe_3]_2]Co(CO)_2W\{1,2\text{-}cyclo\text{-}[Se\text{-}Co\text{-}\{C_5H_3[CMe_3]_2\}\text{-}Se]\}_2$ | S, X, H, IR | [847] |

| Compound | Information | References |
|---|---|---|
| [1,2-{*cyclo*-SRu[$MeC_6H_4CHMe_2$]S}$C_2B_{10}H_{10}$]$_2$Mo(CO)$_2$[1,2-{*cyclo*-SRu(CO)$_3$S}$C_2B_{10}H_{10}$] (FF) | S, X, H, B, C, IR | [669] |
| [1,2-(*cyclo*-$S_2C_2B_{10}H_{10}$)$_2$W(CO)$_2$(μ-RhCp*) (FF) | S, X, H, B, C, IR | [962] |
| [(1,2-*cyclo*-E-RhCp*-E)$C_2B_{10}H_{10}$]$_2$Mo(μ-CO)$_2$ E = S, Se (FF) | S, X, H, B, C, IR | [672] |
| {1,2-*cyclo*-SeRh{$C_5H_3$[$C(Me)_3$]$_2$}W(CO)$_4$Se}-$C_2B_{10}H_{10}$ (FF) | S, X, H, B, C, IR | [672] |
| Mo(μ-CO)$_2$[CpCo(*cyclo*-E$_2$)$C_2B_{10}H_{10}$]$_2$ E = S, Se (FF) | S, X(S), H, B, C, IR | [879] |
| ($C_2B_{10}H_{11}$-$CH_2$-$NHCHMe_2^+$)$_4$$W_{10}O_{32}^{4-}$($H_2O$)$_2$($Me_2CO$)$_4$ iminium carborane cations, decatungstate anions hydrophilic/hydrophobic lamellar structure (FF) | S, X | [1394] |
| ***Manganese and rhenium*** | | |
| 1-MeO-CMe[=Mn(CO)$_5$]-2-R M = Cr, W; R = Me, Ph | S, X(Ph), H, B, C, IR, MS | [880] |
| 1-(CO)$_4$M*n*=C(OMe)Me-2-R R = H, Me | S, X(Ph), H, B, IR, MS | [881] |
| 1-$C_5H_4$Mn(CO)$_3$-2-C(O)OHgMe | S, H ($J_{Hg\text{-}Me}$), p$K_a$ | [906] |
| 1,2-*cyclo*-{—($PPh_2$)$_2$MnCp(CO)—} | S | [1490] |
| 1,2-*cyclo*-[—Mn(2,2′-bipyridine)—] | S | [1415] |
| 1,9-*cyclo*-[$CH_2NEt_2$-Re(CO)$_4$] | S | [883] |
| 1,9-*cyclo*-[N=NPh-Re(CO)$_4$]-2-R R = Me, Ph, $CH_2$=CMe, $Me_2CH$ | S | [883] |
| 1-[*cyclo*-(CO)$_2$($CF_3$)M(CO)$_4$]-2-R R = H, Me; M = Mn, Re | S, ESR | [1453] |
| 1,2-*cyclo*-[—$CB_{10}H_{10}$C–MeAs-$CB_{10}H_{10}$C–AsMeMnCp(CO)$_2$—] (FF) | S | [1490] |
| Mn(μ-$H_2O$)[μ-Me($CO_2$)$C_2B_{10}H_{10}$]$_n$·2$H_2O$ polymer (FF) | S, X, H, B, C, IR, MAG, E | [1816] |
| Mn($H_2O$)[μ-($CO_2$)$C_2B_{10}H_{11}$]$_n$.2$H_2O$ polymer (FF) | S, X, H, B, C, IR, MAG, E | [1816] |
| Mn$_2$[R($CO_2$)$C_2B_{10}H_{10}$]$_4$(bpy)$_2$ R = Me, H (FF) | S, X, H, B, C, IR, MAG, E | [1816] |
| Mn[R($CO_2$)$C_2B_{10}H_{10}$]$_2$(bpy)$_2$ R = Me, H (FF) | S, X, H, B, C, IR, MAG, E | [1816] |
| Mn[Me($CO_2$)$C_2B_{10}H_{10}$]$_2$(bipyrimidine)$_n$ R = Me, H polymer (FF) | S, X, H, B, C, IR, MAG, E | [1816] |
| 3-Re(CO)$_5$ | S | [886] |
| 1-$CHMe_2$-2-N=NPh-2-Re(CO)$_4$ Re—N | X | [1482] |
| $Re[CN-3-(1,2-C_2B_{10}H_{11})]_6^+$ (FF) | S, X, H, B, C, MS | [717] |
| 1-$SiMe_2ReH_2$[$PPh_3$]$_2$-2-$SiMe_2H$ | S, X, H, B, C, P, IR | [1384] |
| ***Iron*** | | |
| 1-$CH_2$(CO)Fe(CO)Cp | S | [1382] |
| 1-$CH_2$Fe(CO)$_2$Cp-2-R R = H, Me, Ph | E | [891] |
| 1-$CH_2$($C_5H_4$)FeCp-2-R R = Me, $CHMe_2$ | S, E | [892] |
| 1-C≡CFe(CO)$_2$Cp | S | [996] |

*Continued*

| Compound | Information | References |
|---|---|---|
| 1,2-$[(\eta^4\text{-}C_5H_5)Fe(CO)_3]_2$ | S, H, IR | [893] |
| 1-C(O)$(\eta^4\text{-}C_5H_5)Fe(CO)_3$ | S, H, IR | [893] |
| 1-C(O)$Fe(CO)_2$Cp | S, H, IR | [893] |
| 1-$CH_2Fe(CO)_2$Cp-2-Me | S, H, IR | [893] |
| 1-CH(SPh)$(C_5H_4)$FeCp | S, H, B, IR | [1843] |
| 1-CH═CH$(C_5H_4)$FeCp | S, H, B, IR | [1843] |
| 1-$CH_2$CR(OH)$(C_5H_4)$FeCp R = H, Me | S, H, B, IR | [1843] |
| 9-$(CH_2)_n$CH(OH)$(C_5H_4)$FeCp $n = 0$, 1 | S, H, B, IR | [1843] |
| 9-$CH_2$CR(OH)$(C_5H_4)$FeCp R = H, Me | S, H, B, IR | [1843] |
| 1-PCl$(C_5H_3\text{-}o\text{-}CHRNMe_2)$FeCp R = H, Me | S, X(pure enantiomer), H, B, C, P, IR, MS | [603] |
| $Fe\{[N_2(O)_2(C_6H_8)]_3B-CB_{10}H_{10}CR\}_2^{2+}$ R = $CHMe_2$, Et *o*-carboranyl capping agents for Fe (II) clathrochelates | S, X(Et), H, B, C, UV, MS, IR, Mössbauer | [894] |
| 1,2-*cyclo*-[—$C_5H_4Fe(CO)(\mu\text{-}CO)_2Fe(CO)C_5H_4$—] | S, H, IR | [893] |
| 1,2-*cyclo*-[$CH_2PPh_2Fe(CO)_2PPh_2$] | S | [1492] |
| 1,2-*cyclo*-[—$Ph_2P\text{-}Fe(CO)_3\text{-}PPh_2$—] | S | [895] |
| 1,2-[S—C(═$CH_2$)—$CpFe(C_5H_4)]_2$ vinyl sulfide | S, X, H, B, C, IR, MS | [645] |
| 1,2-*cyclo*-[—SC(R)═CH—S—] R = Ph, $(C_5H_4)$FeCp vinyl sulfides | S, X[$(C_5H_4)$FeCp], H, B, C, IR, MS | [645] |
| 1,2-*cyclo*-[—SC($C_5H_4$FeCp)═CH—S—] influence on native conformation of myoglobin protein | S, E, CD, UV, fluorescence | [1524] |
| 1,2-*cyclo*-[—SC($C_5H_4$FeCp)—($\mu\text{-}CH_2$)—S—] ($CH_2$—B) influence on native conformation of myoglobin protein | S, E, CD, UV, fluorescence | [1524] |
| 1-*cyclo*-[—$(CO)_2(CF_3)$FeCp(CO)—]-2-Me | S, ESR | [1453] |
| 1,2-*cyclo*-[EMCp*$Fe(CO)_3$E] M—Fe E = S, Se; M = Rh, Co | S, X(S,Rh,Co; Se,Rh), H, B, C, IR | [896] |
| 1,2-$Me_2$-3-C(O)Fe(CO)Cp | S | [897] |
| 1,2-$Me_2$-3-Fe(CO)Cp | S | [897] |
| 1-CpRe$(CO)_3$FeCPh$(CO)_2$ | S, X, H, IR, MS | [884] |
| 1-$Fe(CO)_2$Cp-2-R R = H, $Fe(CO)_2$Cp | MS (electron impact fragmentation) | [1402] |
| $Fe[C_5H_4\text{-}1,2\text{-}Me\ C_2B_{10}H_{10}]_2$ (FF) | S, X, H, B | [898] |
| $Fe\{(terpyridine)[SiMe_2(t\text{-}C_4H_9)]\ C_2B_{10}H_{10}\}_2^{2+}$ (FF) | S, H, B, C, IR, MS | [275] |
| 1,2-$(\mu\text{-}S)_2Fe_2(CO)_6$ FeFe hydrogenase active site model | S, X, B, C, IR, E | [899] |
| 1,2-[SCH═CHC(O)$C_5H_4$FeCp] 3 *cis*/*trans* isomers | S, X(1 isomer), H, B, C, IR, MS | [1583] |
| 1,2-*cyclo*-SCH═C[C(O)$C_5H_4$FeCp]S | S, X, H, B, C, IR, MS | [1583] |
| 1-SCH═CHC(O) $C_5H_4$FeCp 2 *cis*/*trans* isomers | S, X, H, B, C, IR, MS | [1583] |
| 1,2-[$(C_5H_4)$FeCp]$_2$-3-X X = Cl, Br, I | S, X, H, B, C, MS | [1615] |
| 1,2-*cyclo*-[CpFe$(C_5H_4)C_2]_2S_2C_2B_{10}H_{10}$ C—B(3) | S[insertion of HC≡C—$C_5H_4$FeCp into CpCo ($S_2C_2B_{10}H_{10}$)], X | [1644] |
| 1,2,3-*tricyclo*-{—S-Ru$(MeC_6H_4CHMe_2)(\mu\text{-}CH_2)$C[$(C_5H_4)$FeCp]—} Ru—B | Reversal of biofilm antibiotic resistance | [1669] |

| Compound | Information | References |
|---|---|---|
| (+1),(-1) $Cl_3Fe^{III}{}_2[HOCH(C_5H_4N)\text{-}C_2B_{10}H_{11}]_3$ 3Fe—N pure enantiomers | S, X, H, B, CD, MAG, second harmonic generation | [1731] |
| $Fe[N{=}C(Ph){-}C(Ph){=}N]_2[N{=}CH\text{-}C(C_2B_9H_{11}){=}N](BFO_3)_2$ quasi-aromatic Fe(II) cage complex | S, X, H, B, C, F, IR, MS, Raman, UV | [1755] |
| $\{1,2\text{-}[C_6H_4\text{-}p\text{-}C{\equiv}C{-}C_6H_4{-}p\text{-}C_5H_2N\text{-}(C_5H_4N)_2]_2C_2B_{10}H_{10}\}_nFe^{II}{}_n$ $n=2$–4 (FF) | S[self-assembly of bis(terpyridyl) *o*-carboranes with metal ions to form cyclic dimers, trimers and tetramers], H (var. temp.), C, MS | [1765] |
| B-$(CO)Fe(CO)_2Cp$ | S | [900] |
| B-$Fe(CO)_2Cp$ | S | [900] |
| 9-$(C_5H_4)Fe(CO)_2Br$ | S, H, B, IR | [901] |
| 3-$(C_5H_4)Fe(CO)_2Cl$ | S | [897] |
| B-$(C_5H_4)Fe(CO)_2Br$ | $^{35}Cl$ NQR | [1326] |
| $Fe(1,2\text{-}C_2B_{10}H_{11}\text{-}3\text{-}C_5H_4)_2$ (FF) | S | [1500] |
| $(THF)Fe(1,2-S_2C_2B_{10}H_{10})_2^-$ (FF) | X | [902] |
| 1-$[C_6H_4\text{-}p\text{-}CH{=}CH\text{-}C_6H_4FeCp]$ | S, UV, E, NLO [β (hyperpolarizability)] | [903] |
| 1,2-*cyclo*-$[{-}Cp'(CO)_3Fe_2\text{-}(\mu\text{-}Se)_2{-}]$ | S, X | [905] |
| 1,2-*cyclo*-$[{-}C_5H_3\text{-}(tert\text{-}C_4H_9)_2]_2Fe_2(CO)_3Se_2{-}]$ | S, X | [1389] |
| 1-$C_5H_4FeCp$-2-C(O)OHgMe | S, H ($J_{Hg\text{-}Me}$), p$K_a$ | [906] |
| *Trans*-[1,2-*cyclo*-$C(NH\text{-}CHMe_2){=}N(CHMe_2)\text{-}C_2B_{10}H_{10}]_2Fe^{III}Cl$ 2 Fe—C, 2 Fe—N amidinates | S, X, IR | [1797] |
| *Trans*-[1,2-*cyclo*-$C(NH\text{-}CHMe_2){=}N(CHMe_2)\text{-}C_2B_{10}H_{10}]_2Fe^{II}$ 2 Fe—C, 2 Fe—N amidinates | S, X, IR | [1797] |
| 1,2-*cyclo*-$C(CH_2OH)CH(C_5H_4\text{-}FeCp)Ru\text{-}(MeC_6H_4CHMe_2)$S Ru—B | S, X, H, B, C | [1825] |
| ***Ruthenium and osmium*** | | |
| 1-Me-2-RuCpLL′ (L,L′ = $PMe_2Ph$; L,L′ = $PMePh_2$; LL′ = $Ph_2CH_2CH_2PPh_2$) | S, X($PMe_2Ph$), H, C, P, MS | [908] |
| 1,2-*cyclo*-$\{CMe_2(C_5H_4)RuH(PPh_3)_2\}$ direct $C_5H_4\text{-}C_2B_{10}$ cage linkage | S, X, H, P, IR | [909] |
| 1-$CH_2$-O-*bicyclo*-$C_7H_4O(CHMe_2)$ $RuCl_2(C_3H_4N_2mes_2)$ mes = mesitylene; catalyst for ring-opening metathesis | S, H, B, C | [910] |
| 1,2-*cyclo*-$Me_2C(C_5H_4)RuL_2$ $L_2 = 2P(OEt)_3$, $2PPh_2(OEt)$, $NH_2(CH_2)_2CHMe_2$, NH $2CHMe_2$, $H_2N(CH_2)_2NH_2$, $HMeN(CH_2)_2NHMe$, tetramethylimidazole, $Me_2N(CH_2)_2NMe_2$, 2NCMe | S, X[except $H_2N(CH_2)_2CHMe_2$], H, B, C, P, I, E | [911] |
| $\{1,2\text{-}[cyclo\text{-}Me_2C(C_5H_4)Ru(OH_2)]C_2B_{10}H_{10}\}_2$ Ru-Ru (FF) | S, X, H, B, C, P, IR, E | [911] |
| 1,2-*cyclo*-$Ru(C_4R_4)(C_5H_4)CMe_2$ R = Et, Ph cyclobutadiene | S, X(Et), H, B, C, IR | [1861] |
| 1,2-*cyclo*-$Ru(C_7H_6R_2)(C_5H_4)CMe_2$ R = Me, Et cyclopentatriene | S, X(Me), H, B, C, IR | [1861] |
| 1,2-*cyclo*-$Me_2C(C_{11}H_7R_3)Ru(NCMe)$ R = Ph, *p*-$C_6H_4Me$, *p*-$C_6H_4Cl$, *p*-$C_6H_4Br$ | S(Ru-mediated coupling and *cyclo*addition of alkynes), X, H, B, C | [1446] |
| 1,2-*cyclo*-$(MeC_6H_4CHMe_2)Ru(\mu\text{-}Cl)_2Ru\text{-}(MeC_6H_4CHMe_2)$ | S, X, H, B, IR | [1470] |

*Continued*

| Compound | Information | References |
|---|---|---|
| 1,2-*cyclo*-[$Me_2C(C_5H_4)Ru(H)_2P(CHMe_2C_6H_4Me)_3$] | S, X, H, B, C, P, IR | [1387] |
| 1,2-*cyclo*-ERu($C_8H_{12}$)(μ-Cl)$_2$RhCp*E E = S, Se | S, X, H, B, IR | [913] |
| 1,2-cyclo-ERu($C_8H_{12}$)(μ-Cl)$_2$ RhCp*E—$C_2B_{10}H_9$ L E = S, Se; L = H, OMe | S, X(S, H; Se, OMe), H, B, IR | [913] |
| 1,2-*cyclo*-$S_2$Ru($MeC_6H_4CHMe_2$)($C_3N_2H_3$Me-NHCH=$CH_2$) imidazoline; carbene | S, X, H, B, C | [914] |
| [($MeC_6H_4CHMe_2$)$Ru_2$(μ-$S_2$—$C_2B_{10}H_9$)(μ-$S_2$—$C_2B_{10}H_{10}$)]$_2$ S—Ru | S, X, H, B, IR, MS | [1535] |
| ($MeC_6H_4CHMe_2$)$_2Ru_2$Ru(μ-$S_2$)(μ-$S_2$Cl)-(μ-$S_2$—$C_2B_{10}H_{10}$)$_2$ S—Ru | S, X, H, B, IR, MS | [1535] |
| ($MeC_6H_4CHMe_2$)$_2Ru_2$Ru(μ-$S_2$)(μ-$S_4$)(μ-$S_2$—$C_2B_{10}H_{10}$)$_2$ S—Ru | S, X, H, B, IR, MS | [1535] |
| ($MeC_6H_4CHMe_2$)Ru(μ-E)$_2$(*cyclo*-$S_2B_{10}H_{10}$)$_2$ E = S, Se (FF) | S, X(S), H, B, C, IR | [915] |
| ($MeC_6H_4CHMe_2$)Ru(μ-Se)$_2$(*cyclo*-$S_2B_{10}H_{10}$)$_2$ (FF) | X | [916] |
| 1,2-*cyclo*-[SM($MeC_6H_4CHMe_2$)$CH_2$C($C_5H_4$FeCp)S] M = Ru, Os | S, X(Ru), H, B, C, IR, MS | [917] |
| 1,2-*cyclo*[SCH($C_5H_4$FeCp)$CH_2$Ru-($MeC_6H_4CHMe_2$)S] | S, X, cytotoxicity toward cancer cells | [918] |
| (CO)ClM{*cyclo*-[—$Ph_2PCH_2$]$C_2B_{10}H_{11}$-B(3)H—}$_2$ M = Ru, Os (FF) | S, H, P, IR, Raman (actual spectra) | [919] |
| (CO)$_2$ClRu{*cyclo*-[—$Ph_2PCH_2$]$C_2B_{10}H_{11}$-B(3)H—}{$Ph_2PCH_2$]$C_2B_{10}H_{11}$} (FF) | X | [1414] |
| *Trans*-H(Cl)Ru[($Ph_2P$)$_2C_2B_{10}H_{10}$]$_2$ (FF) | S, X, H, P | [920] |
| 1,2-*cyclo*-C($CH_2OH$)CH($C_5H_4$-FeCp)Ru($MeC_6H_4CHMe_2$)S Ru—B | S, X, H, B, C | [1825] |
| (CO)Cl(2,2′-bipyridine)Ru{*cyclo*-[—$Ph_2PCH_2$]$C_2B_{10}H_{11}$-B(3)H—} (FF) | S, H, P, IR, Raman (actual spectra) | [919] |
| $Cl_2$Ru[($R_2P$)$_2C_2B_{10}H_{10}$]$_2$ R = Et, EtO (FF) | S, X(EtO), H, B, P, IR | [921] |
| 1,2-*cyclo*-{($CH_2C_5H_4N$)RuCl[$MeC_6H_4CMe_2$]—}$CH_2C_5H_4N$=picolyl | S, X, H, B, C, IR | [523] |
| ($N_2C_4H_4$){1,2-[*cyclo*-SRu[$MeC_6H_4CH$-$Me_2$]S]-$C_2B_{10}H_{10}$}$_2$ (FF) | S, X, H, B, IR | [673] |
| Ru[(terpyridine)-O-($CH_2$)$_n$$C_2B_{10}H_{11}$]$_2$ $n$ = 1,3 (FF) | S, H, B, C, MS | [198] |
| (terpyridine)Ru{(terpyridine)[$SiMe_2$(t-$C_4H_9$)]-$C_2B_{10}H_{10}$}$^{2+}$ (FF) | S, H, B, C, IR, MS | [275] |
| [*p*-$MeC_6H_4$-$CHMe_2$]M(μ-S)$_2C_2B_{10}H_{10}$ M = Ru, Os (FF) | S, X[Ru, $PPh_3$], H, B, C, IR | [922] |
| [*p*-$MeC_6H_4$-$CHMe_2$]Ru(μ-S)$_2C_2B_{10}H_{10}$ (FF) | Anticancer activity toward human ovarian cancer cells A2780 and cisplatin-resistant A2780cisR, with and without BNCT | [1900] |
| *exo, nido*-Cl$Ph_3P$)$_2$Ru-(μ-H)$_3$-7,8-*nido*-$C_2B_9H_8$-10-Hg-(9-$C_2B_{10}H_{11}$) (FF) | S, X, H, B, P | [1069] |
| 1,2-[(μ-S)$_2$CPh$CH_2$M[*p*-$MeC_6H_4$-$CHMe_2$]$C_2B_{10}H_{10}$ M = Ru, Os M–B (FF) | S, X(Ru), H, B, C, IR, MS | [961] |
| *Exo*-Cp*M[-S-HC≡CH[C(O)OMe]-](μ-S)-1,2-$C_2B_{10}H_{10}$ Ru-B M = Ru, Os (FF) | S, H, B, C, IR, MS | [965] |

| Compound | Information | References |
|---|---|---|
| $(MeC_6H_4CHMe_2)Ru^{I}(\mu\text{-}S_2)Ru^{III}[(\mu\text{-}S)_2C_2B_{10}H_{10}]_2$ (FF) | S, X, H, B, C, IR, MS | [1475] |
| *exo*-{-S-C[C(O)OMe]=[C(O)OMe}-M[*p*-$CHMe_2C_6H_4Me$]-S-]-1,2-$C_2B_{10}H_{10}$ (M-S) M=Ru, Os (FF) | S, H, B, C, IR, MS | [965] |
| 1,2[*p*-$MeC_6H_4CHMe_2$]Os$(\mu\text{-}S)_2$ | X | [923] |
| 1,2-*cisoid*/*transoid*-Cp*[*p*-$MeC_6H_4CHMe_2$]M (RC≡CH)$(\mu\text{-}S)_2$ M=Ru, Os; R=H, Me | S, X(Ru, H), H, B, C, IR, MS | [923] |
| 1-$CMe_2C_5H_4$-2-Ru{=C=C[$SiMe_3]_2$}$_2$ Ru—$C_5H_4$ bis(vinylidene) complex | S, X, H, B, C, IR | [1445] |
| 1,2-LRu$(\mu\text{-}S)_2$ L=$C_6Me_6$, *p*-$MeC_6H_4CHMe_2$ | S, H, C. E, UV, IR, MS | [924] |
| 1,2-(Ar)LRu$(\mu\text{-}S)_2$ Ar=$C_6Me_6$, *p*-$MeC_6H_4CHMe_2$; L=$PEt_3$, CN($CMe_3$), CO | S, X[$PEt_3$, CN(*t*-$C_4H_9$), $C_6Me_6$], E | [924] |
| 1,2-(Ar)[$HSiMe)_3$]Ru$(\mu\text{-}S)_2$ Ar=$C_6Me_6$, *p*-$MeC_6H_4CHMe_2$ | S, X[$C_6Me_6$], H, C. E, UV, IR, MS | [924] |
| 1-$Me_2C(\eta^5\text{-}L)$-2-Ru($C_8H_{12}$) ($C_5H_4$–Ru) L=$C_5H_4$, $C_9H_6$, $C_{13}H_8$ | S, X, H, B, C. E, IR | [253] |
| 1-($C_5H_4$)RuD$(PPh_2)_2$ synthesized via nucleophilic substitution of carborane on Cp ring | S, X, H, C | [926] |
| [(*p*-$MeC_6H_4CMe_2)Ru_2Se_4$)($C_2B_{10}H_{10})_2$]-[(*p*-$MeC_6H_4CMe_2$)$RuSe_2$($C_2B_{10}H_9$] (FF) | S, X, H, B, IR, MS | [1538] |
| [(*p*-$MeC_6H_4CMe_2$)$RuSe_2$($C_2B_{10}H_9$)-$RuSe_2$($C_2B_{10}H_{10}]_2$ (FF) | S, X, H, B, IR, MS | [1538] |
| (*p*-$MeC_6H_4CMe_2)_2Ru_2Se_2$($C_2B_{10}H_{10}$)-$Ru_2Se_6$($C_2B_{10}H_{10})_3$ (FF) | S, X, H, B, IR, MS | [1538] |
| 1,2-*cyclo*-{S—Ru($MeC_6H_4CHMe_2$)C$(\mu\text{-}CH_2)$-[($C_5H_4$)FeCp]—S} promotes apoptosis in human lung cancer HCC287 cells (*in vivo*/*in vitro*) (FF) | Cell growth inhibition, flow cytometry, (tumor growth inhibition) | [1573] |
| 1,2-*cyclo*-[SCR$(\mu\text{-}CH_2)$Ru($MeC_6H_4CHMe_2$)S] Ru—B R=$C_6H_4C$≡CH, ($C_{24}H_{16}O_4$)C≡CH, ($C_4H_2S$)Br, $C_4H_2SC$≡CH | S, X[($C_6H_4C$≡CH, ($C_4H_2S$)Br], H, B, C, IR, MS | [1589] |
| 1,3-*cyclo*-[RuCp*NR=C(NHR)]-1,2-$C_2B_{10}H_9$-μ-(C,Ru)—Se R=$CHMe_2$, *cyclo*-$C_6H_{13}$ (FF) | S, X(*cyclo*-$C_6H_{13}$), H, B, C, IR | [1652] |
| ($MeC_6H_4CHMe_2$)$RuS_2Ru[(\mu\text{-}S)_2C_2B_{10}H_{10}]_2(\mu\text{-}CH$=CR R=*cyclo*-$C_6H_{12}$, C(O)Ph, and related derivs (FF) | S, X, H, B, C, IR, MS | [1653] |
| 1,2,3-*tricyclo*-{—S-Ru($MeC_6H_4CHMe_2$)$(\mu\text{-}CH_2)$C-[($C_5H_4$)FeCp]—} Ru—B | Reversal of biofilm antibiotic resistance | [1669] |
| $(Ph_3P)_2Ru[(\mu\text{-}S)(\mu\text{-}O)_2C_2B_{10}H_{10}][S—C_2B_{10}H_{11}]$ promotes $H_2$ cleavage | S, X, H, B, ESR, XPS | [1677] |
| $(Ph_3P)Ru[(\mu\text{-}S)_2C_2B_{10}H_{10}][S—C_2B_{10}H_{11}]_2$ | S, X, H, B | [1677] |
| $(Ph_3P)Ru[(\mu\text{-}S)(\mu\text{-}OC_2B_{10}H_{10}][S—C_2B_{10}H_{11}]_2$ | S, X, H, B | [1677] |
| (*p*-$MeC_6H_4CHMe_2)Ru(\mu\text{-}Se)_2$-($S_2C_2B_{10}H_{10})_2$(RC=CR′) R=H, R′=*cyclo*-$C_6H_9$ (two isomers) | S, X(one isomer), H, B, MS | [1688] |
| 1,2-*cyclo*-SRu($MeC_6H_4CHMe_2$)($PPh_3$)S | Solid state $^1H$, $^{11}B$, $^{13}C$, $^{31}P$ MAS (magic angle spinning) NMR | [1738] |
| 1,2-*cyclo*-$SeRu_2$($MeC_6H_4CHMe_2$) | S, X, H, B, C, IR, MS | [1771] |

*Continued*

| Compound | Information | References |
|---|---|---|
| *Cobalt* | | |
| 9-$CH_2$—$C_2Co_2(CO)_6$ | S | [335] |
| 1-SCoCp*(μ-S)$NC_5H_4$ | S, X, H, B, C, IR | [929] |
| 1,2-(μ-S)$_2$[Co($C_5Me_4$)$CH_2$—S-$C_5H_4N$—] | S, X, H, B, C, IR | [929] |
| $C_3N_3$[$C_5H_4N$—CoL(μ-S)$_2$($C_2B_{10}H_{10}$)]$_3$ $C_3N_3$ = triazine L = Cp*, *p*-$MeC_6H_4CMe_2$ (FF) | S, X, H, B, IR | [930] |
| 1,2-*cyclo*-CpCoS(RC═CR′) R = MeOCO,H; R′ = MeOCO, Ph, $SiMe_3$ | S, X(MeOCO), H, C, IR, MS | [932] |
| 1 1,2-*cyclo*-SCoCpS-3-CH═CH-C(O)Ph-6-CH═CHR R═CH═CH-C(O)Ph, CH═CH-C(O)Me, C[C(O)OMe]═CH-C(O)OMe | S, X, H, B, C, IR | [933] |
| 1,2-*cyclo*-CpCoSCH$SiMe_3$ | S, X, H, C, IR | [932] |
| 1,2-*cyclo*-[—S(CoCp)($C_4Ph_2$)S—] | S, X, H, B, C, MS | [667] |
| 1,2-*cyclo*-[—Se(CoCp)$_2$Se—] | S, X, H, B, C, MS | [667] |
| 1,2-*cyclo*-[—Se(CoCp)$H_2$CPhSe—] | S, H, B, C, MS | [667] |
| 1,2-*cyclo*-[—SCoCp*I-S═$PMe_2$—] | S, X, H, C, P, IR | [664] |
| 1,2-*cyclo*-[—SCoCP—S(*bicyclo*-[2.2.1]heptene-C-(O)Ph] | S, X, H, B | [1385] |
| 1,2-*cyclo*-SCo($C_5Me_4$H)S | S, X, H, B, MS | [1907] |
| 1,2-*cyclo*-SCo($C_5Me_4$H)—CH═C[C(O)($C_5H_4$)FeCp]CH═C[C(O)($C_5H_4$)FeCp]—S S→Co | S, X, H, B, MS | [1907] |
| 1,3-*tricyclo*-SCoCp*C(S)($CO_2$Me)$CH_2$ S—C, S—Co | S, X, H, B, C, IR, MS | [1862] |
| 1,3-*bicyclo*-SCoCp*CH═C($CO_2$Me)CH═C($CO_2$Me)—S S—Co | S, X, H, B, C, IR, MS | [1862] |
| 1,3-*bicyclo*-SCoCp*CH═C($CO_2$Me)C($CO_2$Me)═CH—S S—Co | S, X, H, B, C, IR, MS | [1862] |
| 1,3-*bicyclo*-SCoCp*C($CO_2$Me)═CH—C($CO_2$Me)═CH-S S—Co | S, H, B, C, IR, MS | [1862] |
| 1,3-*bicyclo*-SCoCp*CH═CR—CH═CR—S S—Co R = C(O)Me, C(O)Ph | S, X, H, B, C, IR, MS | [1862] |
| 1,3-*bicyclo*-SCoCp*CR═CH—CH═CR-S S—Co R = C(O)Me, C(O)Ph | S, X, H, B, C, IR, MS | [1862] |
| μ(1,2)-(S-$Co_2Cp_2$-S) | S, H, C, E, IR | [934] |
| μ(1,2)-(S-CoLCp-S[$CHSiMe_3$]) | S, X, H, C, IR | [934] |
| 1,2-*cyclo*-[ECoCp*Fe($CO_3$E] M—Fe E = S, Se | S, X(S), H, B, C, IR | [896] |
| $Co(S_2C_2B_{10}H_{10})_2^{2-}$ (FF) | S | [1503] |
| 1,2-[*cyclo*-SCo(L)Cp*S-] L = CNC$Me_3$, $PMe_3$, $PEt_3$, $PHEt_2$ | S, X[$PHEt_2$], H, C, E, IR | [1374] |
| 1,2-{*cyclo*-EC[C(O)OMe]═CH—C[C(O)OMe]═CH—CoCP—E} E = S, Se | S, X, H, B, C, IR, MS | [935] |
| $Co\left[(\mu-S)_2CH_2CH-CH_2-CB_{10}H_{10}CR\right]_2^{2-}$ R = H, Ph, $CHMe_2$ (FF) | S | [1373] |
| ($N_2C_4H_4$){1,2-[*cyclo*-SCo[$MeC_6H_4$CH-$Me_2$]S] $C_2B_{10}H_{10}$}$_2$ (FF) | S, X, H, B, IR | [673] |

| Compound | Information | References |
|---|---|---|
| 1-$CpRe(CO)_5CoCPh(CO)_2$ | S, X, H, IR, MS | [884] |
| 1-Co(2,2′-bipyridine) | S | [937] |
| 1,2-Co(2,2′-bipyridine) | S | [937] |
| $Cl_2Co\{1\text{-}P[NMe_2]_2\text{-}2\text{-}PPh_2$ | S, IR, UV | [1334] |
| $Cl_2Co\{1\text{-}PPh_2C_2B_{10}H_{11})\}_2$ (FF) | S, IR, UV | [1334] |
| *Cyclo*-$Me_2Si(CB_{10}H_{10}C)_2Co$(2,2′-bipyridine) (FF) | S | [798] |
| $O[(CH_2)_2(C_5H_4)Co(PPh_3)(1,2\text{-}cyclo\text{-}E_2C_2B_{10}H_{10})_2$ E = S, Se (FF) | S, X(S), H, B, C, P, IR | [940] |
| *cyclo*-$C_2N_2O[(C_5H_4N)CoL(\mu\text{-}S)_2(1,2\text{-}C_2B_{10}H_{10})]_2$ $C_2N_2O$ = oxadiazole L = Cp, Cp* (FF) | S, X(Cp*)H, B, C, IR | [941] |
| $\{Ph_2P]_2C_2B_{10}H_{10}\}Co(S_2C_2B_{10}H_{10})$ (FF) | S, MAG | [942] |
| $Co(S_2C_2B_{10}H_{10})_2^{2+}$ (FF) | S, MAG, UV, COND | [942] |
| 1,2-*cyclo*-{—E-Co[*cyclo*-$C_5H_4(CH_2)_2$SEt]-E—} E = S, Se | S, X(S), H, B, IR | [943] |
| 1,2-*cyclo*-{—E-Co[$C_5H_4(CH_2)_2$OMe](CO)-E—} E = S, Se | S, H, B, IR | [943] |
| {1,2-*cyclo*-[—E-Co[$C_5H_4(CH_2)_2$OMe]-E—]}$_2$ E = S, Se | S, X(Se), H, B, IR | [943] |
| 1,2-*cyclo*-[Se-Co{$C_5H_3[CMe_3]_2$}-Se] | S, X, H, IR | [847] |
| 1,2-*cyclo*-[SeRh($C_8H_{12}$)CoCp*Se] | S, X, H, B, IR | [952] |
| 1,2-*cyclo*-[—E$Co_3$Cp′$(CO)_5$E—] Cp′ = Cp, Cp*; E = S, Se | S, X(S,Cp*), H, B, C, IR | [879] |
| $Me_2Si[C_5H_4—Co(\mu\text{-}S)_2C_2B_{10}H_{10}]_2$ (FF) | S, H, B, C, IR | [944] |
| $(\mu\text{-}Me_2Si)_2(C_5H_3)_2[Co(\mu\text{-}S)_2C_2B_{10}H_{10}]_2$ (FF) | S, X, H, B, C, IR | [944] |
| 1-$SCH_2C(O)OEt$-3-CH[C(O)OEt]$CH_2C(O)OEt$-2,4-*cyclo*-1,2-SCHC(O)OEtCoCp O → P | S, X, H, B, C, IR, MS | [1561] |
| 1,3-*cyclo*-SCoCpCHC(O)OEt-2-S(→Co)$CH_2C(O)$-OEt | S, X, H, B, C, IR, MS | [1561] |
| 1-$SCH_2C(O)OEt$-2,3-*cyclo*-S[CH[C(O)OEt] CoCpCH[C(O)OEt] S → Co | S, X, H, B, C, IR, MS | [1561] |
| 1,2-{*cyclo*-SC[C(O)$NHC_{10}H_7$]=CH-CH=C[C(O)-$NHC_{10}H_7$]CoCp*S}CoCp*S} S → Co | S, X, H, B, C, IR, MS | [1563] |
| 1,2-{*cyclo*-SCR=CH-CH=CRCoCp*S} S → Co R = $C(O)C_4H_8(O)$ (2 isomers), $C(O)C_5H_4$FeCp (2 isomers), Ph | S, X, H, B, C, IR, MS | [1563] |
| 1,2-*tricyclo*-CpCo(CHCFc)$S_2$ Fc = $CpFeC_5H_4$ | S, X, H, B, C, IR, MS | [1595] |
| 1,2-*bicyclo*-CpCo(FcC=CH-CH=CFc)$S_2$ Fc = $CpFeC_5H_4$ | S, X, H, B, C, IR, MS | [1595] |
| Co[NR = C(NHR)$CB_{10}H_{10}C—]_2$ 2 C—Co, 2 Ni—Co R = $CHMe_2$, *n*-$C_6H_{11}$ | S, X($CHMe_2$), IR | [1609] |
| 1,2,3-*bicyclo*-{SCH[$CH_2C(O)OMe$]-Co($C_5H_4$)—}-S—Co-promoted B—H and C—H activation | S, X, H, B, C | [1616] |
| 1,3-*cyclo*-[SCo($CH_2CHCCR(O)OEt)C_5H_4$]-2-SCH=CHC(O)OMe R = $CH_2$Ph, $CH_2C(O)OEt$ Co-promoted B—H and C—H activation | S, X, H, B, C | [1616] |

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| Compound | Information | References |
|---|---|---|
| 1,3-*cyclo*-{SCo[*cyclo*-S—$CB_{10}H_{10}C$—S-($C_7H_6$)C(O)OMe)$C_5H_4$]-2-SCH═CHC(O)OMe Co-promoted B—H and C—H activation | S, X, H, B, C | [1616] |
| 1,2-*bicyclo*-SCoCpSNC(R)O R = OMe, Ph | S, X, H, B, C, IR, MS | [1636] |
| 1,2-*bicyclo*-SCoCpN(R)S(R′C═CR″) R = Ts, Ms R′, R″ = H, C(O)OMe, Ph Ts = *p*-toluenesulfonyl Ms = methanesulfonyl | S, X[Ts,C(O)OMe], H, B, C, IR, MS | [1636] |
| 1,2-*bicyclo*-SCoCpSN(R)(R′C═CR″) R = Ts, Ms R′, R″ = H, C(O)OMe, Ph Ts = *p*-toluenesulfonyl Ms = methanesulfonyl | S, X, H, B, C, IR, MS | [1636] |
| 1,2-*bicyclo*-SCoCpSN(R)C═CHCMe$_3$ R = Ts, Ms R′,R″ = H, C(O)OMe, Ph Ts = *p*-toluenesulfonyl Ms = methanesulfonyl | S, X(Ms), H, B, C, IR, MS | [1636] |
| [R′$CB_{10}H_{10}C$—CH(OH)R]$_2CoCl_2$ chelates R′ = H, Me; R = *o*/*m*/*p*-$C_5H_4N$, $C_{10}H_6N$ (2-/4-quinoline) | S, X(H, *o*/*m*/*p*-$C_5H_4N$; Me, *p*-$C_5H_4N$), H, C, B, IR, MAG (H, *o*/*m*/*p*-$C_5H_4N$), UV(H, *o*-$C_5H_4N$), TGA | [1641] |
| [H$CB_{10}H_{10}C$—CH(OH)(*p*-$C_5H_4N$)]$_4CoCl_2$ chelate | S, X, H, B, C | [1641] |
| [H$CB_{10}H_{10}C$—CHO(*o*-$C_5H_4N$)]$_2$Co chelate | S, X, H, B, C | [1641] |
| 1,2-[*cyclo*-SCo ($C_5H_4$Me)S]-3,6-[CH═CHC(O)OMe]$_2$ | S, H, B, C, IR, MS | [1642] |
| 1,2-*cyclo*-SCH═C[C(O)OMe]CH═C[C(O)OMe]-Co($C_5H_4$Me)S}-3-CH═CHC(O)OMe S → Co | S, X, H, B, C, IR, MS | [1642] |
| 1,2,3-{*cyclo*-SCo(L)C[C(O)OMe](S)$CH_2$} L = $C_5H_4$Me, $C_5HMe_4$ S → Co | S, X, H, B, C, IR, MS | [1642] |
| 1,2-{*cyclo*-SCo($C_5Me_4H$)C[C(O)OMe]═CH-C[C(O)OMe]═CHS} S → Co | S, X, H, B, C, IR, MS | [1642] |
| 1-SCH═CHC(O)OMe-2-SCoL$S_2$C-(μ-CR) L = Cp, $C_5H_4$Me, Cp* R = $CHMe_2$, $NC_4H_8$ | S, H, X(Cp,$CHMe_2$), B, C, IR, MS | [1642] |
| 1-SCo[$S_2$C—$CHMe_3$]$_2$-SCH═C[C(O)OMe] CoCp$S_2$C—$CHMe_2$ | S, X, H, B, C, IR, MS | [1642] |
| (μ-CpCo$S_2$)$_2$($C_2B_{10}H_{10}$)$_2$ (FF) | S, X, H, B, IR, MS, E | [1660] |
| $Cp_4Co_4$(u-Se)$_4Co_3$(u-Se)$_8$($C_2B_{10}H_{10}$)$_4$ (FF) | S, X, H, IR, MS | [1813] |
| Co[*cyclo*-S—$CB_{10}H_{10}C$—$SC_7H_5$—C(O)R]$_2$ (FF) $C_7H_5$ = norbornyl R = Me, Ph, styryl, ferrocenyl $2C_{norbornyl}$—B, Co—O | S, X(Ph), H, B | [1679] |
| $Cl_2$Co{*anti*-[($NC_5H_4$)CH(OH)]$_2C_2B_{10}H_{10}$} (FF) 2 Co—N, 2 Co—O | S, X, H, B, IR | [1682] |
| CpCo(μ-Se)$_2C_2B_{10}H_9$-3-$CH_2$C(O)$C_4H_3O$ (FF) | S, X, H, B, C, IR, MS | [1705] |
| CpCo$S_2$($C_2B_{10}H_{10}$)[(*n*-$C_4H_9$)$S_2$-($C_2B_{10}H_{10}$) $S_2Co_2Cp_2$ (FF) | S, X, H, B, IR, MS | [1707] |
| Co$S_2$($C_2B_{10}H_{10}$)$_2^-$ [CpCo$S_3$(*n*-$C_4H_9$)$_3$]$_2$Co$^+$ (FF) | S, X, H, B, IR, MS | [1707] |
| Co$S_2$($C_2B_{10}H_{10}$)$_2^-$ [CpCo$S_3$(*n*-$C_4H_9$)$_3$]Co-[CpCo$S_3$(*n*-$C_4H_9$)$_2$($C_2B_{10}H_{11}$)]$^+$ (FF) | S, X, H, B, IR, MS | [1707] |
| Co$S_2$($C_2B_{10}H_{10}$)$_2^-$ N(*n*-$C_4H_9$)$_4$]$^+$ (FF) | S, X, H, B, IR, MS | [1707] |
| CpCo($S_2C_2B_{10}H_8$)[$CH_2$C═C(O)OMe]-[HC═CHC-(O)OMe (FF) | S, X, H, B, C, IR, MS | [1709] |
| Co($S_2C_2B_{10}H_8$)$_2$[CH = CCH(O)OMe]$_4^-$ (FF) | S, X, H, B, C, IR, MS | [1709] |
| CpCo($S_2C_2B_{10}H_8$)[CH═CHC(O)OMe]$_2$-(HC═C-Fc)[MeO(O)CC═CC(O)OMe] Fc = $CpFeC_5H_4$ (FF) | S, X, H, B, C, IR, MS | [1709] |

| Compound | Information | References |
|---|---|---|
| $[CpCo(\mu\text{-}S)_2C_2B_{10}H_9][C_{12}H_{10}O_2]$ 2-furylpropynone; paramagnetic (FF) | S, X, H, B, IR, MS | [1769] |
| $Cp^*Co(S_2C_2B_{10}H_{10})(C\text{-}CO_2Me)(CHCO_2Me)(NHTs)$ | S, X, H, B, C, IR, MS | [1827] |
| $Cp^*Co(S_2C_2B_{10}H_{10})(CHCO_2Me)(CHCO_2Me)\text{-}(N_3Ts)$ | S, X, H, B, C, IR, MS | [1827] |
| $CpCo(S_2C_2B_{10}H_{10})(CHCO_2Me)$ | S, X, H, B, C, IR, MS | [1827] |
| $CpCo(S_2C_2B_{10}H_{10})(NTs)$ | S, H, B, C, IR, MS | [1827] |
| $CpCo(S_2C_2B_{10}H_{10})(CHCO_2Me)(NTs)$ | S, X, H, B, C, IR, MS | [1827] |
| 1,3-*cyclo*-[S-CoCp-(μ-CHCOOEt)-RCH-CHR′]-2-$SCH_2C(O)OEt$ R = Ph, COOMe R′ = H, COOMe, $C_5H_4FeCp$ | S, X, H, B, C, IR, MS | [1830] |
| 1,3-cyclo-[$S(CH_2COOEt)$-CoCp-RC=CR′]-2-$SCH_2C(O)OEt$ 2(S→Co) R = Ph, COOMe R′ = H, COOMe, $C_5H_4FeCp$ | S, X, H, B, C, IR, MS | [1830] |
| 1,2-*cyclo*-SCoMCp*OCR = NS S→Co | S, X, H, B, C, IR, MS | [1844] |
| $9,12\text{-}\{(CH_2)_3O[(CH_2)_2O]_2-8'-(1',2'\text{-}C_2B_9H_{10})Co(1',2'-C_2B_9H_{11})\}_2^{2-}$ (FF) | S, H, B, C, IR, MS | [1898] |
| $8,9,10,12\text{-}\{(CH_2)_3O[(CH_2)_2O]_2-8'-(1',2'\text{-}C_2B_9H_{10})Co(1',2'-C_2B_9H_{11})\}_4^{4-}$ (FF) | S, H, B, C, IR, MS | [1898] |
| 1,2-*cyclo*-$SCo(MeC_5H_4)S$ | S, H, B, C, IR, MS | [1899] |
| 1,2-*bicyclo*-$SCo_2(MeC_5H_4)_2S$ | S, X, H, B, C, IR, MS | [1899] |
| 1,2-*tricyclo*-$SCo(MeC_5H_4)(CPh)S$ B(3)—CPh | S, X, H, B, C, IR, MS | [1899] |
| 1,2-*cyclo*-S[(OMe)C(O)—C=C—C(O)(OMe)]Co-$(MeC_5H_4)SS$—Co | S, X, H, B, C, IR, MS | [1899] |
| 1-S(CH=CH)C(O)OMe-2,3-*cyclo*-S—Co(S=CR-SH)$(C_5H_3R')$ R = $NC_4H_4$, $CHMe_2$ R′ = H, Me | S, X(R = $CHMe_2$; R′ = H, Me), H, B, C, MS | [1909] |
| 1,2-*bicyclo*-$SCHCH_2C(OMe)=OCo(C_5H_3R)S$ R = H, Me | S, X(H), H, B, C, MS | [1909] |
| 1-SCH=CH[C(O)OMe]-2,3-*cyclo*-S-Co[$CH_2$ $CHC(CH_2R)(CO_2Et)](C_5H_3R')$ R = Ph, Et R′ = H, Me | S, X(R = Ph, R′ = H), H, B, C, MS | [1909] |
| 1-[SCH=CH-C(O)OMe]-2,3-*cyclo*-S-Co{*cyclo*-S—$CB_{10}H_9C$—S[$C_7H_9C(O)OMe$]}$Co(C_5H_3R)$ R = H. Me | S, X(H), H, B, C, MS | [1909] |
| ***Rhodium and iridium*** | | |
| 1,2-$Me_2$-3-$NCRhCl_2Cp^*$ R = H, Me | S, X(Me), IR | [945] |
| 1-$Rh(PPh_3)_2$-2-R R = Me, Ph | S, H, IR, UV | [948] |
| 1,2-$(PPh_2)_2Rh(Cl)L$ L = CO, $PPh_3$ | S, IR | [1354] |
| 1,2-[*cyclo*-(2′-$NC_5H_4$)-$Rh(PPh_3)_2$—S—] | S, X, H, B, C, IR | [269] |
| 1-(terpyridine)RhCl-2-$SiMe_2(t\text{-}C_4H_9)$ | S, X, H | [1336] |
| 1,2-$(\mu\text{-}S)_2RhCp^*(S\text{—}C_5H_4NH)$ | S, X, H, B, C, IR | [929] |
| 1,2-$(\mu\text{-}S)_2RhCp^*C_3N_2Me_2H_3$ imidazole | S, X, H, B, C, IR | [949] |
| 1,2-*cyclo*-[$(CH_2C_5H_4N)RhCp^*L$—S—] L = Cl, $SC_2B_{10}H_{11}$ $CH_2C_5H_4N$ = picolyl (FF) | S, X, H, B, C, IR | [523] |

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| Compound | Information | References |
|---|---|---|
| {$(C_8H_{12})Rh(C_{20}H_{12})_2$-$O_2$P-S—$C_2B_{10}H_{10}$}$^+$ $BF_4^-$ chiral 'thiophosphite (FF) | S, H, B, P | [323] |
| (μ-Cl)$_2${Rh[1,2-*cyclo*-$(OR)_2$P]$_2C_2B_{10}H_{10}$}$_2$ R = *cyclo*-$C_6H_9Me_2(CHMe_2)$, *cyclo*-$C_6H_4$-*p*-$CMe_3$ (FF) | S, X, H, B, C, P, IR, MS | [591] |
| *Cyclo*-$N_3C_3$[$SCH_2C_5H_4N$—Cp*Rh(μ-E)$_2C_2B_{10}H_{10}$]$_3$ E = S, Se helical supramolecular assemblies (FF) | S, H, B, IR | [950] |
| N[$CH_2CH_2$—$N_2$(Me)$C_3$—RhCp*(μ-E)$_2C_2B_{10}H_{10}$]$_3$ E = S, Se imidazolium (FF) | S, X(Se), H, B, C, IR | [1476] |
| 1,2-*cyclo*-(E-Cp*Rh-CpCo-E) E = S, Se | S, X(S, Se), H, B, C, IR | [936] |
| 1,2-*cyclo*-[SeRh($C_8H_{12}$)CoCp*Se] | S, X, H, B, IR | [952] |
| [Cp*M(μ-E)$_2C_2B_{10}H_{10}$]$_2$(*cyclo*-CHNMeCH=CH-N)$_2(CH_2)_2$ E = S, Se; M = Ir, Rh (FF) | S, X(Se,Ir), H, IR | [953] |
| Cp*(L)Rh(μ-S)$_2C_2B_{10}H_{10}$ L = $NC_5H_4$-4-$CH_2Cl$, $NC_5H_4$-4-$CH_2SMe$ (FF) | S, X, H, IR | [954] |
| O[$(CH_2)_2(C_5H_4)$Rh($PPh_3$)(1,2-*cyclo*-$E_2C_2B_{10}H_{10}$)$_2$ E = S, Se (FF) | S, X(Se), H, B, C, P, IR | [940] |
| [Cp*MCl-S(1,2-$C_2B_{10}H_{11}$)]$_2$ M = Rh, Ir CpM*-bridged dimers (FF) | S, X, H, B, IR | [1518] |
| 1-SMClLCp* L = $PPh_3$, *n*-$C_4H_9PPh_2$ | S, X, H, B, IR | [1518] |
| 1-Cp*MLS-$C_2B_{10}H_{11}$ L = $PPh_3$, *n*-$C_4H_9PPh_2$ | S, X, H, B, IR | [1518] |
| μ(1,2)-(S-$M_2$Cp*$_2$-S) M = Rh, Ir | S, H, C, E, IR | [934] |
| 1,2-*cyclo*-LM(μ-Cl)$_2$ML M = Rh, Ir; L = Cp*, 1,3-$C_5H_3(CMe_3)_2$ | S, X, H, B, IR | [1470] |
| {1,2-*cyclo*-CMe(=$CH_2$)—RhCl($PPh_2$)$C_2B_{10}H_{10}$}$_2$ (FF) | S | [1368] |
| *Cis*-1,2-[-$PR_2$-Rh(Cl)(CO)-R′$_2$P—] R = Ph, $NMe_2$; R′ = Ph, $NMe_2$, H | S, C, P, IR | [1341] |
| X(H)Rh(-E,-B)($NC_5H_4R$)$_2$[1-$Ph_2ECH_2$—$C_2B_{10}H_{11}$] R = H, Me, C(O)OMe; E = P, As; X = Cl, I (FF) | S, H, B, P, IR | [956] |
| (CO)ClRh[1-$Ph_2PCH_2$-$C_2B_{10}H_{11}$]$_2$ (square planar) (FF) | S, H, P, IR | [956] |
| 1,2-*cyclo*-[ERhCp*Fe$(CO)_3$E] (M—Fe) E = S, Se | S, X(S,Se), H, B, C, IR | [896] |
| Cl{($Ph_3P$)Rh[$Ph_2P$]$_2C_2B_{10}H_{10}$ (FF) | S, H, B, P, IR | [921] |
| 1,2-*cyclo*-[S-$ML_2$-$NMe_2$-$CH_2^-$] M = Rh, Ir; $L_2$ = $(CO)_2$, $\eta^4$-$C_8H_{12}$ | S, X(Rh), H, B, C, MS | [957] |
| 1,2-*cyclo*-[-S-$M_2(C_8H_{12})_2$-S-] M = Rh, Ir | S, X(Rh), H, C, IR, E | [664] |
| [(1,2-*cyclo*-E-RhCp*-E)$C_2B_{10}H_{10}$]$_2$Mo(μ-CO)$_2$ E = S, Se (FF) | S, X, H, B, C, IR | [672] |
| 1,2-*cyclo*-$S_2$RhCp*$C_3N_2H_3$Me-NHCH=$CH_2$) imidazoline; carbene | S, X, H, B, C | [914] |
| {1,2-*cyclo*-SeRh{$C_5H_3$[C(Me)$_3$]$_2$}W$(CO)_4$Se} $C_2B_{10}H_{10}$ (FF) | S, X, H, B, C, IR | [672] |
| *Exo*-Cp*Rh(μ-S)$_2$-1,2-$C_2B_{10}H_8$-3,6-[CH=CHC(O)OMe)$_2$ (FF) | S, X, H, B, C, Rh, MS | [959] |

| Compound | Information | References |
|---|---|---|
| {1,2-*cyclo*-[-S-M(CO)-$PPh_{2^-}$]$C_2B_{10}H_{10}$}$_2$ M = Rh, Ir (FF) | S, X, H, C, P, IR | [960] |
| 1,2-*cyclo*-[-S-M(CO)$PEt_3$-$PPh_{2^-}$]$C_2B_{10}H_{10}$ M = Rh, Ir (FF) | S, X, H, C, P, IR | [960] |
| {1,2-*cyclo*-Cp*Rh[HC≡C[C(O)OMe]-(μ-Se)$_2$$C_2B_{10}H_{10}$}$_2$ (FF) | S, H, B, C, Se, IR, MS | [970] |
| Cp*Rh(μ-Se)[μ-CH═C[C(O)OMe]CH═C[C(O)-OMe]Se]$C_2B_{10}H_{10}$ (two isomers) (FF) | S, H, B, C, Se, IR, MS | [970] |
| 1,2-*cyclo*-[(μ-S)$_2$CPhCH$_2$Cp*M]$C_2B_{10}H_{10}$ M—B M = Rh, Ir (FF) | S, X, H, B, C, Rh, IR, MS | [961] |
| 1,2-*cyclo*-(E-Cp*Rh-E)$C_2B_{10}H_{10}$ E = S, Se (FF) | S | [1357] |
| 1,2-*cyclo*-E-Rh{$C_5H_3$[$CMe_3$]$_2$}-E E = S, Se | S, X(Se), H, B, C, IR | [991] |
| [1,2-(*cyclo*-ERhCp*S)$C_2B_{10}H_{10}$]$_2$(μ-CO)$_2$W E = S, Se (FF) | S, X, H, B, C, IR | [962] |
| M{[μ-Se(*n*-$C_4H_9$)Cp*Rh](μ-Se)$_2$$C_2B_{10}H_{10}$}$_2$ M = Ni, Pd (FF) | S, X, H, B, C, IR | [850] |
| $N_3C_3$[($C_5H_4N$)RhCp*(*cyclo*-$S_2C_2B_{10}H_{10}$)]$_3$ $N_3C_3$ = triazine (FF) | S, X, H, B, IR | [670] |
| L[($C_5H_4N$)MCp*(*cyclo*-$S_2C_2B_{10}H_{10}$)]$_2$ M = Rh, Ir; L = pyrazine, 1,2-di(4-pyridylethylene, 4,4′-dipyridine, diisonicotinic acid 1,4-phenylene diester (FF) | S, X (Rh, pyrazine; Ir, dipyridylethylene; Ir, diisonicotinic acid phenylene diester), H, B, IR | [670] |
| 1,2-[*cyclo*-SRh($C_8H_{12}$)IrCp*S]$C_2B_{10}H_9$ (B-Ir) (FF) | S, X, H, B, C, IR | [1466] |
| 1,2-*bicyclo*-[S—RhCp*—S—NS(O)$_2$- *p*-$C_6H_4$Me] O→Rh cytotoxic activity toward A549 and NCI-8460 cancer cell lines | S, X, H, B, C, IR, MS | [1629] |
| 1,2-*cyclo*-$E_2Ir_2$($C_8H_{12}$)$_2$ E = S, Se | S, X(S), H, B, C, IR | [963] |
| Cp*Ir(μ-E)$_2$($C_2B_{10}H_{10}$)Rh($C_8H_{12}$) E = S, Se (FF) | S, H, B, MS | [964] |
| Cp*Ir(u-E)$_2$($C_2B_{10}H_9$)$Rh_2$($C_8H_{12}$)Cp*Ir(μ-S)$_2$($C_2B_{10}H_{10}$) E = S, Se (FF) | S, X, H, B, MS | [964] |
| 1-{$C_6H_3$-3′,5′-[$C_6H_2$-2″,4″,6″-($CHMe_2$)$_3$]$_2$}-2-P($CHMe_2$)$_2$-Rh($CO$)$_3$} terphenyl | S, H, IR | [1841] |
| *Exo*-Cp*Rh{-S-HC═C[C(O)OMe]CH═C[C(O)-OMe]}(μ-S)-1,2-$C_2B_{10}H_{10}$ (FF) | S, X, H, B, C, Rh, IR, MS | [965] |
| (*cyclo*-N═C–O-C═N)($C_5H_4N$)$_2$[1,2-*cyclo*-ECp*IrE($C_2B_{10}H_{10}$)]$_2$ E = S, Se oxadiazole (FF) | S, X, H, B, IR | [673] |
| 1,2-[μ-$Ph_2P$][μ-$CH_2NMe_2$]M($C_8H_{12}$)$^+$ M = Rh, Ir | S, X, H, B, C, P, IR | [572] |
| 1,2-*cyclo*-[-S-M($C_8H_{12}$)$PPh_{2^-}$] M = Rh, Ir | S, X, H, C, P, IR | [1383] |
| 1,2-*cyclo*-Cp*Rh(HC≡CH)(μ-S)$_2$ | S, H, B, C, Rh, IR, MS | [923] |
| 1,2-*cisoid*/*transoid*-Cp*(RC≡CH)Rh(μ-S)$_2$ R = Me, $CH_2OMe$ | S, X(*trans*, $CH_2OMe$), H, B, C, Rh, IR, MS | [923] |
| μ(1,2)-{—ERh[$C_5H_3$(*t*-$C_4H_9$)$_2$]E—} E = S, Se | S, X(S), H, B, IR, MS | [1379] |
| 1,2-*cyclo*-[($CH_2C_5H_4N$)ClCp*Ir—] picolyl catalyst for $C_2H_4$ polymerization with MAO | S, X, H, B, C, IR | [523] |
| Cp*(L)Ir(μ-S)$_2$$C_2B_{10}H_{10}$ L = $PMe_3$, CN(*t*-$C_4H_9$), CO (FF) | S, X ($PMe_3$), H, C, IR | [967] |
| 1-Ir(H)(X)(CO)$L_2$-2-R R = H, Me, Ph; X = Cl, Br, I; L = $PPh_3$, $PMePh_2$ | S, H, IR | [1388] |

*Continued*

| Compound | Information | References |
|---|---|---|
| 1-$(PPh_3)_2$Ir(CO)-2-R R = H, Me | S, H, IR | [519] |
| 1-$(PPh_3)_2$Ir(CO)-2-$C_6H_4$-[Ir] | S, H, IR | [519] |
| 3-IrHCl[$EPh_3$]$_2$ E = P, As | S, H, B, IR | [551] |
| 1,2-Cp*Ir(S)(HRC=CR′-S) R, R′ = H, Ph, C(O)OMe | S, X(H, Ph), H, B, C, IR | [969] |
| 1,2-*cyclo*-Cp*Ir(S)[$Me_3$Si-$CH_2$-S] | S, X, H, B, C, IR | [969] |
| 1,2-*cyclo*-Cp*Ir(μ-Se)CH[C(O)OMe]CH(μ-Se)-$C_2B_{10}H_{10}$ Ir—B (2 isomers) (FF) | S, H, B, C, Se, IR, MS | [970] |
| 1,2-*cyclo*-[(μ-Se)$_2$CPh$CH_2$Cp*Ir]$C_2B_{10}H_{10}$ Ir—B (FF) | S, X, H, B, IR, MS | [961] |
| $C_3N_3$[($C_5H_4$N)Cp*Ir(μ-S)$_2C_2B_{10}H_{10}$]$_3$ $C_3N_3$ = triazine (FF) | S, X, H, B, IR, UV | [971] |
| $C_3N_3$[($C_5H_4$N)RhCp*(*cyclo*-$S_2C_2B_{10}H_{10}$)]$_3$ $C_3N_3$ = triazine (FF) | S, X, H, B, IR | [670] |
| Cl(H)Ir(-E,-B)(1,5-$C_8H_{12}$)$_2$[1-$Ph_2ECH_2$-$C_2B_{10}H_{11}$] R = H, Me, C(O)OMe; E = P, As (FF) | S, H, B, P, IR | [956] |
| (CO)Cl($Ph_3P$)Ir[C≡C–$C_2B_{10}H_{11}$][CH=CH-$C_2B_{10}H_{11}$] (FF) | S, X, H, IR | [973] |
| ($Ph_3P$)$_2$(CO)(Cl)Ir[CH=CH-1,2-$C_2B_{10}H_{11}$][C≡C–$C_2B_{10}H_{11}$] (FF) | S, X, B, IR, UV, MS | [261] |
| *Exo*-Cp*Ir(μ-E)$_2$-1,2-$C_2B_{10}H_9$-3-CH=CHC(O)-OMe E = S, Se (*cis*, *trans*) (FF) | S, X(Se), H, B, C, Se, IR, MS | [974] |
| *Trans*-($C_8H_{12}$)Ir[(μ-Se)$_2$-$C_2B_{10}H_8$(OEt)]Ir[(μ-Se)$_2$-$C_2B_{10}H_{10}$)]IrCp* (FF) | S, X, H, B, IR | [975] |
| *Cis*-($C_8H_{12}$)Ir[(μ-Se)$_2$-$C_2B_{10}H_8$(OEt)]Ir[(μ-Se)$_2$-$C_2B_{10}H_9$)]IrCp* (FF) | S, X, H, B, IR | [975] |
| 1,2-*cisoid*/*transoid*-Cp*(RC≡CH)Ir(μ-E)$_2$ R = H, Me, $CH_2$OMe; E = S, Se | S, X(H,S), H, B, C, Se, IR, MS | [923] |
| [($Me_3$C)NC]$_2$($\eta^2$-$C_{60}$)Ir[*cyclo*-($CH_2$P)$C_2B_{10}H_{11}$-] [B(3)-$C_{60}$] fullerene complex (FF) | S, X, H, P, IR, UV | [1454] |
| *Cyclo*-1,B(4)-[Cp*Ir$H_2$-SiH$R_2^-$]$C_2B_{10}H_{10}$ R = Me, Et (FF) | S, X(Me), H, B, C, Si, IR | [1384] |
| 1,2-*cyclo*-[EIrCp*$Co_2$(CO)$_5$E] E = S, Se | S, X, H, B, C, IR | [907] |
| {1,2-*cyclo*-[Se-Cp*Ir-Se]$C_2B_{10}H_{10}$}$_2$Mo(CO)$_2$ (FF) | S, X, H, B, IR | [978] |
| $C_6S_4H_2$[$C_5H_4$N-IrCp*(μ-E)$_2$-1,2-$C_2B_{10}H_{10}$]$_2$ (FF) E = S, Se $C_6S_4H_2$ = 1,4,5,8-tetrathiafulvalene | S, X(S), H, B, IR | [979] |
| 1,2-*cyclo*-$Ph_2$P=S—M($C_5Me_5$)—$C_2B_{10}H_{11}$ M = Rh, Ir | S, X, H, P, I | [1736] |
| 1,2-*cyclo*-$Ph_2$P=S—Rh[($C_5Me_5$)—$C_2B_{10}H_{11}$]—S | S, X, H, P, I | [1736] |
| 1,2-*cyclo*-$Ph_2$P=S—RhCp*($C_2B_{10}H_{11}$)—S | S, X, H, P, I | [1736] |
| 1,2-*cyclo*-$Ph_2$P=S—MCp*Cl M = Ir, Rh M = Ir, norbornene polymerization catalyst | S, X(Ir), H, B, C, P, IR | [1596] |
| 1,3,2-*bicyclo*-$Ph_2$P=S—IrCp*S— S→C(2) | S, X, H, B, C, P, IR | [1596] |
| *Cis*-[($Me_3$C)$_2$P—$C_2B_{10}H_9$-3-Rh(CO)]$_2$(μ-Cl)$_2$ Rh—Rh | S, X, H, B, C, P, MS | [1607] |
| *Cis*-($Me_2C_3HO_2$)Ir($NC_5H_4$-$C_6H_3$—$CB_{10}H_{10}CMe$)$_2$ (2 isomers) color tuning | S, X, H, B, C, UV, E, phosphorescence emission | [1651] |

| Compound | Information | References |
|---|---|---|
| 1,3-*cyclo*-[IrCp*NR=C(NHR)]-1,2-$C_2B_{10}H_9$-μ(C, Ir)-Se R=$CHMe_2$, *cyclo*-$C_6H_{13}$ (FF) | S, X($CHMe_2$, *n*-$C_6H_{13}$), H, B, C, IR | [1652] |
| $(N_2C_{12}H_8)Ir(N_2C_{10}H_8-1,2-CB_{10}H_{10}CH)_2^+$ $PF_6^-$ (FF) | S, X, H, B, C, MS, UV, phosphorescence | [1666] |
| 1,2-*cyclo*-Ir(RR′)$_2$($NC_5H_4$) $C_{carborane}$—$C_5H_4N$ RR′=O-$C_6H_4$Ph-$C_5H_4$NMe, 2′-Me-4′,6′-$F_2C_6H_2$-1′-$C_5H_4$NMe | S, X, U, E, luminescence | [1676] |
| $(NC_5H_5$-$CN_4)Ir[NC_5H_5$—*m*/*p*-$C_6H_4$—$C_2B_{10}H_9]^{n+}$ *n*=0,1 (FF) | S, X, H, B, C, MS, E, UV, phosphorescence/luminescence | [1824] |
| 1,2-*cyclo*-$OIr_2Cp^*_2$(μ-S) Ir—Ir, Ir—B | S, X, H. B, IR | [1706] |
| $(Me_2C_3HO_2)Ir(NC_5H_4$-$C_6H_3$-$CB_{10}H_{10}CR)$ 2 Ir-$C_6H_3$ acetylacetonate R=H, Me, $CHMe_2$, *i*-$C_4H_9$, Ph, $C_6H_4CF_3$, $C_6F_5$ (FF) | S, X, UV, E, phosphorescence | [1848] |
| [R—$CB_{10}H_{10}$C—$NC_5H_4$—$C_8H_4S]_2Ir(O_2C_3Me_2H)$ R=Me, *n*-$C_4H_9$ pyridyl, benzothienyl, acac phosphorescence (FF) | S, H, B, C, UV, E, electroluminescence | [1710] |
| $(SC_4H2$—$C_5H_4N)Ir[(N_2C_{10}H_6(CH$═C—$CB_{10}H_{10}CH)_2]^+$ $PF_6^-$ thienylpyridyl, 2,2′-bipyridyl | S, X, H, B, C, UV(absorption and emission), MS | [1859] |
| *Cyclo*-{1,2-$(O_2C)_2C_2B_{10}H_8$-4,10-[IrCp*(*cyclo*-$NC_4H_4N)IrCp^*]_2$-4,10-$H_8B_{10}C_2(CO_2)_2$} 4 B—Ir (FF) | S, X, H, B, MS | [1729] |
| 1,2-*cyclo*-S—$IrCp^*NHC_6H_3(NO_2)$—S S→Ir (two isomers) | S, X, H, B, IR, MS | [1748] |
| 1,2-cyclo-S—Ir[$C_5Me_4$—$CH_2$—$C_6H_3(NO_2)(NH_2)$] —S | S, X, H, B, IR, MS | [1748] |
| 1,2-*bicyclo*-S—Ir[$C_5Me_4$—$CH_2$—$C_6H_3(NO_2)$ $(NH_2)$]—S—$C_6H_3(NO_2)$NH two isomers S→Ir N→Ir | S, X(1 isomer), H, B, IR, MS | [1748] |
| 1,3-*cyclo*-C(═NPh)—S—MCp*(CNPh) M=Rh, Ir | S, X, H, B, IR | [1837] |
| 1,2-*cyclo*-C(NHPh)═S—MCp*Cl M=Rh, Ir | S, X, H, B, IR | [1837] |
| 1,2-*cyclo*-SN$(SO_2C_6H_4Me)$RhCp*N-$(SO_2C_6H_4Me)$-S S→Rh | S, X, H, B, C, IR, MS | [1844] |
| 1-$SNHSO_2C_6H_4Me$-2,3-cyclo-SN$(SO_2C_6H_4Me)$ IrCp* | S, X, H, B, C, IR, MS | [1844] |
| 1,2-*cyclo*-SMCp*OCR═NS S→M M=Co, Rh, Ir | S, X, H, B, C, IR, MS | [1844] |
| 1,2-*cyclo*-SIr($C_5Me_4$-$CH_2$NHCPh═O)S O→Ir | S, X, H, B, C, IR, MS | [1844] |
| 1,3-*cyclo*-$P(CHMe_2)_2Ir(C_8H_{12})$ | S, X, H, B, C, P, IR, MS | [1929] |
| μ(1,1′)-Cp*M-(2,2′-$C_2B_{10}H_{11})_2$ M=Rh, Ir | S, X(Ir), H, B(Ir), IR(Ir) | [1914] |
| μ(1,1′)-Cp*(CO)Ir-(2,2′-$C_2B_{10}H_{11})_2$ | S, H, IR, MS | [1914] |
| *Nickel* | | |
| 1,2-*cyclo*-$ClNi_2(PPh_2)_2$ | S | [980] |
| $(μ\text{-}Br)_2Ni_2[1,2\text{-}(PPh_2)_2C_2B_{10}H_{10}]_2$ (FF) | S, X, H, C, IR | [981] |
| $Ni_2(μ\text{-}E)_3(C_2B_{10}H_{10})_3^{2-}$ E=S, Se (FF) | S, X(S), IR | [982] |
| $Cl_2Ni[Ph_2P$—$CB_{10}H_{10-n}Br_nC$—$PPh_2]_2$ *n*=0,1,2,3 (FF) | S, UV, COND, MAG | [980] |

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| Compound | Information | References |
|---|---|---|
| 1,2-*cyclo*-(μ-S)$_2$Ni(PPh$_2$)$_2$ | S, MAG, COND | [942] |
| 1,2-*cyclo*-Cl$_2$Ni(PPh$_2$)$_2$ | S, MAG | [942] |
| {Ph$_2$P]$_2$C$_2$B$_{10}$H$_{10}$}Ni(S$_2$C$_2$B$_{10}$H$_{10}$) (FF) | S, MAG, COND | [942] |
| 1,2-*cyclo*-Ni[Ph$_2$P(CH$_2$)$_2$PPh$_2$] carboryne complexes | S, X, H, B, C, P, IR | [1527] |
| 1,2-*cyclo*-Ni(PR$_3$)2-3-X carboryne complexes X = Ph, Br; R = Ph, Me | S, X, H, B, C, P, IR | [1527] |
| 1,2-Ni(PR$_3$)$_2$-9-I carboryne complexes R = Ph, Me | S, X, H, B, C, P, IR | [1527] |
| 1,2-*cyclo*-Ni(PR$_3$)$_2$-9,12-I$_2$ carboryne complexes R = Ph, Me | S, X, H, B, C, P, IR | [1527] |
| 1,2-*cyclo*-[-Me)$_2$Si-N(PEt$_3$)$_2$-SiMe$_2$-] | S, X, H, C, P, Si | [313] |
| 1,2-{*cyclo*-(PPh$_2$)$_2$NiX$^{3-}$ X = Cl, Br, I | S | [1310] |
| 1,2-*cyclo*-I$_2$NiPh$_2$P]$_2$ X = Cl, Br | S, MAG, UV, COND, IR | [931] |
| Ni(S$_2$C$_2$B$_{10}$H$_{10}$)$_2^{2-}$ (FF) | S | [1503] |
| 1-R-2-CS$_2$Ni(S$_2$C–C B$_{10}$H$_{10}$C–R)(PR′$_3$)$_n$ R, R′ = Me, Ph; $n$ = 1, 2 (FF) | S, H(var. temp.), UV | [985] |
| *cyclo*-Me$_2$Si(CB$_{10}$H$_{10}$C)$_2$Ni(2,2′-bipyridine) (FF) | S | [798] |
| [2,2′-(1,1′-C$_2$B$_{10}$H$_{10}$)$_2$]$_2$Ni$^{2-}$ (FF) | S, H, B, E, IR, UV | [938] |
| $\mathrm{Ni}\left[(\mu-\mathrm{S})_2\mathrm{CH_2CH}-\mathrm{CH_2}-\mathrm{CB_{10}H_{10}CR}\right]_2^{2-}$ R = H, Ph, CHMe$_2$ (FF) | S | [1373] |
| X$_2$Ni{*cyclo*-(PPh$_2$)[PMe$_2$N)$_2$]C$_2$B$_{10}$H$_{10}$} X = Cl, Br, I, NCS (FF) | S, MAG, COND, IR, Raman | [986] |
| $[1,2-cyclo-\mathrm{PPh_2}-\mathrm{Ni}-\mathrm{Ph_2P}-\mathrm{C_2B_{10}H_{10}}]_2^{2-}$ (FF) | S, MAG, COND, UV | [987] |
| 1,2-Ni(2,2′-bipyridine) | S | |
| Ni[(1-CH$_2$C$_5$H$_4$N)C$_2$B$_{10}$H$_{10}$]$_2$ catalyst for addition polymerization of norbornene in the presence of MAO (FF) | S, X, H, IR | [522] |
| 1,2-*cyclo*-(CH$_2$)$_2$Ni(PPh$_3$)$_2$ | S | [743] |
| X$_2$Ni{(Ph$_2$P)C$_2$B$_{10}$H$_{11}$}$_2$ X = Cl, Br, SCN (FF) | S | [1413] |
| 1-CpNiPPh$_3$ | S | [988] |
| L$_2$Ni{[OC(O)]C$_2$B$_{10}$H$_{11}$}$_2$ (L$_2$ = 2H$_2$O, 2,2′-bipyridine) (FF) | S | [988] |
| 1,2-*cyclo*-[CH$_2$PPh$_2$Ni(CO)$_2$PPh$_2$] | S | [1492] |
| (C$_2$B$_{10}$H$_{10}$)$_3$Ni$_3$(CH$_2$CHC$_6$H$_4$N)$_3$Cl$^-$ | S, X | [309] |
| 1,2-*cyclo*-CH$_2$CH[C(O)OMe]NiPPh$_3$ | S, H, B, C | [309] |
| (porphyrin)Ni[*m*/*p*-C$_6$H$_4$-(CH$_2$)$_n$-CB$_{10}$H$_{10}$CMe]$_4$ $n$ = 0,1 (FF) | S, H(activation energy for rotation) | [989] |
| (CO)$_2$Ni[PPh$_2$)]C$_2$B$_{10}$H$_{10-n}$X$_n$ $n$ = 0–3; X = Cl, Br; Y = CO, Cl, Br (FF) | S, IR | [560] |
| 1,2-*cyclo*-[—Ph$_2$P-NiX$_2$-PPh$_2$—] X = CO, Cl, I | S | [895] |
| 1,2-*cyclo*-{(GeMe$_2$]$_2$Ni(PEt$_3$)$_2$} | S, X, H, C, P | [990] |

| Compound | Information | References |
|---|---|---|
| 1,2-*cyclo*-{$(GeMe_2]_2$-Ni$(PEt_3)_2$-$(GeMe_2]_2$} | S, X, H, C, P, MS | [812] |
| {1,2-*cyclo*-E-Rh[$C_5H_3CMe_2$-E]$C_2B_{10}H_{10}$}$_2$Ni Rh—Ni—Rh E = S, Se (FF) | S, X, H, B, C, IR | [991] |
| Ni[CpCo)(1,2-*cyclo*-$E_2$)$C_2B_{10}H_{10}]_2$ E = S, Se (FF) | S, X(S), H, B, C, IR | [879] |
| Ni{[μ-Se(*n*-$C_4H_9$)Cp*Rh](μ-Se)$_2C_2B_{10}H_{10}\}_2$ (FF) | S, X, H, B, C, IR | [850] |
| 1,2-*cyclo*-[$PPh_2$—$NiCl_2$—$Ph_2P$] | S, X, H. B, IR | [1548,1574] |
| | C, P | [1574] |
| 1,2-*cyclo* –$(Ph_2P)_2$Ag(μ-Cl)$_2$Ni[*nido*-7,8-$(Ph_2P)_2C_2B_9H_{12}]_2$(μ-Cl)$_2Ag_2$ | S, X, H. B, IR | [1548] |
| (μ-Cl)$_2Ag_2[(Ph_2P)_2C_2B_{10}H_{10}]_2$ (FF) | S, X, H, B, IR | [1548] |
| (μ-$SO_3CF_3)_2Ag_2[(Ph_2P)_2C_2B_{10}H_{10}]_2$ (FF) | S, X, H, B, IR | [1548] |
| Review of transition metal-carboryne complexes | | [1546] |
| Ni[$CB_{10}H_{10}$-$PPh_2$═S—]$_2$ 2 Ni—S | S, X, H, P, IR | [1591] |
| Ni[NR═C(NHR)$CB_{10}H_{10}$C—]$_2$ | | |
| 2 C—Ni, 2N—Ni R = $CHMe_2$, *n*-$C_6H_{11}$ | S, X($CHMe_2$), IR | [1609] |
| 1,2-μ-[Ni$(PPh_2)_2C_2H_2$Ni$(PPh_2)_2C_2H_4$] carboryne complex | S, X, H, B, C, P, IR | [1701] |
| ***Palladium and platinum*** | | |
| 1,2-*cyclo*-{$(Ph_3P)_2PdCl_2$} | S | [1435] |
| 1-$Ph_2P$-2-(P[$NMe_2]_2$)$PdCl_2$ | S | [1435] |
| 1,2-[*cyclo*-(2′-$NC_5H_4$)-PdCl$(PPh_3)$—S—] | S, X, H, B, C, IR | [269] |
| 1-Pd(2,2′-bipyridine)-2-$C_6H_4$ | S | [1155] |
| 1-$PdBr_2$(2,2′-bipyridine)-2- $C_6H_4$ | S | [1155] |
| 1,2-*cyclo*-[—$Ph_2P$-$PdCl_2$-$PPh_2$—] | S | [895] |
| *Cyclo*-$Me_2Si(CB_{10}H_{10}C)_2$Pd(2,2′-bipyridine) (FF) | S | [798] |
| 1-R-2-$CS_2M(S_2C$–$CB_{10}H_{10}C$–R)$(PR'_3)_n$ M = Pd, Pt; R, R′ = Me, Ph; *n* = 1, 2 (FF) | S, H(var. temp.), UV | [985] |
| 1-*cis*-$(Et_2MeP)_2$PtH-2-R R = H, Me, Ph | S, H, IR | [994] |
| 1-*cis*-$(PhMe_2P)_2$PtH-2-Ph | S, H, IR | [994] |
| 1,2-*cyclo*-M$(NEt_2CH_2)$ M = Pd, Pt | S | [995] |
| [*cyclo*-$AsMe_2CH_2$-$CB_{10}H_{10}C$–]$_2$M M = Pd, Pt (FF) | S | [742] |
| 1,2-*cyclo*-$(CH_2)_2M(PPh_3)_2$ M = Pd, Pt | S | [743] |
| $(Ph_3P)_2$M(1-C≡C–1,2-$C_2B_{10}H_{11})_2$ M = Pd, Pt (FF) | S | [996] |
| (2,2′-bipyridine)Pd$(C_2B_{10}H_{11})_2$ (FF) | S | [997] |
| 1,2-*cyclo*-[(2,2′-bipyridine)Pd | S | [997] |
| 1,2-*cyclo*-Pd$(CO_2)$OCO | S | [997] |
| *Trans*-$Cl_2M[Ph_2PCH_2C_2B_{10}H_{11}]_2$ M = Pd, Pt (FF) | S | [998] |
| [ClPd$Ph_2PCH_2C_2B_{10}H_{10}$-4]$_2$ (FF) | S | [998] |
| $L_2$ClPd[1,4-*cyclo*-$Ph_2PCH_2C_2B_{10}H_{10}$-] L = 2,2′-pyridine, $PEt_3$ (FF) | S | [998] |

*Continued*

| Compound | Information | References |
|---|---|---|
| $[Ph_2PCH_2CH_2PPh_2]Pd[1,4\text{-}cyclo\text{-}Ph_2PCH_2C_2B_{10}H_{10}\text{-}]^+$ (FF) | S | [998] |
| $\{1,2\text{-}(PPh_2)_2C_2B_{10}H_{10}\}_nPd^0$ dual-mode catalysts for synthesis of allenes from aryl iodides (FF) | S | [1401] |
| 1-R-2-$CH_2NR'_2Pd$ (Cl)($NC_5H_4$-*p*-Me) N—Pd—B R = H, Ph; R′ = Me, Et | S | [1369] |
| 1,2-*cyclo*-[-$Ph_2P$-$PdX_2$-$PPh_2$-] X = Cl, Br? | S, IR, Raman, UV, MAG, COND | [999] |
| 1,2-*cyclo*-[-$[(Me)_2N]_2P$-$PdX_2$-$PPh_2$-] X = Cl, Br? | S, IR, Raman, UV, MAG, COND | [999] |
| *Cyclo*-$\{R[(CH_2)_nPPh_2]C_2B_{10}H_{10}\text{-}Pd(Cl)\}_2$ R = $(Me)_2CH$, Me, H; *n* = 3, 7 (FF) | S, H, B, P | [1420] |
| $(PEt_3)(Et_2PCH_2CH_2)Pd(RC_2B_{10}H_{10})$ R = Me, Ph (FF) | S, H, P, IR | [1000] |
| 1-R-2-SM($PMe_2Ph$)pyCl R = H, Ph; M = Pd, Pt | S, X(Pd,py), H, P | [1002] |
| *Trans*-Pd($PEt_3$)L(S-$CB_{10}H_{10}C$-Ph)$_2$ L = $PEt_3$, py (FF) | S, X, H, P | [1002] |
| $\{(Ph_2P)(Me_2Sn)C_2B_{10}H_{10}\}_2Pd$ (FF) | S, X, H, C, P, Sn | [824] |
| 1,2-*cyclo*-[$R_2P$-PdClMe-$PR_2$] R = Ph, $CHMe_2$ | S, X, H, C, P, IR | [1412] |
| 1,2-*cyclo*-{-$MMe_2$-$Pd(PPh_3)_2$-$MMe_2$-} M = Ge, Sn | S, H, C, P, Sn, MS | [809] |
| $[Me_2M\text{-}CB_{10}H_{10}C\text{–}PPh_2]_2Pd$ M = Si, Ge (FF) | S, X(Si), H, C, P, Si | [1004] |
| $(C_3H_7)Pd(1,2-Me_2-9-O-\text{bicyclo}-PC_5H_9N_2Ph)_2^+$ diamidophosphite asymmetric catalyst for allylic alkylation | S, B, C, P | [1392] |
| *Cis*-Pd$\{(Me_2Si)(L_2P)C_2B_{10}H_{10}\}_2$ L = Me, Et, Ph (FF) | S, X(Ph), H, C, P | [584] |
| $Pd\{[\mu\text{-}Se(n\text{-}C_4H_9)Cp^*Rh](\mu\text{-}Se)_2C_2B_{10}H_{10}\}_2$ (FF) | S, X, H, B, C, IR | [850] |
| $(Et_3P)_2Pd(Se—CB_{10}H_{10}C—Ph)_2$ | S, X, H, P, Se | [1534] |
| $(R_3P)_2Pd(Se—CB_{10}H_{10}C—Ph)_2$ $R_3P = PMe_2Ph$, $PMePh_2$ | S, X($PMe_2Ph$), H, P, Se | [1534] |
| $Cl_3M_2(R_3P)_2$-μ-Se—$CB_{10}H_{10}C$—Ph M = Pd, $PR_3 = PMe_2Ph$; M = Pt, $PR_3 = PEt_3$ | S, X(Pd,$PMe_2Ph$), H, P, Se, Pt | [1534] |
| Ph—$CB_{10}H_{10}C$—Se—$Pd_2(PEt_3)_2Cl_2$-μ-Se—$CB_{10}H_{10}C$—Ph | S, X, H, P, Se | [1534] |
| 1-SPtCl(bipyridyl) | S, H(2d), B, C, Pt | [1006] |
| 1-SPtCl(phenanthroline) | S, H(2d), B, C, Pt | [1006] |
| (NN)Pt(S-$C_2B_{10}H_{11})_2$ NN = bipyridyl, phenanthroline (FF) | S, X(bipyridyl), H(2d), B, C, Pt | [1006] |
| *Cis*-$Cl_2Pt\{2,2'\text{-}N_2C_{10}H_6[C(O)O(CH_2)_3CB_{10}H_{10}CR]_2\}$ R = H, Me bipyridyl | S, H, B, C, IR | [510] |
| 1-$(CH_2)_n$S-Pt(terpyridyl)$^+$ $OSO_2CF_3^-$ *n* = 0–3 | S, H, B, C, MS, cytotoxicity | [633] |
| 1-$CH_2OCH(CH_2OH)_2$-2-SPt(terpyridyl)$^+$ $OSO_3CF_3^-$ | S, H, B, C, Pt, MS | [1335] |
| 1-$CH_2$SPt(terpyridyl)$^+$ $OSO_3CF_3^-$ | S, H(2d), B, C, Pt, MS, cell toxicity | [1474] |
| 1-*cis*-Pt($PEt_3)_2H$ | S, H | [1008] |
| 1-*trans*-Pt($PEt_3)_2$H-2-R R = Me, Ph | S, H | [1008] |
| 1-*cis*-Pt($PEt_3)_2$H-2-R R = H, Ph | S, H, IR | [994] |
| 1-*cis*-Pt[$PEt_2Me]_2$H-2-R R = H, Me, Et | S, H, IR | [994] |
| 1-*trans*-$(PEt_3)_2$PtH-2-R R = Me, Ph | S, H, IR | [994] |

| Compound | Information | References |
|---|---|---|
| 1-*cis*-Pt($PPh_2Me$)(*cyclo*-$CH_2PPh_2$—)-2-Ph | S, H, P, IR | [1009] |
| 1-$(CH_2)_n$$NH_2$-*cis*-Pt$(NH_3)_2Cl^+$ $n=1$, 3 | S, H, B, C, N, Pt, MS | [1010] |
| 1-$(CH_2)_n$$NH_2$-*trans*-Pt$(NH_3)_2Cl^+$ $n=1,3$ | S, H, B, C, N, Pt, MS | [1010] |
| *Trans*-Pt{$(Me_2Si)(R_2P)C_2B_{10}H_{10}$}$_2$ R = Me, OEt (FF) | S, X(Me), H, C, P | [584] |
| *Cis*-Pt{$(Me_2Si)(R_2P)C_2B_{10}H_{10}$}$_2$ R = Me, OEt, Ph (FF) | S, X(Ph), H, C, P | [584] |
| *Cis*-$PdCl_2$-1-CH(py)$NHCH_2$Ph-2-Me | S, X, H, B, C, IR, MS | |
| 1-{Pt($PPh_3$)[$PEt_2CHMe$]}-2-Me Pt-CH | X | [1325] |
| 1-2-$(CH_2)_n$HgR-Ph {$n=0$, 1; R = $PtBr(PPh_3)_2$, PtCl$(PPh_3)_2$} | S | [1011] |
| 1-Pt[$P(CH_2Ph)_3$][*cyclo*-(CHPh)$(CH_2Ph)$]-2-Me [Pt-P-C(benzyl)] | S, X | [1323] |
| $HCB_{10}H_{10}C$–$PPh_2$-Pt(Cl){*cyclo*-[-$PPh_2$-$CB_{10}H_{10}C$–]} (FF) | S, X | [1013] |
| 1,2-[*cyclo*-$Ph_2P$]$PtCl_2$[PRR′] R = R′ = Ph, $NMe_2$, F; R = $NMe_2$, R′ = F | S | |
| ($PEt_3$)[$Et_2PCH_2CH_2$]Pd($RC_2B_{10}H_{10}$) R = Me, Ph (FF) | S, H, P, IR | [1000] |
| 1-[(P(*n*-$C_3H_7)_3$]$Pt^{II}$[P(*n*-$C_3H_7)_2CHCH_2Me$]-2-Ph | X | [1324] |
| $L_2Pt(CB_{10}H_{10}C$–$Me)_2$ L = $PPh_3$, $PMe_2Ph$, $PMePh_2$ (FF) | S, H, P, IR | [1015] |
| 1,2-*cyclo*-[$Ph_2$-1,10-phenanthroline]Pt$(\mu-S)_{2^-}$] | S, UV, E | [1016] |
| [$Ph_2$-1,10-phenanthroline]Pt(S-1,2-$C_2B_{10}H_{11})_2$ (FF) | S, UV, E | [1016] |
| 1,2-*cyclo*-[$Ph_2$-1,10-phenanthroline]Pt$(\mu-S)_{2^-}$] | S, NLO | [1017] |
| 1,2-*cyclo*-{$[Ph_3]_2$Pt($SiMe_2$)-} | S, X, H, C, P, Si, MS | [315,790] |
| 1-$CH_2$S-Pt(terpyridine)$^+$ $(O_3SCF_3)^-$ intercalative DNA binding | S, H, B, C, Pt | [632] |
| $(Ph_3P)_2$Pt(μ-Se)$_2C_2B_{10}H_{10}$ (FF) | S, Se, Pt, H, B, C | [843] |
| Pt[μ-*trans*-$(PR_2)(SiMe_2)$(1,2-$C_2B_{10}H_{10})]_2$ R = Me, OEt, Ph (FF) thermal isomerization to *cis* isomer | S, X(Me), H, C, P | [1018] |
| 1,2-{*cyclo*-$Me_2$Si-Pt[($PEt_3$)]-$SiMe_2$} | S, X, H, C, P, Si, IR | [768] |
| *cis*-$Cl_2Pd(NC_5H_4)$CH(NH$CH_2$Ph)—$CB_{10}H_{10}$CH catalyst for Suzuki coupling (FF) | S, H, S, MS | [1587] |
| XPt($RC_5H_2$N-$C_5H_4$N)—$CB_{10}H_{10}$C—R′ R = Ph, Me, $BrC_6H_4$; R′ = Me, Ph; X = Cl, C≡CPh (FF) | S, X($BrC_6H_4$,Me,C≡CPh), UV(absorbance, emission) | [1588] |
| LM(E—$CB_{10}H_{10}$CPh)$_2$ L = $Me_2P(CH_2)_nPMe_2$, $n=1$–3; M = Pd, Pt; E = S, Se (FF) | S, X($n=1$, Pt, S, Se), H, P, Se, Pt | [1602] |
| 1,2-*cyclo*-SMLS L = $Me_2P(CH_2)_nPMe_2$, $n=1$–3; M = Pd, Pt | S, H, P, Pt | [1602] |
| 1,2-*cyclo*-SM$(PR_3)_2$S $R_3$ = $Et_3$, $Ph_3$, $MePh_2$, $Me_2Ph$; M = Pd, Pt | S, X(Pt, $Me_2Ph$, $MePh_2$), H, P, Pt | [1602] |
| *Trans*-[$(Me_3C)_2$P—$C_2B_{10}H_9$-3-Pd]$_2$(μ-Cl)$_2$ | S, X, H, B, C, P, MS | [1607] |
| [$(Me_3C)_2$P]$C_2B_{10}H_9$-3-Pd($PEt_3$) Pd—P | S, X, H, B, C, P, MS | [1607] |
| 1,2-(μ-$Ph_2P)_2$M(μ-S)$_2$($C_2B_{10}H_{10}$) M = Pd, Pt | S, H, P | [1758] |

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| Compound | Information | References |
|---|---|---|
| $H_{10}B_{10}C_2(\mu\text{-}S)_2M(\text{–}M'PPh_3)$-7,8-$(\mu\text{-}PPh_2)_2$-7,8-*nido*-$C_2B_9H_{10}$ M = Pd, Pt, Ni; M′ = Cu, Ag, Au heterobimetallic $d^8$–$d^{10}$ interactions | S, X(Pd, Au; Pt, Au; Pd, Ag; Pd, Cu; Ni, Au), H, P, MS, diffuse reflectance UV, emission | [1758] |
| 1,2-*cyclo*-PtX—$NC_5H_2(C_6H_4OMe)(C_6H_3OMe)$ X = $SEt_2$, $PPh_3$, $CNCMe_3$ Pt—$C_6$ $O_2$ sensor | S, X($SEt_2$, $PPh_3$), UV, phosphorescence | [1761] |
| 1,2-[CH(OH)—$C_5H_3RN]_2PdCl$ R = H, Me 2 N → Pd, B(3) → Pd pincer complexes catalysts for Suzuki coupling | S, X, H, B, C | [1772] |
| 1,2-*cyclo*-$S_2Pt^{II}$-L L = *o*-phen, bipyr, $Me_2$bipyr, $(CMe_3)_2$bipyr, $Ph_2$bipyr, $Ph_2$phenan | S, X[*o*-phen, $(CMe_3)_2$bipyr],H, B, C, UV, IR, E | [1801] |
| *Copper* | | |
| $Cl\{(Ph_3P)Cu[Ph_2P]_2C_2B_{10}H_{10}$ (FF) | S, H, B, P, IR | [921] |
| *cyclo*-$Me_2Si(CB_{10}H_{10}C)_2Cu$(2,2′-bipyridine) (FF) | S | [798] |
| *cyclo*-$[1,2\text{-}(Ph_2P)_2C_2B_{10}H_{10}]_2Cu_2M(\mu\text{-}S)_4$ M = Mo, W (FF) | S, X, H, C, IR, UV | [1019] |
| $Cu\{[OC(O)]C_2B_{10}H_{11}\}_2$ (FF) | S, X, H, B, C, IR, X-ray photoelectron | [878] |
| $Cu\{[OC(O)]_2C_2B_{10}H_{10}\}_2$ (FF) | S, H, B, C, IR | [878] |
| 1,2-*cyclo*-[-Cu-$NEt_2CH_2$⁻] | S | [995] |
| 1,2-*cyclo*-Cu(2,2′-bipyridine) | S | [1409] |
| $HCB_{10}H_{10}C\text{–}PPh)_2$-Cu(μ-X)$_2$-Cu$[Ph_2P(C_2B_{10}H_{11})_2]$ X = Cl, Br, I (FF) | S, IR, Raman, UV, MAG, COND | [1020] |
| $ClCu(PPh_3)[(PR_2)_2C_2B_{10}H_{10}]$ R = OEt, Et, $CHMe_2$ (FF) | S, X(OEt) | [1377] |
| $Cu\left[(C_2B_{10}H_{10})_2\right]_2^{n-}$ *n* = 1, 2 (FF) | S, X | [928] |
| *Rac*/*meso*-1,2-$(PPh_3)ClRu[PPhH]_2$ | S, H, B, C, P, IR | [578] |
| 1-Cu-2-R R = H, Cu | S | [471] |
| 1-C≡CCu-2-R R = H, Ph acetylide | S | [296] |
| $Cu_2[(PhC_3N_3\text{-}C_5H_4N)MeC_2B_{10}H_{10}]_2Cl_4$ triazinyl (FF) | S, X | [273] |
| 1,2-*cyclo*-$(Ph_2P)Cu(\mu\text{-}X)_2Cu(PPh_2)$ X = Cl, Br, I | S, X, H, C, IR | [1022] |
| {1,2-*cyclo*-[PCl(t-$C_4H_9$)-Cu-P(*t*-$C_4H_9$)Cl] $C_2B_{10}H_{10}\}_2(\mu\text{-}Cl)_2$ (FF) | S, H, B, C, P, IR | [1040] |
| Porphyrin$(C_6H_4\text{-}p\text{-}C_2B_{10}H_{11})_4Cu$ (FF) | S, X | [515] |
| | Microdistribution in tissue for BNCT | [1443] |
| Cu[porphyrin(4-$C_5H_5N$)]$_4$[Cp*Ir(μ-$S)_2(C_2B_{10}H_{10})]_4(THF)_2$ (FF) | S, X, H, B, IR, UV | [1023] |
| Corrole(Cu)[*m*/*p*-$C_6H_4$-1,2-$CB_{10}H_{10}CH]_2$ (FF) | S, X(*m*-$C_6H_4$), UV | [518] |
| Cu[NR═C(NHR)$CB_{10}H_{10}C\text{—}]_2$ 2 C—Cu, 2 N—Cu R = $CHMe_2$, *n*-$C_6H_{11}$ | S, X($CHMe_2$), IR | [1609] |
| $Cu_6N_8S_6$(1,10-phenanthroline)$_4$(1,2-$C_2B_{10}H_{10})_2$ (FF) | S, X, H, DNA binding, in vivo cytotoxicity | [1662] |
| $H_{10}B_{10}C_2(\mu\text{-}S)_2M(\text{–}CuPPh_3)$-7,8-$(\mu\text{-}PPh_2)_2$-7,8-*nido*-$C_2B_9H_{10}$ M = Pd, Pt, Ni heterobimetallic $d^8$–$d^{10}$ interactions | S, X(Pd), H, P, MS, diffuse reflectance UV, emission | [1758] |
| $L_4Cu_2[(O_2C)C_2B_{10}H_{11}]_4$ L = N $C_5H_5$, NC5H4Me paddle-wheel complexes | S, X, H, B, IR, UV, E | [1873] |

| Compound | Information | References |
|---|---|---|
| $(C_5H_3Me_2N)Cu[(O_2C)C_2B_{10}H_{11}]$ | S, X, H, B, IR, UV, E | [1873] |
| $(hfac)_2Cu[1\text{-}(C_{12}H_7N_2\text{-}2'\text{-}C_2B_9H_{11})]_2$ 1′,10′-phenanthrolinyl hfac = hexafluoroacetylacetone (FF) | S, X | [1915] |
| ***Silver*** | | |
| $(phen)Ag\{1,2\text{-}(PPh_2)C_2B_{10}H_{10}\}^+ ClO_4^-$ (FF) | S, X, P | [1024] |
| $Ag_4(\mu_3\text{-}S\text{-}C_2B_{10}H_{11})_2(O_3SCF_3)_2(PPh_3)_4$ (FF) | S, X, H, P, IR, MS | [1025] |
| $L\text{-}Ag[(NC_5H_5\text{-}S)_2C_2B_{10}H_{10}]^+$ L = $PPh_3$, $PPh_2Me$, $AsPh_3$ (FF) | S, X($PPh_3$), H, P, COND | [1026] |
| $1\text{-}Se[AgPPh_3]_2$ | S, P, IR, MS, COND | [836] |
| $(\mu\text{-}SCN)_2\{1,2\text{-}cyclo\text{-}[(Me_2CH)_2P\text{—}Ag\text{—}P\text{-}(CHMe_2)_2]C_2B_{10}H_{10}\}_2$ (FF) | S, X, IR | [1555] |
| $(H_{10}B_{10}C_2)[\mu\text{-}P(C_6H_{11})_2]_2Ag\{SC{\equiv}Nag(SC{\equiv}N)\text{-}[\mu\text{-}P(C_6H_{11})_2]_2C_2B_{10}H_{10}\}\{N{\equiv}CSAg[(\mu\text{-}P\text{-}(C_6H_{11})_2]_2C_2B_{10}H_{10}\}$ supramolecular network (FF) | S, X, H, B, C, P, IR | [1581] |
| $Me\text{—}CB_{10}H_{10}C\text{—}PPh_2\text{—}Ag[nido\text{-}7,8\text{-}(\mu\text{-}PPh_2)_2C_2B_9H_{10}]$ | S, X, H, P, IR, UV(luminescence emission) | [1763] |
| 1,2-$[(CHMe_2)_2P\text{-}Ag\text{-}(N_2C_{11}OH_6)\text{-}P(CHMe_2)_2]$ phosphanes; diazafluorene-9-one | S, X, H, P, emission/excitation luminescence | [1794] |
| ***Gold*** | | |
| $1\text{-}Se[AuPPh_3]_2$ | S, P, IR, MS, COND | [836] |
| $1\text{-}Me\text{-}2\text{-}SeAu(PPh_3)$ (FF) | S, X, H, B, C, P, IR | [838] |
| $1\text{-}Au(PPh_3)Br_2\text{-}2\text{-}Ph$ | S | [1028] |
| $1\text{-}(2'\text{-}NC_5H_4)\text{-}2\text{-}SAu(PPh_3)$ | S, X, H, B, C, IR | [269] |
| $\mu,\mu'\text{-}Au\{(Ph_2P)_2C_2B_{10}H_{10}\}_2$ (FF) | S, P, IR, COND | [1029] |
| 1-R-2-AuR′ R = $MeOCH_2$, Ph; R′ = $Ph_3P$, $MeC_6H_4$, $(C_6H_{11})_3P$, $Et_3P$, $Et_3As$, $(o\text{-tol})_3P$ | S, X[$MeOCH_2$, $Et_3As$], H, B, P | [1030] |
| $Au_4(S_2C_2B_{10}H_{10})_2\{[Et_2P]_2C_2B_{10}H_{10}\}_2$ (FF) | S, X, P, IR, MS | [1031] |
| $1,2\text{-}cyclo\text{-}\{[Et_2P]_2Au[cyclo\text{-}[PEt_2]_2L]\}^+$ L = $CH_2$, $CH_2CH_2$, $C_6H_4$, CH═CH, NH | S, P, IR | [1032] |
| $\{[AuPPh_3]_2C_2B_{10}H_{10}\}_2$ (Au-Au) (FF) | S, X, H, C, B, P, MS | [1033] |
| $Au_2(\mu - S_2C_2B_{10}H_{10})_2^{2-}$ (FF) | S, P, H, IR, COND | [1034] |
| $Au(\mu - S_2C_2B_{10}H_{10})_2^{2-}$ (FF) | S, B, E, MS, COND | [1035] |
| $(\mu\text{-}S_2C_2B_{10}H_{10})Au(nido\text{-}C_2B_9H_{10})^{2-}$ (FF) | S, H, B, C | [1035] |
| $1,2\text{-}\mu(R_2AuS_2)\text{-}C_2B_{10}H_{10}^-$ R = $C_6F_5$, $C_6F_3H_2$, Cl (FF) | S, X(Cl), F, IR, COND | [1036] |
| $Ph_2P(CH_2)_nPPh_2[Au\text{-}S\text{-}C_2B_{10}H_{11}]_2$ $n$ = 2, 3 (FF) | S, X($n$ = 2), H, C, P, IR, MS | [1037] |
| $Au(S - C_2B_{10}H_{11})_2^+$ (FF) | S, H, C, P, IR, MS | [1037] |
| $Ph_3PAu(NC_5H_5)\text{-}S)_2C_2B_{10}H_{10}^{2+}$ (FF) | S, H, P | [1026] |
| $1,2\text{-}[Si(t\text{-}C_4H_9)Me_2][LAu]$ L = $PPh_3$, $PPh_2Me$, $AsPh_3$ | S, X($PPh_3$), H, P, COND | [1038] |
| $1,2\text{-}cyclo\text{-}[Ph_2PAuX]_2$ X = Cl, $C_6F_5$ | S, P, F, COND | [1039] |
| $1,2\text{-}cyclo\text{-}[Ph_2P\text{-}AuX\text{-}PPh_2]$ X = Cl, Ph, THF, $PPh_3$, $PPh_2(C_6H_4Me)$, $P(C_6H_4OMe)_3$, $PPh_2Me$, $CHPPh_3$, $CH_2PPh_2Me$, $SPPh_3$, $AsPh_3$, $C_5H_4NSH$, *o*-phenanthroline | S, P, F, COND | [1039] |

*Continued*

| Compound | Information | References |
|---|---|---|
| 1,2-*cyclo*-[PCl(*t*-$C_4H_9$)(AuCl-P(*t*-$C_4H_9$)Cl] | S, H, B, C, P, IR | [1040] |
| 1-SeAuL L = $PPh_3$, $AsPh_3$ | S, X[$Ph_3$], H, P, MS, COND | [836] |
| $HCB_{10}H_{10}C$—Se—Au—L—Se—$CB_{10}H_{10}CH$ L = dppf, dppe (FF) | S, P, IR, MS, COND | [836] |
| 1,2-cyclo-(E—Au—X—Au—E) Au···Au X = dppf, dppe E = Se, Te L = $PPh_3$, $PPh_2Me$, $PPh_2Py$ dppf = bis(diphenylphosphino)ferrocene | S, H, P, Se, IR | [1685] |
| Au[(μ-E)$_2C_2B_{10}H_{10}$]$_2$ E = Se, Te (FF) | S, H, P, Se, IR | [1685] |
| $Au_2$[$Se_2(C_2B_{10}H_{10}$Au(u-$PPh_2)_2C_2B_{10}H_{10}$] E = Se, Te (FF) | S, H, P, Se, IR | [1685] |
| Au($SC_{12}H_{13}$)$_4$[S-$(CH_2)_{10}$—$N_3C_2H$—$C_6H_4$—$CB_{10}H_{10}$CMe]$_4$ dendrons (FF) | S, H, UV, TEM | [1692] |
| Au($SC_{12}H_{13}$)$_4$[S$(CH_2)_{10}$—$N_3C_2H$—$C_6H_4$—$(OCH_2CH_2)_n$OMe]$_4$[S$(CH_2)_{10}$—$N_3C_2H$—$C_6H_4$—$CB_{10}H_{10}$CMe]$_4$ $n$ = 7, 40–44 dendrons (FF) | S, H, UV, TEM | [1692] |
| Au{$SC_6H_2$[$OCH_2$-$C_2HN_3$-$C_6H_4$-$CH_2$-$N_3C_2H$-$C_6H_4CB_{10}H_{10}$CMe][$OC_2HN_3(CH_2OCH_2)_n$-$CH_2$OMe]$_2$}$_4$ $n$ = 40-44 dendrons (FF) | S, H, UV, IR, TEM | [1692] |
| 1-Me-2-$PPh_2$AuX X = Cl, $SC_4H_8^+$, $PPh_3^+$ For X = Cl, pyrolysis and deposit on Si → Au crystals microcrystalline materials | S, H, P, F, IR | [1763] |
| Au($Ph_2P$—$CB_{10}H_{10}C$—Me)$_2$ | S, H, P, IR | [1763] |
| Me—$CB_{10}H_{10}C$—$PPh_2$—Au[*nido*-7,8-(μ-$PPh_2)_2C_2B_9H_{10}$] | S, H, P, IR, UV(luminescence emission) | [1763] |
| 1-Me-2-$PPh_2$Au(μ-$PPh_2)_2C_2B_{10}H_{10}^+$ $OTf^-$ | S, H, P, F, IR | [1763] |
| 1,2-[$AuPh_2P$—$CB_{10}H_{10}C$—Me)$_2$ | S, H, P, IR | [1763] |
| 1,12-($AuPPh_2$-1,2-$CB_{10}H_{10}$CMe)$_2$-1,12-$C_2B_{10}H_{10}$ pyrolysis and deposit on Si → Au crystals microcrystalline materials | S, H, P, IR, UV(luminescence emission) | [1763] |
| 1,2-*cyclo*-{[($Me_2CH$)N($CH_2$)$_2$N($CHMe_2$)]P}$_2$AuX-$C_2B_{10}H_{10}^-$ X = Cl, $NTf_2$ Tf = trifimidate = $CF_3SO_2NH^-$ (FF) oxidative addition of aryl iodides | S, X($NTf_2$), H, P | [1802] |
| 1,2-*cyclo*-{[($Me_2CH$)N($CH_2$)$_2$N($CHMe_2$)]P}$_2$AuIY-$C_2B_{10}H_{10}$ Y = aryl, naphthyl, iodopyridyl, iodothiophenyl (FF) | S, X(naphthyl), H, P | [1802] |
| ***Zinc*** | | |
| (porphyrin)Zn[*m*/*p*-$C_6H_4$-$(CH_2)_n$-$CB_{10}H_{10}$CMe]$_4$ $n$ = 0,1 (FF) | S, X($n$ = 1), H(activation energy for rotation) | [989] |
| Zn[$CB_{10}H_{10}$C–Ph]$_2$ (FF) | S | [1042] |
| $Zn^{2+}$[(tetraphenylporphyrin)$C_2B_{10}H_{11}^{2-}$] (FF) | S, H, MS (for BNCT application) | [1043] |
| Zn[porphyrin(4-$C_5H_5N$)]$_4$[Cp*Ir(μ-S)$_2$($C_2B_{10}H_{10}$)]$_4$($THF)_2$ (FF) | S, X, H, B, IR, UV | [1023] |
| {Zn[porphyrin(4-$C_5H_5N$)]$_4$[Cp*Ir(μ-S)$_2$($C_2B_{10}H_{10}$)]$_2$-($CHCl_3$)$_6$}$_n$ polymer (FF) | S, X, H, B, IR, UV | [1023] |
| Zn(porphyrin){3-[1,2-(MeO)$PhC_2B_{10}H_9$]}$_4$ lipophilic porphyrins (FF) | S, fluorescence, boron distribution in mice | [1691] |

| Compound | Information | References |
|---|---|---|
| Zn(phthalocyanine)[$OC_6H_4$-(*cyclo*-CH-O-$CH_2$)$C_2B_{10}H_{10}$) photocatalysis of oxidation of citronellol (FF) | S, H, UV, IR, MS | [1710] |
| Zn(phthalocyanine)[$C_5H_4N$-$(CH_2)_3CB_{10}H_{10}CMe]_3(OC_5H_4N)$ photocatalysis of oxidation of citronellol (FF) | S, H, UV, IR, MS | [1710] |
| *Mercury* | | |
| 1-HgMe-2-Ph | S | [555] |
| 1-HgMe-2-$CH_2F$ | S, F | [179] |
| 1-HgMe-2-$CH_2Ph$ | X | [1046] |
| 1-HgMe-2-$CH_2OEt$ | X | [1047] |
| 1-HgMe-2-R R = Me, C≡CPh | H ($J_{Hg-H}$); polarity of R group and solvent] | [1346] |
| 1-HgMe-2-R R = HgMe, $CHMe_2$, Et, $CH_2Cl$, $CH_2Br$, C(O)OMe | S, H | [1048] |
| 1-HgR R = Me, Ph | S (thermal decarboxylation) | [1049] |
| 1-HgR-2-R R = Me, Ph | S, E | [203] |
| 1-$HgGeEt_3$-2-R R = H, Me, $CH_2Cl$, Ph | S | [807] |
| 1-HgCl-2-Ph | S, E | [891] |
| 1-HgCl-2-C≡CH | S | [296] |
| 1-R-2-HgR′-B-$X_n$ R = H, Me, Ph; R′ = Me, Ph; X = Br, Cl; $n$ = 0, 2, 4 | S | [1053] |
| 1-HgR-2-R′ R, R′ = Ph, H | S | [684] |
| 1-$CH_2HgR$ R = Cl, Me, Ph | S | [684] |
| $ClHg(CH_2CB_{10}H_{10}CH)$ (FF) | S | [593] |
| 1-$HgC_5H_4FeCp$-2-Ph | S | [203] |
| 1-HgX-2-Ph X = Cl, Br | S | [203] |
| 1-HgCH=$CMe_2$-2-R | H (Hg-CH coupling constants variation with substituents) | [1054] |
| 1-R-9-HgX R = H, Ph | E | [1055] |
| 1-R-9-HgX X = Cl, Br, I; R = H, Me, Ph | MS (detailed) | [1456] |
| $Hg(\text{-}9\text{-}RC_2B_{10}H_{10})_2$ R = H, Me (FF) | MS (detailed) | [1456] |
| $Hg(CH_2{=}CH\text{-}CB_{10}H_{10}C)_2$ (FF) | S, E | [203] |
| $RHg(PhC_2B_{10}H_{10})$ R = Ph, $CpFe(C_5H_4)$ (FF) | S | [1057] |
| $Hg(RC_2B_{10}H_{10})_2$ R = Me, Ph,$CH_2Cl$ (FF) | S | [1058] |
| $Hg(C_2B_{10}H_9\text{-}10,12\text{-}Cl_2)_2$ (FF) | S, E ($pK_a$) | [1059] |
| $[CB_{10}H_{10}C{-}HgMe]_2$ (FF) | S | [362] |
| $Hg\{[Me_2NCH_2]C_2B_{10}H_{11}\}_2$ (FF) | S, X, H, B, C, IR, MS | [820] |
| $Hg(CH_2CB_{10}H_{10}CH)_2$ (FF) | S | [593,684] |
| | S, E | [891] |
| $Hg[PhC_2B_{10}H_{11}]_2$ (FF) | S | [1060] |
| $Hg(CB_{10}H_{10}CR)_2$ R = Ph, $CH{=}CH_2$, Me, H (FF) | S | [575] |
| $MeHg(CB_{10}H_{10}CR)$ R = Ph, $CH{=}CH_2$, H (FF) | S | [575] |

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| Compound | Information | References |
|---|---|---|
| $Hg(n\text{-}C_2B_{10}H_{11}\}_2$ $n=1$, 9 (FF) | Raman | [760] |
| $(RC_2B_{10}Cl_{10})HgR'$ R = H, Me; R′ = Me, Ph (FF) | S | [1061] |
| 1,2-$(HgMe)_2C_2B_{10}Cl_{10}$ (FF) | S | [1061] |
| 1,2-$RBrC_2B_{10}Cl_{10}$ R = Me, Cl (FF) | S | [1061] |
| $(RC_2B_{10}Cl_{10})_2Hg$ R = H, Me (FF) | S | [1061] |
| $(MeC_2B_{10}Cl_{10})HgR$ R = OC(O)Me, Cl (FF) acetate | S | [1061] |
| $RCB_{10}H_{10}CHgX\cdot$*o*-phenanthroline R = H, Me, Et, Ph; X = Cl, Br, Me (FF) | S | [1062] |
| $(RCB_{10}H_{10}C)_2Hg\cdot$*o*-phenanthroline R = Me, Ph (FF) | S | [1062] |
| $(HCB_{10}H_{10}CCH_2)_2Hg\cdot$*o*-phenanthroline (FF) | S | [1062] |
| $Hg(9\text{-}RC_2B_{10}H_{10})_2$ R = H, Ph (FF) | E | [1055] |
| B-$[HgC(O)OCF_3]_n$ $n=1$–5 | S | [1065] |
| B-HgR R = Et, I | S | [1066] |
| 9-$HgOC(O)CF_3$ | S | [1056,1067,1068] |
| | H | [241] |
| 9-$HgCl\cdot$*o*-phenanthroline | S | [1501] |
| $L_2Hg[C(O)O\text{-}CB_{10}H_{10}CH]_2$ L = *o*-phenanthroline, 2,2′-bipyridine, $C_5H_5N$, $PPh_3$ (FF) | S | [1410] |
| *Exo*, *nido*-$ClPh_3P)_2Ru(\mu\text{-}H)_3$-7,8-*nido*-$C_2B_9H_8$-10-Hg-(9-$C_2B_{10}H_{11}$) (FF) | S, X, H, B, P | [1069] |
| 3,1,2-$ClPh_3P)_2Ru(C_2B_9H_{10})$-10-Hg(9-$C_2B_{10}H_{11}$) (FF) | S, H, B, P | [1069] |
| (9-$C_2B_{10}H_{11}$)Hg(10-*nido*-7,8-$C_2B_9H_{10}$-7-R)$^-$ R = H, Ph, $CHMe_2$ (FF) | S, X(H), H, B | [1070] |
| (9-$C_2B_{10}H_{11}$)Hg(10-*nido*-7,8-$C_2B_9H_{10}$-6-F)$^-$ (FF) | S, H, B, F | [1070] |
| $Li_2[HgC_2B_{10}H_8I_2]_4\cdot I_2$ (FF) microporous solid | S, X, H, B, C, MS | [1071] |
| $Hg\{9\text{-}[Me_3Si]C_2B_{10}H_{10}]\}_2$ (FF) | S | [1072] |
| $Hg[9\text{-}Me_2C_2B_{10}H_{10}]_2$ (FF) | S | [1072] |
| $Hg[9-C_2B_{10}H_{11}]_2^{4-}$ (FF) | S | [1072] |
| 9-$HgSn\{CH[MeC(O)O]_2\}_2R$ R = Me, Cl, 9-$C_2B_{10}H_{11}$ (FF) | S | [826] |
| 9-Me-12-HgR R = $CF_3C(O)O$, Cl | S, B | [1073] |
| $Hg(12\text{-}C_2B_{10}H_{10}\text{-}9\text{-}Me)_2$ (FF) | S, B | [1073] |
| 1-C(O)OHgMe-2-R R = $C_5H_4FeCp$, $C_5H_4Mn(CO)_3$ | S, H ($J_{Hg\text{-}Me}$), p$K_a$ | [906] |
| 1-$(CH_2)_n$HgR-2-Ph {$n$ = 0, 1; R = $PtBr(PPh_3)_2$, $PtCl(PPh_3)_2$} | S | [1011] |
| 1,2-cyclo-[—$P(CHMe_2)_2$—$HgCl_2$—$P(CHMe_2)_2$—] | S, X, IR | [1074] |
| $Hg_2(C_2B_{10}H_9\text{-}3\text{-}Ph)_3\cdot EtOH$ (FF) | S, X, H, B, C, Hg, IR, MS | [1075] |
| *Cyclo*-$Hg_3(C_2B_{10}H_{10})_3$ (FF) | S, X(MeCN complex), H, B, C, Hg, IR | [174,1481] |
| *Cyclo*-$Hg_3(C_2B_{10}H_8\text{-}9,12\text{-}Me_2)_3\cdot X^-$ X = Cl, Br, I (FF) | S, X(Br, I), H, B, C, Hg(detailed) | [1076] |
| {*cyclo*-$Hg_3[C_2B_{10}H_8\text{-}9,12\text{-}(Me)_2]_3\}\cdot 2I^-$ (FF) | S, X, H, B, C, Hg, MS | [1077] |

| Compound | Information | References |
|---|---|---|
| *Cyclo*-$Hg_3[(Me)_2C_2B_{10}H_8]_3 \cdot X^-$ X = Cl, Br, I (FF) | S, X, H, B, C, Hg, IR, MS | [1078] |
| *Cyclo*-$Hg_3(C_2B_{10}H_{10})_3 \cdot H_2O \cdot [C(O)(Me)_2]_3$ (FF) | X | [1079] |
| *Cyclo*-$Hg_3(C_2B_{10}H_{10})_3 \cdot (H_2O)_2 \cdot C_6H_6$ (FF) $H_2O$-benzene π-complex | X | [1079] |
| *Cyclo*-$Hg_4(C_2B_{10}H_8$-9-I-12-Et$)_4 \cdot (Hg\text{-}C_2B_{10}H_{11})_4$ (FF) | S, X, H, B, C, Hg, IR | [174,1081] |
| *Cyclo*-$Hg_4(C_2B_{10}H_{10})_4 \cdot Cl^-$ (FF) | S, X, H, B, C, Hg, IR | [174,1082] |
| *Cyclo*-$Hg_4(C_2B_{10}H_{10})_4 \cdot Br^-$ (FF) | S, X, H, B, C, Hg, MS | [174] |
| *Cyclo*-$Hg_4(C_2B_{10}H_{10})_4 \cdot I^-Li^+$ (FF) | S, H, B, C, Hg, IR, MS | [174,1479] |
| *Cyclo*-$Hg_4(C_2B_{10}H_9$-3-Ph$)_4 \cdot I^-$ $Li^+$ (FF) | S, X, H, B, C, Hg, IR, MS | [1075,1504] |
| *Cyclo*-$Hg_4(C_2B_{10}H_{10})_4{I_2}^{2-}$ (FF) | S, X, H, B, C, Hg, IR, MS | [174] |
| *Cyclo*-$Hg_4[C_2B_{10}H_8$-9,12-$Et_2]_4 \cdot (C_2B_{10}H_{10}$-9, 12-$I_2)_2$ (FF) | S, X, B, Hg, IR | [174] |
| *Cyclo*-$Hg_4(C_2B_{10}H_8$-9,12-$R_2)_4 \cdot [B_{10}H_{10})^{2-}]_2$ R = H, Et (FF) | S, X(Et), B, Hg, IR | [646] |
| *Cyclo*-$Hg_4(C_2B_{10}H_8$-9-I-12-Et$)_4 \cdot [B_{10}H_{10})^{2-}]_2$ (FF) | S, X, B, Hg, IR | [174] |
| *Cyclo*-$Hg_4[C_2B_{10}H_{10-x})R_x]_4{I_2}^{2-}$ R = Et, $x$ = 2; R = Me, X = 2,4 (FF) | S, X(Me), H, B, Hg, MS | [1083] |
| *Cyclo*-$Hg_4(C_2B_{10}H_{10})_4 \cdot (NO_3)_2{}^{2-}$ [K(18-crown-$6^+]_2$ (FF) | S, X, H, B, Hg, IR | [1507] |
| **Theoretical Studies** | | |
| *Molecular and electronic structure calculations* | | |
| Parent | EI (energy indexes), stabilities | [1098] |
| | Electron delocalization | [1091] |
| | Electron affinities, acidity | [1086] |
| | Electron density on carbon | [1399] |
| | HOMO-LUMO gap in films on Cu(100) | [80] |
| | IR, vibrational frequencies | [1100] |
| | C—H bond length compared with halomethanes | [1101] |
| | Molecular motion in two plastic phases; comparison with 1,12-$C_2B_{10}H_{12}$ | [1316] |
| $C_2B_{10}H_{11}^{\bullet}$, $C_2B_{10}H_{10}^{\bullet\bullet}$ radicals | DFT, CASPT2 | [1103] |
| *n*-R *n* = 1, 3, 9; R = CH, N | *Ab initio*; carbenes, nitrenes | [1104] |
| 1-Me | DFT: natural bond orbital cluster charge distribution | [1095] |
| 1,2-$R_2$ R = H, Me, $NH_2$, OH, F, $SiH_3$, $PH_3$, SH, Cl | DFT; unusually long C–C bond distances; influence of substituents on C–C length | [1106] |
| 1,2-$(R^-)_2$ R = H, Me, $NH_2$, OH, F, $SiH_3$, $PH_3$, SH, Cl | DFT; unusually long C–C bond distances; influence of substituents on C–C length | [1106] |
| $H_2C_2B_{10}Me_{10}$ (FF) | DFT: natural bond orbital cluster charge distribution | [1095] |
| 1-$B(OH)_2$-2-R R = H, Ph | DFT: geometry of anionic reduction product | [1878] |
| $H_2C_2B_{10}Me_8$-9-X-12-Y X,Y = H, I, Cl (FF) | Mulliken charges; Me electron-donating properties | [268] |
| 1-*cyclo*-$C_3H_5$-2-R R = H, CH(OH)Ph | Stability of $C_3$ ring conformations | [1452] |

*Continued*

| Compound | Information | References |
|---|---|---|
| $C_7H_6^+$ $C_2B_{10}H_{11}^-$ tropenyliumyl ion (FF) | *Ab initio* charge-transfer | [1109] |
| 1-$CH_2CH{=}CH_2^-$ (allylcarboranyl anion) | Electron density distribution | [1399] |
| 1,2-{*p*-$C_6H_4$-C[*cyclo*-C═N(O)$CMe_2CMe_2$N(O)]}$_2$ nitronyl nitroxide radical | DFT (optimized geometry) | [477] |
| 1-DDQC (DDQC = an amidoquinoline group) (two rotamers) | *Ab initio*, rotamer geometries | [1328] |
| XM[$Me_2PCH_2$-$C_2B_{10}H_{10}$]$_2$ (M—B) M = Al, Ga, In; X = Cl, Br (FF) | DFT (geometry) | [752] |
| 1-$AsH_3Au$ | Geometry | [1030] |
| *Cis*-$Cl_2Pd[(H_2P)_2C_2B_{10}H_{10}]$ (FF) | DFT: plasticity of 5-membered chelate ring | [1447] |
| *Trans*-Pt{$(Me_2Si)(R_2P)C_2B_{10}H_{10}$}$_2$ R = Me, OEt (FF) | DFT | [584] |
| $C_6H_2$-1,4-[9′-(1′,2′-$C_2B_{10}H_{12}$)]$_2$-2,5-$R_2$ R = H, Me | DFT: stability, photoemission binding energies; carborane-aromatic copolymers | [1916] |
| $C_6$-1,2,4,5-[9′,12′-(1′,2′-$C_2B_{10}H_{10}$)]$_2$-3,6-$R_2$ R = H, Me | DFT: stability, photoemission binding energies; carborane-aromatic copolymers | [1916] |
| 9,12-$I_2$ | DFT: electronic structure, NMR shifts, ring currents | [1923] |
| **Aryl Derivatives** | | |
| 1-Ph-2-R R = F, OH, $NH_2$, $O^-$, $NH^-$ | *Ab initio*, icosahedral cage distortions caused by π-bonded substituents | [343] |
| —[$C_{13}H_6$(*n*-$C_6H_{13}$)$_2$—$CB_{10}H_{10}C$—$C_{13}H_6$(*n*-$C_6H_{13}$)$_2$]$_n$— polyfluorene derivatives (FF) | HOMO-LUMO | [1610] |
| 1,2-($C_6H_4$-*p*-$C_6H_4$-$NC_{12}H_6R_2$)$_2$ carbazole R = H, $NH_2$ second order NLO, substituent effects, redox switching | DFT: geometry; first order hyperpolarizability | [1725] |
| 1′,4′-$(RCB_{10}H_{10}C)_2C_6H_4$ R = 3′,5′-$(F_3C)_2C_6H_3$, Ph, *p*-$C_6H_4$-*n*-$C_4H_9$, *p*-$C_6H_4$-$NMe_2$ | DFT: electronic transitions | [1741] |
| 1,6-$C_6H_2(C_6H_4)_2$-*trans*-(1′,2′-*cyclo*-$C_2B_{10}H_{10})_2$ terphenyl | DFT: energy levels | [1754] |
| *p*-$C_6X_4(CB_{10}H_{10}C-Ph)_2^{n-}$ *n* = 2,4 X = H, F 2*n*+3 SE clusters | DFT: electronic and molecular structure | [1759] |
| 1-$(C_6H_4)_n$-*p*-$NC_{12}H_8$ *n* = 1,2 N-carbazolyl donor-acceptor dyad complexes photoelectron donor-acceptor charge transfer | DFT: energy levels | [1762] |
| {1,2-[$C_6H_4$-*p*-C≡C—$C_6H_4$—*p*-$C_5H_2$N-$(C_5H_4N)_2$]$_2C_2B_{10}H_{10}$}$_n$$M^{II}{}_n$ *n* = 2–4 M = Zn, Fe (FF) | Molecular modeling of metal ion-promoted cyclo-oligomerization | [1765] |
| $(C_6H_4)_2$-2,2′-$(CB_{10}H_{10}CH)_2$ (FF) | DFT: electronic structure | [1773] |
| $C_6H_4$-1,4-$(CB_{10}H_{10}CH)_2$ (FF) | DFT: electronic structure | [1773] |
| $(C_6H_4)_2$-4,4-$(CB_{10}H_{10}CH)_2$ (FF) | DFT: electronic structure | [1773] |
| $C_{22}H_{12}$-6,13-(C≡C-$CB_{10}H_{10}CR)_2$ pentacenyl R = H, Me, Et, *n*-$C_4H_9$ | DFT: HOMO/LUMO energies | [1892] |
| 1-$C_5H_{11}$—12-$C_6H_4$-*p*-R R = C≡C—$C_6H_4$-$OC_8H_{17}$, N = CH—$C_6H_4$—$OC_8H_{17}$, N = N—$C_6H_4$—C(O)O—$C_5H_{11}$* | DFT: dipole moment, polarizability, geometry | [1919] |
| 1-$C_5H_{11}$—O—$C_6H_4$-$C_2B_{10}H_{10}$-12-L—$C_6H_4$—*p*-$OC_5H_{11}$ L = $CH_2CH_2$, CH═CH (FF) | DFT: dipole moment, polarizability, geometry | [1919] |
| 1-R-2-$C_6H_4$-*m*-$B(C_6H_2Me_3)_3$ R = Ph, $B(C_6H_2Me_3)_3$ | DFT: energy levels | [1912] |
| 1-R-2-$C_6H_4$-*p*-$B(C_6H_2Me_3)_3$ R = Ph, $B(C_6H_2Me_3)_3$ | DFT: energy levels | [1912] |

| Compound | Information | References |
|---|---|---|
| ***Amines and imines*** | | |
| 1,2-*cyclo*-C($CMe_3$)—N[$C_6H_3(CHMe_2)_2$]—B[$Me_2C_3N_2(CHMe_2)_2$ | DFT: structure and energies | [1931] |
| 1,2-*cyclo*-C($CMe_3$)═N[$C_6H_3(CHMe_2)_2$]—$B(OAc)_2$ carbene-stabilized iminocarborane | DFT: structure and energies | [1931] |
| ***Heterocyclic amines*** | | |
| 1,2-{*cyclo*-[B—N(R)—*o*-$C_6H_4$—N(R)—]}$_2$ R = Et, Ph diazaborolyl | Molecular geometry | [1684] |
| Porphyrin[$S(CH_2)_6$-$C_2B_{10}H_{11}$ deactivation following photoexcitation, due to flexibility of alkylthio chains | DFT: molecular orbital energy levels | [1927] |
| 1,2-$C_2B_{10}H_{10}$ | Mechanism of [5 + 2] nitrone addition to carboryne | [1906] |
| ***Silicon*** | | |
| 1,2-$(SiH_3)_2$ | DFT optimized structure of singlet and triplet states of neutral species and dianions formed by $H^+$ removal from R groups | [1107] |
| 1,2-$(SiH_3^-)_2$ | DFT; unusually long C–C bond distances; influence of substituents on C–C length | [1106] |
| 1,2-*cyclo*-(—$Me_2Si$—$SiMe_2$—) | DFT: energies | [768] |
| *cyclo*-1,B(4)-[Cp*$IrH_2$-$SiHMe_2^-$]$C_2B_{10}H_{10}$ (FF) | Geometry | [1384] |
| 1,2-*cyclo*-[$SiR_2$-Cp*$IrH_2$-$SiHMe_2^-$]$C_2B_{10}H_{10}$ (FF) | Geometry | [1384] |
| $O_{12}Si_8$[CH═CH—$C_6H_4$—*p*-$CH_2$—$CB_{10}H_{10}C$—R]$_8$ octasilsesquioxanes R = H, Me, Ph (FF) | DFT: HOMO/LUMO | [1718] |
| 1-SiH[$(CHMe_2)_2N_2CPh]_2$ 6-coordinate silicon complex | DFT: molecular structure | [1819] |
| ***Phosphorus*** | | |
| 1,2-$(PH_3)_2$ | DFT optimized structure of singlet and triplet states of neutral species and dianions formed by $H^+$ removal from R groups | [1107] |
| 1,2-$(PH_3^-)_2$ | DFT; unusually long C–C bond distances; influence of substituents on C–C length | [1106] |
| *Rac*-1,2-*cyclo*-$P_2R_2$ R = $CMe_3$, $N(CHMe_2)_2$ 1,2-diphosphetanes | DFT, molelcular structure | [1578] |
| 1,2-$(PIR)_2$ R = $CMe_3$, $N(CHMe_2)_2$ diphosphetanes | DFT, molelcular structure | [1578] |
| *trans*-[$(Me_3C)_2P$—$C_2B_{10}H_9$-3-Pd]$_2$(μ-Cl)$_2$ | DFT, molecular structure | [1607] |
| 1,2-*cyclo*-(S—R—S) R = $P(CMe_3)$, $P(S)(CMe_3)$, $P(Se)(CMe_3)$ | DFT: structures and NMR shifts | [1744] |
| (1,2-$S_2C_2B_{10}H_{10}$)$_2$[μ-S—$P(CMe_3)$-S]$_2$ (FF) | DFT: structures and NMR shifts | [1744] |
| (1,2-$C_2B_{10}H_{10}$)$_2$(μ-S—PR—S)$_2$ R = $CHMe_2$, $CH_2C_6H_3Me_2$, *n*-$C_6H_{11}$, Ph (FF) | DFT: structures and NMR shifts | [1744] |
| 1,2-[$SP(CMe_3)Cl]_2$ | DFT: structures and NMR shifts | [1744] |
| $CH_2$[P(μ-S)$_2C_2B_{10}H_{10}]_2$ (FF) | DFT: structures and NMR shifts | [1744] |
| (1,2-$C_2B_{10}H_{10}$)$_2$[μ-SPCl—$CH_2$—PClS]$_2$ (FF) | DFT: structures and NMR shifts | [1744] |

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| Compound | Information | References |
|---|---|---|
| 1,2-$[SP(CMe_3)Cl]_2$ | DFT: structures and NMR shifts | [1744] |
| 1,2-$[Au(PPh_3)]_2$ | DFT | [67] |
| ***Sulfur*** | | |
| 1,2-$(SH^-)_2$ | DFT optimized structure of singlet and triplet states of neutral species and dianions formed by $H^+$ removal from R groups | [1107] |
| | DFT; unusually long C–C bond distances; influence of substituents on C–C length | [1106] |
| 1,2-*cyclo*-$C_8H_4S_2$ (dithiophene) | DFT: non-aromaticity of $C_6$ ring | [1637] |
| 1,2-*cyclo*-SeP(S)PhSe | DFT, molecular structure | [1711] |
| 1,2-*cyclo*-SeP(R)(S)PhSe R = $CHMe_2$, OEt | DFT, molecular structure | [1711] |
| [-*cyclo*-$C_8S_2H_2(C_2B_{10}H_{10})$-Ar-]$_n$ dithiophene polymers Ar = (*n*-$C_{12}H_{25})_2C_8S_2$, $(octyldodecyl)_2N_2C_6O_2(C_4H_2S)_2$ | DFT: HOMO/LUMO | [1721] |
| 1,2-*cyclo*-(S—R—S) R = $SiMe_2$, $P(CMe_3)$, P(S)$(CMe_3)$, P(Se)$(CMe_3)$ | DFT: structures and NMR shifts | [1744] |
| $(1,2\text{-}S_2C_2B_{10}H_{10})_2[\mu\text{-}S—P(CMe_3)\text{-}S]_2$ (FF) | DFT: structures and NMR shifts | [1744] |
| 1,2-*cyclo*-(S—PX—S) X = Cl, Br, I, H, F, $NCH_2PhH$ | DFT: structures and NMR shifts | [1744] |
| 1,2-*cyclo*-(S—SbF—S) | DFT: structures and NMR shifts | [1744] |
| 1,2-*cyclo*-(S—BBr—S) | DFT: structures and NMR shifts | [1744] |
| 1,2-*cyclo*-(S—PR—S) R = $NEt_2$, OEt, $CHMe_2$, $CH_2C_6H_3Me_2$, Ph | DFT: structures and NMR shifts | [1744] |
| 1,2-$[SP(CMe_3)Cl]_2$ | DFT: structures and NMR shifts | [1744] |
| 1,2-*cyclo*-[S—P($CH_2PCl_2$)—S] | DFT: structures and NMR shifts | [1744] |
| $CH_2[P(\mu\text{-}S)_2C_2B_{10}H_{10}]_2$ (FF) | DFT: structures and NMR shifts | [1744] |
| $(1,2\text{-}C_2B_{10}H_{10})_2[\mu\text{-}SPCl—CH_2—PClS]_2$ (FF) | DFT: structures and NMR shifts | [1744] |
| 1,2-$[SP(CMe_3)Cl]_2$ | DFT: structures and NMR shifts | [1744] |
| 9,12-cyclo-S-CH=CR-S 1,4-dithiin R = Ph, *o*/*m*/*p*-$C_6H_4F$, $C_5H_4FeCp$, C(O)Me, C(O)furyl, C(O)Ph, C(O)OMe, $C(O)C_5H_4FeCp$ | DFT: electronic structure | [1750] |
| ***Selenium*** | | |
| 1-$SeC_{10}H_7$-2-R R = Me, Ph naphthyl selenides | DFT, structures and energies | [1571] |
| *Spirocyclo*-$[B(1,2-Se_2C_2B_{10}H_{10}]_2^-$ (FF) | DFT, molecular structure | [1575] |
| 1,2-(Se-cyclo-$Pse_2$-$C_2B_{10}H_{10})_2$ (FF) | DFT, molecular structure | [1619] |
| 1,2-*cyclo*-SeC($CMe_3$)=CH—BCl—Se— | DFT: $^{11}B$ and $^{77}Se$ NMR shifts; cage geometry | [1640] |
| 1,2-cyclo-SeCEt=CEt—BX—Se—X = Cl, Br, I, Ph | DFT: $^{11}B$ and $^{77}Se$ NMR shifts; cage geometry | [1640] |
| 1,2-*cyclo*-SeCPh=CEt—BCl—Se— | DFT: $^{11}B$ and $^{77}Se$ NMR shifts; cage geometry | [1640] |
| 1,2-*cyclo*-SeCPh=CEt—BCl—CEt=CPh—Se— | DFT: $^{11}B$ and $^{77}Se$ NMR shifts; cage geometry | [1640] |
| [1,2-*cyclo*-SeCR=CEt—B—CEt=CR—Se—]$_2$ B—O R = Et, Ph | DFT: $^{11}B$ and $^{77}Se$ NMR shifts; cage geometry | [1640] |
| 1,2-*cyclo*-SeCR=CEt—B(OH)—CEt=CR—Se— R = Et, Ph | DFT: $^{11}B$ and $^{77}Se$ NMR shifts; cage geometry | [1640] |
| 1,2-*cyclo*-SeP(R)(Se)PhSe R = $CHMe_2$, OEt | DFT, molecular structure | [1711] |
| 1,2-*cyclo*-$Se_2P(Se)PhSe_2$ (2 isomers) | DFT, molecular structure | [1711] |

| Compound | Information | References |
|---|---|---|
| 1,2-*cyclo*-$Se_2P(Se)(CHMe_2)Se_2$ | DFT, molecular structure | [1711] |
| 1,2-*cyclo*-[S—P(Se)($CMe_3$)—S] | DFT: structures and NMR shifts | [1744] |
| 1,2-*cyclo*-SeP(R)Se R = $CHMe_2$, *cyclo*-$C_6H_{11}$, $CMe_3$, $CH_2C_6H_3Me_2$, Ph, OEt, $NEt_2$, $(CH_2)_nPCl_2$ $n$ = 1,2 | DFT: molecular structure, NMR | [1751] |
| $(CH_2)_n[P(\mu\text{-}S)_2C_2B_{10}H_{10}]_2$ | DFT: molecular structure, NMR | [1751] |
| $(H_{10}B_{10}C_2)[\mu\text{-}SeP(R)Se]_2(C_2B_{10}H_{10})$ R = $CHMe_2$, *cyclo*-$C_6H_{11}$, $CMe_3$ (FF) | DFT: molecular structure, NMR | [1751] |
| 1,2-*cyclo*-$Se_2P(=Se)CH_2C_6H_3Me_2$ | DFT: molecular structure, NMR | [1751] |
| 1,2-*cyclo*-SeP(S)PhSe | DFT, molecular structure | [1711] |
| 1,2-*cyclo*-SeP(R)(S)PhSe R = $CHMe_2$, OEt | DFT, molecular structure | [1711] |
| ***Tellurium*** | | |
| 1,2-cyclo-TeP(R)P(R) R = $CHMe_2$, $CMe_3$, Ph | DFT: molecular structure, NMR | [1751] |
| 1,2-*cyclo*-$Te_2PR$ R = $CHMe_2$, $CMe_3$ | DFT: molecular structure, NMR | [1751] |
| $(H_{10}B_{10}C_2)[\mu\text{-}P(R)TeP][\mu\text{-}TeP(R)](C_2B_{10}H_{10})$ R = $CHMe_2$, $CMe_3$ (FF) | DFT: molecular structure, NMR | [1751] |
| $H_2C[P(\mu\text{-}Te)_2C_2B_{10}H_{10}]_2$ (FF) | DFT: molecular structure, NMR | [1751] |
| ***Mercury, silver, and gold*** | | |
| [*cyclo*-$\{\mu\text{-}1,2\text{-}C_2B_{10}H_{10})_nM_nAg_m\}^{z-}$ M = Au, Hg; $n$ = 3, 4; $m$ = 0, 1, 2 | DFT: electronic & geometric structures | [1649] |
| 1,2-*cyclo*-$\{[(Me_2CH)N(CH_2)_2N(CHMe_2)]P\}_2AuIY\text{-}C_2B_{10}H_{10}$ Y = aryl, naphthyl, iodopyridyl, iodothiophenyl | DFT: energies | [1802] |
| ***Iridium*** | | |
| (*cyclo*-$O_2C_3HMe_2$)Ir($N_2C_{10}H_8$—1,2-$CB_{10}H_{10}CH)_2$ | DFT: HOMO-LUMO levels | [1666] |
| $(N_2C_{12}H_8)Ir(N_2C_{10}H_8-1,2-CB_{10}H_{10}CH)_2^+$ $PF_6^-$ | DFT: HOMO-LUMO levels | [1666] |
| [R—$CB_{10}H_{10}C$—$NC_5H_4$—$C_8H_4S$]$_2$Ir($O_2C_3Me_2H$) R = Me, *n*-$C_4H_9$ pyridyl, benzothienyl, acac phosphorescence | DFT: HOMO/LUMO | [1710] |
| $(Me_2C_3HO_2)Ir(NC_5H_4\text{-}C_6H_3—CB_{10}H_{10}CR)$ 2 Ir—$C_6H_3$ acetylacetonate R = H, Me, $CHMe_2$, *i*-$C_4H_9$, Ph, $C_6H_4CF_3$, $C_6F_5$ | DFT: HOMO-LUMO levels | [1848] |
| $(Me_2C_3HO_2)Ir(NC_5H_4\text{-}Ph)_2[CB_{10}H_{10}C\text{-}(CH_2)_n\text{-}CB_{10}H_{10}C]$ $n$ = 4,6 cyclometalates (FF) | DFT: molecular orbital energies | [1875] |
| ***Nickel, palladium, platinum*** | | |
| 1,2-$[CH(OH)—C_5H_3RN]_2PdCl$ R = H, Me 2 N→Pd, B(3)→Pd pincer complexes | DFT: σ-electron donation | [1772] |
| 1,2-*cyclo*-$S_2Pt^{II}$-L L = *o*-phen, bipyr, $Me_2$bipyr, $(CMe_3)_2$bipyr, $Ph_2$bipyr, $Ph_2$phenanthroline | DFT: electronic structure | [1801] |
| $(N_2C_{16}H_{11})Pt—C{\equiv}C—C_2B_{10}H_{11}$ phenylbipyridyl | DFT: influence of carborane on phosphorescence | [1918] |
| **Isomerization Calculations** | | |
| 1,2-$Me_2$-9,12-$Cl_2$ | Cage isomerization via anticubeoctahedron | [1118] |

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| Compound | Information | References |
|---|---|---|
| **NMR Calculations** | | |
| 1,2-{*cyclo*-[B—N(R)—o-$C_6H_4$—N(R)—]}$_2$ R = Et, Ph diazaborolyl | GIAO NMR | [1684] |
| 1-$PPh_2$I-2-Me I–I intermolecular interaction in solid state and solution | DFT-GIAO $^{31}$P NMR | [568] |
| 1-Me-2-NHNHPh | GIAO-NMR; dative *exo*-CN - cage π bonding | [540] |
| 1-Ph-2-$C_6H_4$-*p*-X X = H, F, OMe, $NMe_2$, $NH_2$, OH | DFT-GIAO $^{11}$B and $^{13}$C NMR | [1128] |
| 1,2-*cyclo*-SeC($CMe_3$)═CH—BCl—Se— | DFT: $^{11}$B and $^{77}$Se NMR shifts; cage geometry | [1640] |
| 1,2-cyclo-SeCEt═CEt—BX—Se— X = Cl, Br, I, Ph | DFT: $^{11}$B and $^{77}$Se NMR shifts; cage geometry | [1640] |
| 1,2-*cyclo*-SeCEt═CEt—BX—CEt═CEt—Se— X = Cl, Br, I, Ph | DFT: $^{11}$B and $^{77}$Se NMR shifts; cage geometry | [1640] |
| 1,2-*cyclo*-SeCPh═CEt—BCl—Se— | DFT: $^{11}$B and $^{77}$Se NMR shifts; cage geometry | [1640] |
| 1,2-*cyclo*-SeCPh═CEt—BCl—CEt═CPh—Se— | DFT: $^{11}$B and $^{77}$Se NMR shifts; cage geometry | [1640] |
| [1,2-*cyclo*-SeCR═CEt—B—CEt═CR—Se—]$_2$ B—O R = Et, Ph | DFT: $^{11}$B and $^{77}$Se NMR shifts; cage geometry | [1640] |
| 1,2-*cyclo*-SeCR═CEt—B(OH)—CEt═CR—Se— R = Et, Ph | DFT: $^{11}$B and $^{77}$Se NMR shifts; cage geometry | [1640] |
| 1,2-*cyclo*-SeP(R)Se R = $CHMe_2$, *cyclo*-$C_6H_{11}$, $CMe_3$, $CH_2C_6H_3Me_2$, Ph, OEt, $NEt_2$, $(CH_2)_nPCl_2$ *n* = 1,2 | DFT: molecular structure, NMR | [1751] |
| $(CH_2)_n$[P(μ-S)$_2$$C_2B_{10}H_{10}$]$_2$ | DFT: molecular structure, NMR | [1751] |
| ($H_{10}B_{10}C_2$)[μ-SeP(R)Se]$_2$($C_2B_{10}H_{10}$) R = $CHMe_2$, *cyclo*-$C_6H_{11}$, $CMe_3$ (FF) | DFT: molecular structure, NMR | [1751] |
| 1,2-*cyclo*-$Se_2$P(═Se)$CH_2C_6H_3Me_2$ | DFT: molecular structure, NMR | [1751] |
| 1,2-*cyclo*-(S—R—S) R = P(Se)($CMe_3$) | DFT: structures and NMR shifts | [1744] |
| 1,2-*cyclo*-(S—R—S) R = $SiMe_2$, P($CMe_3$), P(S)($CMe_3$), P(Se)($CMe_3$) | DFT: structures and NMR shifts | [1744] |
| 1,2-*cyclo*-(S—SbF—S) | DFT: structures and NMR shifts | [1744] |
| 1,2-*cyclo*-(S—BBr—S) | DFT: structures and NMR shifts | [1744] |
| (1,2-$C_2B_{10}H_{10}$)$_2$(μ-S—PR—S)$_2$ R = $CHMe_2$, $CH_2C_6H_3Me_2$, *n*-$C_6H_{11}$, Ph (FF) | DFT: structures and NMR shifts | [1744] |
| 1,2-[SP($CMe_3$)Cl]$_2$ | DFT: structures and NMR shifts | [1744] |
| 1,2-*cyclo*-[S—P($CH_2PCl_2$)—S] | DFT: structures and NMR shifts | [1744] |
| $CH_2$[P(μ-S)$_2$$C_2B_{10}H_{10}$]$_2$ (FF) | DFT: structures and NMR shifts | [1744] |
| (1,2-$C_2B_{10}H_{10}$)$_2$[μ-SPCl—$CH_2$—PClS]$_2$ (FF) | DFT: structures and NMR shifts | [1744] |
| 1,2-[SP($CMe_3$)Cl]$_2$ | DFT: structures and NMR shifts | [1744] |
| **Reactivity Calculations** | | |
| 1-C(O)OO$CMe_2$C≡CH-2-R [R = H, $CHMe_2$ peroxy alkynes | $\Delta H_{formation}$, $\Delta G_{formation}$ | [1337] |
| 1,2-*cyclo*-O[$(CH_2)_2S(CH_2)_2^-$]$_2$ | Molecular modeling | [463] |
| 1,2-cycloethers | Molecular modeling | [463] |
| 1-$C_6H_4$(2′-OMe) R = $NO_2$, $NH_2$, OMe | DFT: effect of substituents on intramolecular C—H—O bonding in solid state | [223] |
| 1,2-*bicyclo*-SCoCpSNC(R)O R = OMe, Ph | DFT: insertion pathways | [1636] |

| Compound | Information | References |
|---|---|---|
| 1,2-*bicyclo*-SCoCpN(R)S(R′C═CR″) R = Ts, Ms R′, R″ = H, C(O)OMe, Ph Ts = *p*-toluenesulfonyl Ms = methanesulfonyl | DFT: insertion pathways | [1636] |
| 1,2-*bicyclo*-SCoCpSN(R)(R′C═CR″) R = Ts, Ms R′, R″ = H, C(O)OMe, Ph Ts = *p*-toluenesulfonyl Ms = methanesulfonyl | DFT: insertion pathways | [1636] |
| 1,2-*bicyclo*-SCoCpSN(R)C═CHCMe$_3$ R = Ts, Ms R′,R″ = H, C(O)OMe, Ph Ts = *p*-toluenesulfonyl Ms = methanesulfonyl | DFT: insertion pathways | [1636] |
| 1-$SO_2NH_2$ | QM/MM interaction with human carbonic anhydrase II | [1703] |
| **Other Calculations** | | |
| *n*-TlCl *n* = 1, 9 | Raman (vibrational frequencies) | [760] |
| Hg(*n*-$C_2B_{10}H_{11}$}$_2$ *n* = 1, 9 (FF) | Raman (vibrational frequencies) | [760] |
| 9-HgR R = Cl, Br, Et | Raman (vibrational frequencies) | [760] |
| 1-HgMe | Raman (vibrational frequencies) | [760] |
| 1-$CH_2$X X = Cl, Br, I | Dipole moments | [1342] |
| 1-X X = Cl, Br, I | Dipole moments | [1342] |
| 9,12-$Br_2$ | Dipole moments | [1139] |
| RR′$C_2B_{10}H_{10}^{n-}$ *n* = 0, 1, 2; R = $C_7H_6$, $B_{12}H_{11}$; R = $C_5H_4$, H, Me (FF) | β (first hyperpolarizability); NLO | [1110] |
| 1-($C_4H_2$S-$C_4H_2$S-)$_n$ thiophene polymer | DFT: orbital energies | [1808] |
| 1,2-(SH)$_2$/9,12-(SH)$_2$ attached to surface of Au microcrystals | Dipole moments | [628] |
| 1,2-*cyclo*-[$C_6H_4$-*p*-(CH═CH)$_n$-$C_6H_4$-*p*-$NMe_2$]$_2$ *n* = 1,2 | DFT, second order NLO response | [1635] |
| 1,2-*cyclo*-[$C_6H_4$-*p*-(CH═CH)$_n$-$C_6H_4$-*p*-($C_3HS_2$]$_2$ tetrathiafulvalene | DFT, second order NLO response | [1635] |
| *Cis*-($Me_2C_3HO_2$)Ir($NC_5H_4$-$C_6H_3$-$CB_{10}H_{10}$CMe)$_2$ | DFT: ground and lowest triplet states | [1651] |
| *Cyclo*-{($O_2C$)$_2$$C_2B_{10}H_8$-4,10-[IrCp*(*cyclo*-$NC_4H_4N$)IrCp*]$_2$-4,10-$H_8B_{10}C_2(CO_2)_2$} | DFT: mechanism of formation | [1729] |
| 1-P(═S)$Ph_2$-2-$SCH_2C_6H_2(CMe_3)_2$-$OZrCl_2$Cp ethylene polymerization co-catalyst with MAO | DFT: stereochemistry | [1787] |

[a] *Substituents on the carborane cage. "FF" indicates that the full formula of the compound is given.*
[b] *S, synthesis; X, X-ray diffraction; ED, gas phase electron diffraction; H, $^1$H NMR; B, $^{11}$B NMR; C, $^{13}$C NMR; D, $^2$D NMR; N, $^{15}$N NMR; F, $^{19}$F NMR; P, $^{31}$P NMR; Li, $^7$Li NMR; Al, $^{27}$Al NMR; Si, $^{29}$Si NMR; Sn, $^{119}$Sn NMR; Se, $^{77}$Se NMR; $^{125}$Te NMR, Pt, $^{195}$Pt NMR; 2d, two-dimensional (COSY) NMR; IR, infrared data; MS, mass spectroscopic data; UV, UV-visible data; E, electrochemical data; ESR, electron spin resonance data; MAG, magnetic susceptibility; COND, electrical conductivity; CD, circular dichroism; DSC, differential scanning calorimetry; OR, optical rotation; NLO, nonlinear optical properties; TGA, thermogravimetric analysis; TEM, transmission electron microscopy; XPS, X-ray photoelectron spectroscopy; NQR, nuclear quadrupole resonance; EXAFS, X-ray absorption fine strucrure; NEXAFS, near edge X-ray absorption fine strucrure.*