Appendix F

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

Compound[a]	Information[b]	References
Synthesis and Characterization		
Parent	K_a association constant with β-cyclodextrin	[898]
Nontransition metal derivatives		
1,12-$C_2B_{10}H_{12}$ and $CB_{11}H_{12}^-$ isosteric pairs; nematic liquid crystals	Effect of molecular polarity on nematic phase stability	[933]
	Photo-fragmentation, double cation formation photoelectron-photoion-photoion coincidence (PEPIPICO) spectroscopy; MS (time-of-flight mass analysis)	[866]
H-$(CB_{10}H_{10}C)_n$-H $n=1$–4 (FF)	S, B ($n=1$–3)	[613]
Alkyl derivatives		
1-Me	Heat of formation	[65,81,82]
	S (small scale via pyrolysis of 1,2-$C_2B_{10}H_{12}$)	[937]
1-$CHMe_2$	B (substituent effects), H, IR	[21]
1-C_7H_6-12-C_5H_4	Hyperpolarizability; NLO	[90]
1-C_7H_7-12-[*cyclo*-C_5H_4-1-OH-3,4-Me_2]	S, H, B, C, IR, UV, MS, NLO	[620]
1-C_7H_7-12-[*cyclo*-C_5H_3-3,4-Me_2]	S, X, H, B, C, IR, UV, MS, NLO	[620]
1-C_5H_{11}—$CB_{10}H_{10}C$—$(C_6H_4)_2$R R=C_8H_{17}, OC_8H_{17} (FF)	H, MS, DSC, polarizing microscopy, ferroelectric liquid crystal properties	[622]
1-C_5H_{11}—$CB_{10}H_{10}C$—C_6H_4—$C_6H_2F_3$ nematic liquid crystals	S, H, DSC, opto-electrical properties	[623]
C_5H_{11}—$CB_{10}H_{10}C$—C(O)O—C_6H_4—O—C_3H_6-R liquid crystals—smectic phase induction via fluorination (FF)	S, H, phase transitions	[624]
C_5H_{11}—O—C_6H_4—$CB_{10}H_{10}C$—L—C_6H_4—O_n—C_5H_{11} L=CH_2CH_2, C(O)O, CH=CHC(O)O, CH=N, CH=CH, C(O)NH, CH_2CH_2O(O)C $n=0,1$ liquid crystals—effect of linking group on mesogenic properties (FF)	S, H, C, MS, phase transition temperature	[625]
C_nH_{2n+1}—C(O)O—C_6H_4—$CB_{10}H_{10}C$—L—C_6H_4—C(O)O—C_nH_{2n+1} effects of phenylalkyl connecting groups on mesogenic properties	S	[626]

Continued

Compound	Information	References
$Me_2N—C_6H_4—p\text{-}CB_{10}H_{10}C—p\text{-}C_6H_4—NO_2$	Dipole moment	[627]
Dipentyl derivatives	Molecular dynamics in liquid crystals	[630]
$HCB_{10}Me_{10}C—(CH_2)_3S(O)Me$ (FF)	S, H, B, C, IR, MS	[916]
Haloalkyl derivatives		
1-CH_2X X = Cl, Br, I	Dipole moment	[344]
$[Br(CH_2)_n]HC_2B_{10}Me_{10}$ n = 5, 6 (FF)	S, H, B, C, MS	[106]
1-CH_2Cl-12-R R = H, Me, Ph, I, Cl, CH_2Cl	E (reduction; comparison with 1,2- and 1,7-$C_2B_{10}H_{12}$ derivatives)	[104]
1-(n-C_6H_{12}-6′-Br)	S	[102]
Aryl derivatives		
1-Ph-12-R R = H, Me	Friedel-Crafts acylation (triflic acid catalysis); Taft σ constants.	[633]
	pK_a	[53]
1,12-(p-$CH_2C_6H_4$-Me)$_2$	S	[189]
1,12-(p-$RC_6H_4—C\equiv C—C_6H_4)C_2B_{10}H_{10}$ R = H, 1,12-$C_2B_{10}H_{11}$ (FF)	S, X, H, B, C, IR, MS	[637]
1-(p-C_6H_4Ph)-12-H	S, H, IR, UV, MS	[107]
1,12-(p-C_6H_4Ph)$_2$	S, H, IR, UV, MS	[107]
1-C_6H_4R-12-R′ R = NO_2, CN; R′ = H, $(CH_2)_n$OH, $(CH_2)_n$OSiMe_3, C(O)OMe, C(O)OH	S, H, C, MS, binding affinity	[638]
1-(3′-C_5H_5N)-12-CH_2OH androgen receptor antagonist	S	[639]
1-CH_2OH-12-C_6H_4-p-$cyclo$-(CNHC(=S)ONC) oxadiazole; hydrophilic pharmacore of androgen receptor ligands	S	[640]
1,12-(C_6H_4-o/m/p-OR)$_2$ R = H, Me, n-C_3H_7, n-C_5H_{11}, OMe, OCSiMe_3	S, H, C, binding affinity to estrogen receptor α	[643]
1-(C_6H_4-p-CN)-12-CH_2C(O)R R = Me, Et, $CHMe_2$, cyclopropyl, n-C_5H_{11}, Ph nonsteroidal progesterone (PR) antagonists (cyclopropyl most potent)	S, H, C, binding affinity	[951]
—$[C_{13}H_9(C_6H_{13})_2$-$CB_{10}H_{10}C$-$C_{13}H_9(C_6H_{13})_2]_n$— fluorenyl polymer	S, H, C, DSC, UV, fluorescence	[644]
(m-NC-C_6H_4)-$CB_{10}H_{10}C$-CH(OH)CH_2-X-p-C_6H_4R) X = O, X, SO_2, NH androgen receptor antagonist candidates (FF)	S, H, C, MS, binding affinity, transient transactivation assay	[903]
1,12-(CH_2-C_6H_4-CH=$CH_2)_2C_2B_{10}H_{10}$ (FF)	Cross-linker in micelles, obtained via radical polymerization; carborane-confined nanoparticles for BNCT	[914]
1-C_7H_7-12-$cyclo$-$C_5H_2Me_2CN$	S, X, H(2d), C(2d), IR, MS, UV	[917]
1-C_7H_7-12-$cyclo$-$C_5HMe_2(CN)_2$	S, H(2d), C(2d), IR, MS, UV	[917]
2-R R = CH_2Ph, C_6H_4Me, C_6H_4F	S	[95]
2-(o-C_6H_4R) R = H, OH, OMe proton-driven conformational change; intramolecular H bonding)	S, X(OH), H	[645]
2-C_6H_4-o-OMe	S, H, C, MS	[647]
	Pd-catalyzed demethylation with 2-MeOPhMgBr	[647]
2-C_6H_4-o-OH	S(from Pd-catalyzed reaction of $C_2B_{10}H_{11}$-2-I with 2-MeOPhMgBr), H, C, MS	[647]

Compound	Information	References
1-(C_6H_3-3′-Me-4′-OH)-12-R R = H, CH_2OH, C_6H_3-3′-Me-4′-OH	S	[893]
1-(C_6H_{10}-*p*-OH)-12-R R = H, CH_2OH estrogen receptor-β ligands	S, H, MS	[893]
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	[947]
1-C_5H_{11}—O—C_6H_4-$CB_{10}H_{10}$C—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	[947]
1-CH(C_6H_4-*p*-OH)$_2$	S, H, C. S	[900]
Haloaryl derivatives		
1-$CH_2CH_2C_6H_{10}$—C_6H_4F	S, H, B, C, MS	[619]
1-R-12-*n*-C_5H_{11} R = $CH_2CH_2C_6H_{10}$—C_6H_4F, *p*-C_6H_4Br	S, H, B, C, MS	[619]
1-(*p*-$C_6H_4Br)_2$-12-(C_6H_4-*p*-NC_5H_4-*p*-NC_5H_4) bipyridine	S, H, B	[649]
1,2-(2′,3′-$C_6H_3Cl_2)_2$ for inclusion in TPP TPP = tris(*o*-phenylenedioxy) cyclotriphosphazene dipolar molecular rotors	S, H(2d), C	[922]
[1-(2′,3′-$C_6H_3Cl_2$)-12-($C_6H_4)_2$-*n*-C_5H_{11}]@TPP TPP = tris(*o*-phenylenedioxy)cyclotriphosphazene dipolar molecular rotors	DSC, C(solid state), X-ray powder	[922]
[1,2-(2′,3′-$C_6H_3Cl_2)_2$]@TPP TPP = tris(*o*-phenylenedioxy) cyclotriphosphazene dipolar molecular rotors	DSC, C(solid state), X-ray powder	[922]
2-*m/p*-C_6H_4F	S	[146]
1-R R = ganciclovir (GCV), acyclovir (ACV), cidofovir (CDV) valganciclovir (VCDV) lipophilic anti-HCMV drugs	S, cytotoxicity	[928]
1,12-F_2-2-*p*-C_6H_4OH	S, H, B, C, estrogen receptor β binding affinity	[853]
1-C_6H_4-*p*-$NC_{12}H_8$ *N*-carbazolyl donor-acceptor dyad complexes photoelectron charge transfer	S, H, B, C, MS, UV, E, transient absorption	[865]
(porphyrin)[C_6F_4-*p*-SCH_2-1-(1,12-$C_2B_{10}H_{11}]_4$	S, H, F, UV, MS, dark & phototoxicity toward T98G cells, BBB permeability	[934]
Alkenyl derivatives		
1-R-12-R′ R = CH=CH_2, CMe=CH_2; R′ = $SnMe_3$, $SnEt_3$, Sn(*n*-$C_4H_9)_3$	S, IR	[473]
1,12-[CH_2=CH]$_2C_2B_{10}Me_{10}$ (FF)	S, H, B, C, MS	[153]
2-CH_2CH=CH_2	S	[95]
1-CH=CH—C_6H_4—C≡C–C_6H_4—CH=CH—C_6H_4—NPh_2 two-photon acceptors	UV(absorption, fluorescence)	[915]
Alkynyl derivatives		
1-C≡CR R = H, Ph	S	[161]
1,12-($C\equiv CR)_2$ R = H, Ph	S	[161]
1-C≡C—C≡C—CMe_2OH	S, H, B, C, IR, MS	[652]
1,12-[$Me(CH_2)_3OC(O)C\equiv C]_2C_2B_{10}Me_{10}$ (FF)	S, H, B, C, MS	[153]
1,12-$HCB_{10}Me_{10}C$—C≡C—C≡C—$CB_{10}Me_{10}CH$ (FF)	S, H, B, C, MS, UV	[153]
[1,12-RC≡C—$CB_{10}Me_{10}$C—C≡C—C≡C—$CB_{10}Me_{10}$-C—C≡C—]$_2$ R—H, Me, C(O)O$(CH_2)_3$Me (FF)	S, H, B, C, MS	[153]
1,12-$RCB_{10}Me_{10}$C—C≡C—C≡C—$CB_{10}Me_{10}$CR′ R, R′ = H, C(O)OMe (FF)	S, H, B, C, MS	[153]

Continued

Compound	Information	References
$HCB_{10}H_{10}C{-}C{\equiv}C{-}C_6H_3I{-}C{\equiv}C{-}CB_{10}H_{10}CH$ (FF)	S, H, C, IR, MS	[655]
Thioxanthene(naphtha[2,1-*b*]-thiopyran-$\{C{\equiv}C{-}C_6H_3(C{\equiv}C{-}CB_{10}H_{10}CH)_2\}_2$ (FF) motorized nanocar	S, H, C, IR, MS, kinetics of thermal isomerization	[655]
$(MeCB_{10}H_{10}C{-}C{\equiv}C)_2C_6H_3$-$C{\equiv}C[C_6H_2(OC_{10}H_{21})_2$-$C{\equiv}C]_2C_6H_2[C{\equiv}C{-}C_6H_2(OCC_{10}H_{21})_2C{\equiv}C$-$C_{60}]_2$ nanodragster	S, H, C, IR, MS	[656]
$N_2[C_6H_4{-}C{\equiv}C{-}C_6H_3(C{\equiv}C{-}CB_{10}H_{10}CH)_2]_2$ nanoworm	S, H, C, IR, UV	[658]
$[HCB_{10}H_{10}C{-}C{\equiv}C{-}C_6H_3(OC_3H_7)_2{-}C{\equiv}C{-}C_6H_4]_2N_2$	S, H, C, IR, photo-isomerization	[659]
$HCB_{10}H_{10}C{-}C{\equiv}C{-}C_6H_3(C{\equiv}C{-}C_6H_4{-}N{=}N{-}Ph){-}$ $C{\equiv}C{-}CB_{10}H_{10}CH$	S, H, C, IR, photo-isomerization	[659]
1′,3′,5′-$\{[C{\equiv}C{-}C_6H_2$-2′,5′-$(OC_3H_7)_2]_2$-$C{\equiv}C{-}CB_{10}H_{10}CH\}_3C_6H_3$ nanocar (FF)	S, H, C, IR, UV, fluorescence	[660]
$H_2C_2B_{10}H_9$-2-$C{\equiv}C$-2-$H_2C_2B_{10}H_9$ (FF)	S, H, B, C, MS	[661]
2-I-$H_2C_2B_{10}H_8$-9-$C{\equiv}C$-9-$H_2C_2B_{10}H_8$-2-$C{\equiv}C$-9-$H_2C_2B_{10}H_8$-2-I (FF)	S, H, B, C, MS	[661]
2,5-$(MeO)_2$-1,4-$[C{\equiv}C{-}C_6H_3$-2′,5′-$(C{\equiv}C{-}CB_{10}H_{10}CH)_2]_2C_6H_2$ motorized nanocar (FF)	S, H, C, IR, UV, fluorescence	[660]
2,5-$(C{\equiv}C{-}CB_{10}H_{10}CH)_2$-1,4-$[C{\equiv}C{-}C_6H_3$-2′,5′-$(C{\equiv}C{-}CB_{10}H_{10}CH)_2]_2C_6H_2$ nanocaterpillar (FF)	S, H, C, IR, UV, fluorescence	[660]
1′,4′-(1,12-$HCB_{10}H_{10}C{-}C{\equiv}C)_2C_6H_3$-2′—$C{\equiv}C{-}C_6H_2$-2′,5-$(OMe)_2$-4′-$C_6H_2$-1′,4′-$(C{\equiv}C$—1,12-$CB_{10}H_{10}CH)_2$-2′-tetramethylrhodamine-isothiocyanate and other similarly labeled nanocars (FF)	S, micrometer-scale translation and fluorescence monitoring of nanocars on a glass surface	[904]
C_6H_3-1′,6′-$(CB_{10}H_{10}CH\_2$-2′-$[C{\equiv}C$-$C_6H_2(OMe)_2$-*p*-$C{\equiv}C$-C_6H_2-1′,6′-$(CB_{10}H_{10}CH)_2$-2′-$C_6H_3(OCHMe_2)(CH{=}RuCl_2L)]$ $L = P(C_6H_4$-*p*-$CHMe_2)$, *cyclo*-$CHN_2Mes_2C_2H_4$ ROMP catalysis of 1,5-cyclooctadiene; ROMP-propelled nanocars (FF)	S(olefin metathesis), H, C, P	[907]
1-$CH{=}CH$-*p*-$C_6H_4{-}C{\equiv}C$—*p*-$C_6H_4{-}CH{=}CH$-C_6H_2-4-R-3′,5′-R′ $R = NPh_2$, $R = R' = OC_{12}H_{25}$; $R = R' = O(CH_2CH_2O)_3Me$ (FF) 2-photon absorbing chromophores	S, UV(visible and emission), fluorescence microscopy	[952]
1-$CH{=}CH{-}C_6H_4{-}C{\equiv}C$-$C_6H_4{-}CH{=}CH{-}C_6H_4{-}NPh_2$ two-photon acceptors	UV(absorption, fluorescence)	[915]
1-$(C{\equiv}C{-}C_6H_4$-*p*-I)-12-$C{\equiv}C{=}C_6H_4$-*p*—C_6H_4-*p*- $SiEt_3$	S, X	[919]
1-$(C{\equiv}C{-}C_6H_4$-*p*-$C{\equiv}C{-}C_6H_4$-*p* -R)-12-$(C{\equiv}C{-}C_6H_4$-*p*-$C{\equiv}C{-}C_6H_4$-*p* -R′) $R = C_{37}H_{42}N_2BF_2O_3$ (borondipyrrolemethene), $R' = C_6H_{20}N_2O_2(CH_2Ph)_2(C_6H_4$-*p*-$NMe_2)$ (diketopyrrole) unsymmetrical linker for donor-acceptor dyads	S, H, C, MS, UV, fluorescence	[919]
$RCB_{10}H_{10}C{-}C{\equiv}C{-}C_5H_6{-}C{\equiv}C{-}CB_{10}H_{10}CR$ (FF) $R = Si(C_6H_{13})_3$, H, C(O)OH and related species C_5H_6 = bicyclo[1.1.1]pentane	S, X[C(O)OH], H, C, P, IR, MS	[923]
$R{-}C_6H_4{-}C{\equiv}C{-}[{-}C_6H_4{-}C{\equiv}C{-}CB_{10}H_{10}C{-}$ $C{\equiv}C{-}C_6H_4{-}C{\equiv}C{-}]n$-$C_6H_4{-}R'$ n = 1-5 (FF) R, R′ = dipyrrolopyrrole chromophores dyads for electronic energy transfer	S, H, C, MS, UV, fluorescence	[924]
(dibenzophenazine)$Ir(N_2C_{10}H_8){-}$ $C{\equiv}C{-}C_6H_4{-}C{\equiv}C{-}CB_{10}H_{10}C{-}C{\equiv}C{-}C_6H_4{-}C{\equiv}C{-}N_2$ $C_{10}H_8)Ir(NC_{11}H_6F_2)^{2+}$ donor-acceptor complexes	S, MS, UV, E	[926]
1-$(CH_2)_3C{\equiv}CH$	S, H, B, C, MS	[949]
2-$C{\equiv}C$-uridine	S, H, B, C, MS, UV, IR, cytotoxic activity vs. DNA and RNA viruses	[949]

Compound	Information	References
2-C≡C-deoxyuridine	S, H, B, C, MS, UV, IR, cytotoxic activity vs. DNA and RNA viruses	[949]
2-(deoxy-ribo-beta-D-furanosyl-dihydrofuropyrimidine-one)	S, H, B, C, MS, UV, IR, cytotoxic activity vs. DNA and RNA viruses	[949]
1-$(CH_2)_3$C≡C-nucleosides	S, H, B, C, MS, UV, IR, cytotoxic activity vs. DNA and RNA viruses	[949]
Alcohols and C- and B-hydroxy derivatives		
1-CH_2OH	heats of combustion and formation	[183]
$(HOCH_2)HC_2B_{10}Me_{10}$ (FF)	S, H, B, C, MS	[663]
$(HOCH_2)HC_2B_{10}HMe_9$-2-R R = NHMe, NH_2, CN (FF)	S, H, B, C, MS	[663]
$(HOCH_2)HC_2B_{10}HMe_9$-2-CH=NOH (FF)	S, X, H, B, C, MS	[663]
$[(HOCH_2)HC_2B_{10}HMe_9$-2-CH=NO−$]_2$ (FF)	S, X, H, B, C, MS	[663]
1-OH-12-$CH(OEt)_2$	S, H, B, C	[666]
1-CH_2OH-12-C_6H_4-*p*-*cyclo*-(CNHC(=S)ONC) oxadiazole; hydrophilic pharmacore of androgen receptor ligands	S	[640]
$[HO(CH_2)_3]MeC_2B_{10}Me_{10}$ (FF)	S, H, B, C, MS	[614]
n-*p*-C_6H_4OH *n* = 1,2	S, partition coefficients (log P)]; Hansch-Fujita hydrophobic parameters; drug design	[669]
	pK_a, hydrophobicity, estrogen receptor binding affinity	[191]
1,12-$(CH_2$-*p*-$C_6H_4OH)_2$	S	[188,189]
1-R-12-R′ R = H, R′ = OH, CH_2OH, NH_2; R = R′ = OH complexes with β-cyclodextrin	K_a (association constants)	[195]
1-OH-12-$(CH_2)_2C(O)OH$ propionic acid	S	[670]
1-(*m*-C_6H_4OH)-12-R R = H, OH, $(CH_2)_nOH$ *n* = 1-3 estrogen agonists; hydrophobic pharmacore; estrogen receptor modulation; steroid receptors	S, H, MS	[196]
1-(*m*-C_6H_4OMe)-12-R R = H, OH, $(CH_2)_nOH$ *n* = 1-3	S, H, MS	[196]
1-R-12-CH_2SCMe_3 R = $(CH_2)_3OH$, $CH_2CH_2C(O)OH$	S, H, C, IR, MS	[671]
1,12-$[HO(CH_2)_2]_2C_2B_{10}Me_{10}$ (FF)	S, H, B, C, MS	[153]
1,12-$H[HO(CH_2)_2]C_2B_{10}Me_{10}$ (FF)	S, H, B, C, MS	[153]
1-$(CH_2)_2OCH_2CH(OH)(CH_2)_2OH$-12-$(CH_2)_2$-O-$CH_2C(O)CMe_3$ nonsecosteroidal vitamin D analogs	S, H, HL-60 cell differentiation activity	[931]
1-$(CH_2)_2OCH_2CH(OH)(CH_2)_2OH$-12-$(CH_2)_2$-O-$CH_2CH(OH)CMe_3$ nonsecosteroidal vitamin D analogs	S, H, HL-60 cell differentiation activity	[931]
1-$(CH_2)_4CEt_2OH$-12-$CH_2O(CH_2)_2C(OH)CHR$- CH_2OH R = OH, $O(CH_2)_nOH$ *n* = 2,3,4 tetraols nonsecosteroidal vitamin D analogues very high VDR activity for *n* = 4	S, vitamin D receptor activity	[936]
1-$(CH_2)_4CEt_2OH$-12-$(CH_2)_2OCH_2CH(OH)$-$(CH_2)_2OH$ tetraols nonsecosteroidal vitamin D analogues	S, X	[936]
Alkoxy and aryloxy derivatives		
1-B[$OCPhCH_2CPhO$]-12-R R = $CH(OEt)_2$, C(O)H boronic acids	S	[666]

Continued

Compound	Information	References
Aldehydes		
1-CH(OEt)$_2$ acetaldehyde diethyl acetal	S	[211]
(CF$_3$SO$_2$CH$_2$)$_2$C$_2$B$_{10}$Me$_{10}$ (FF)	S, X, H, B, C, MS	[614]
1-C(O)H-12-(*p*-C$_6$H$_4$-OC$_5$H$_{11}$)	S, dielectric constants, mesogenic properties	[675]
1-C(O)H-12-R R = B(OEt)$_2$, B(OCPhCH$_2$CPhO) boronic acid	S	[666]
Carboxylic acids and carboxylates		
1-C(O)OH-12-*n*-C$_5$H$_{11}$	S, H, B, C, IR	[619,679]
1-C(O)OH-12-CH$_2$CHMeEt	S, H, B, C, IR	[619]
1-C(O)OH-12-Me	pK_a, E (half-neutralization potential)	[226]
1-C(O)OH-12-NHC(O)OC(CH$_2$)$_3$	S, H, C, IR	[234]
1-C(O)OH-12-*p*-C$_6$H$_4$OMe	S, H, MS	[196]
1-C(O)OH-12-(*p*-C$_6$H$_4$OR) R = Me, H liquid crystals	S, H, DSC, mesogenic properties	[680]
1-CH$_2$CH$_2$C(O)OH-12-CH$_2$SH	S, H, C, IR, MS	[671]
1-R-12-CH$_2$SCMe$_3$ R = (CH$_2$)$_3$OH, CH$_2$CH$_2$C(O)OH	S, H, C, IR, MS	[671]
n-SCH$_2$C(O)OH *n* = 1,2	MS, pK_a	[176]
1-C(O)OH-12-Me	S, IR (actual spectrum)	[600]
1,12-[C(O)OH]$_2$	Complex with α-cyclodextrin in aqueous solution; K_a (association constant)	[227]
1-C(O)OH-12-N(boc)NH(boc) boc = *tert*-butyloxycarbonyl]hydrazino	S, X, H, B, C, MS	[268]
[HO(O)C]MeC$_2$B$_{10}$Me$_{10}$ (FF)	pK_a	[237]
{1,12-[OC(O)]$_2$C$_2$B$_{10}$H$_{10}$}$^{2-}$ [Mo(*N*,*N*′-di-*p*-anisyl-formamidinate)$^+$]$_2$ (FF)	S, X, H	[683]
HO(O)C—CB$_{10}$H$_{10}$C—C$_6$H$_4$-*p*-—CB$_{10}$H$_{10}$C—C(O)OH (FF) incorporation in porous 3D Zn(II) coordination polymers	S, X, H, C, B, X-ray powder diffraction, thermogravimetric analysis	[909]
1,12-{3′,5′-C$_6$H$_3$[C(O)OH]$_2$}$_2$ (FF) bis(isophthalic acid) incorporated in Cu-based MOF CH_4 and H_2 storage	S, X, gas absorption	[927]
1-[C(O)OC$_6$H$_4$-*p*-R]CB$_{10}$H$_{10}$C-12-C$_6$H$_{13}$ R = (CH$_2$)$_2$-*bicyclo*-C$_8$H$_{12}$-*p*-C$_5$H$_{13}$, N = N-C$_6$H$_4$-*p*-OC$_6$H$_{13}$, OC(O)C$_8$H$_{17}$; comparison with ionic analogues; effect of coulombic interactions on mesophase stability (FF)	Thermal analysis, X-ray diffraction patterns	[940]
Esters and acyl halides		
1-C(O)OMe-12-*p*-C$_6$H$_4$OMe	S, H, MS	[196]
1-C(O)OCHMeC$_6$H$_{13}$-2-OC(O)-*p*-C$_2$H$_4$C$_6$X$_{13}$ (X = H, P) liquid crystals	S, electrooptical properties	[686]
1-[C(O)OCH$_2$CH=CH$_2$]$_2$	S	[253]
[C(O)Cl]HC$_2$B$_{10}$Me$_{10}$ (FF)	S	[682]
1-[CH$_2$C$_6$H$_4$-*p*-OC(O)Me]	S	[251]
1-[(C$_6$H$_4$)$_2$-*p*-OC(O)Me]	S	[251]
1-C(O)OCH$_2$Ph-12-NHC(O)OC(CH$_2$)$_3$	S, H, C, IR	[234]
1-C(O)OCH$_2$Ph-12-NH$_2$	S, H, C, IR	[234]
1-CH$_2$NH-CH[C(O)OMe]CH$_2$CHMe$_2$	S, H, C, MS	[205]

Compound	Information	References
1-CH═NCH[C(O)OMe]CH_2CHMe_2	S, H, C, MS	[205]
1-C_5H_{11}-12-[C(O)-O-(C_6H_4)$_2$-O-C_8H_{17}] liquid crystal	S, H, B, C, IR, MS, phase transition	[687]
1-C_5H_{11}-12-[C(O)-O-C_6H_4-CH_2CH_2-*cyclo*-C_6H_{10}-*cyclo*-C_5H_{11} liquid crystals - broad nematic phases	S, thermal analysis, optical microscopy	[688]
1-CH(OEt)$_2$-12-X X = Me_3SiO, OH	S, H(OH), B(OH), C(OH),	[666]
1-CH_2═CH-C(O)O$(CH_2)_3$ propyl acrylate	S, H, B, C	[664]
$MeCH_2OC(O)CMe$-[$CH_2CHC(O)O(CH_2)_3CB_{10}H_{10}CH]_n$Br (FF) poly(*p*-carborane) propyl acrylate	S, H, B, C	[664]
p-C_6H_4OR diesters	S, liquid crystalline behavior; conformational analysis	[691]
1-(*p*-C_6F_4OR)-12-Ph	S, X(Et), H, C, F, IR	[138]
1-$(CH_2)_3OSiPh_2CMe_3$-2-R R = H, C(O)OH, $(CH_2)_3OH$, $(CH_2)_2C(O)OH$	S, H, MS, aqueous solubility	[665]
CMe[C_6H_4—OC(O)$(CH_2)_2$-$CB_{10}H_{10}C$—$(CH_2)_2OSiPh_2CMe_3]_3$ (FF)	S, H, MS, aqueous solubility	[665]
2-(C_6H_4-*p*-OMe)	S (Pd-catalyzed cross-coupling), H, B, C	[646]
Nitro and nitroso derivatives and nitrates		
$(ONOCH_2)HC_2B_{10}Me_{10}$ (FF)	S, H, B, C, MS	[663]
1-NO	S	[676]
$(HOCH_2)HC_2B_{10}HMe_9$-2-CH═NOH (FF)	S, X, H, B, C, MS	[663]
[$(HOCH_2)HC_2B_{10}HMe_9$-2-CH═NO−]$_2$ (FF)	S, X, H, B, C, MS	[663]
Amines and imines		
1-NH_2	S, H, C, Ms, complex with α-cyclodextrin in aqueous solution; K_a (association constant)	[227]
1-NH_2	S	[676]
1-NH_2-12-*p*-C_6H_4OH estrogen agonists; hydrophobic pharmacore; estrogen receptor modulation; steroid receptors	S, H, MS	[196]
1-*p*-C_6H_4R R = NMe_2, NH_2	S, B, C, IR, UV, MS	[634]
1,12-(*p*-$C_6H_4R)_2$ R = NMe_2, NH_2	S, B, C, IR, UV, MS	[634]
1-R-12-C(O)OH R = NH_2, NHC(O)$OCMe_3$	S, H, B, C, IR	[230]
1-NH_2-12-C(O)OCH_2Ph	S, H, C, IR	[234]
2-NH_2	pK_a	[237]
[$H_2N(CH_2)_3$]$HC_2B_{10}Me_{10}$ (FF)	S, H, B, C, MS	[106]
[$H_2N(CH_2)_n$]$HC_2B_{10}Me_{10}$ *n* = 5, 6 (FF)	S, H, B, C, MS	[106]
2-NHC_6H_4R R = H, Cl, OMe	S, H, B	[673]
Heterocyclic amines		
2-R R = furyl, 2′/3′-thienyl, methylindolyl, pyridyl, quinolyl, pyridylethynyl, quinolylethynyl	S, H, B, MS	[281]
1-(*p*-$C_6H_4Br)_2$-12-(C_6H_4-*p*-NC_5H_4-*p*-NC_5H_4) bipyridine	S, H, B	[649]
1,12-(C_6H_4-*p*-NC_5H_4-*p*-$NC_5H_4)_2$ bipyridine	S, H, B	[649]
1-C(O)NCH_2-C_6H_4-*p*-*cyclo*-CN_4CH tetrazinyl	S, X, H, B, C, MS	[946]

Continued

Compound	Information	References
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	[946]
NC_5H_4—NC_5H_3—C≡C—C_6H_4—C≡C—$CB_{10}H_{10}C$—C≡C—C_6H_4—C≡C—R R = $SiMe_3$, H, $(N_2C_{10}H_6)Ir(NC_{11}H_6F_2)_2^+$ donor-acceptor complexes	S, MS, UV, E	[926]
1-$(CH_2)_3$-*cyclo*-N_3C_2H-$(CH_2)_3$-2″-*O*-adenosine	S, H, B, MS, U(fluorescence), neutrophil response to PNA stimulation	[935]
1-C≡C-2″-*O*-adenosine	S, H, B, MS, U(fluorescence), neutrophil response to PNA stimulation	[935]
1-H-2-S(8′-BODIPY) BODIPY = $C_9H_2Me_4N_2BF_2$	S, H, C, MS, UV, fluorescence, permeability across hCMEC/D3 cell monolayers	[948]
Amides and imides		
1-NHC(O)OMe methyl carbamate	S, X, H, B, C, IR, MS	[694]
1-$NHC(O)OCMe_3$-12-$C(O)OCH_2Ph$	S, H, C, IR	[234]
ethylene oxide-modified 3-*p*-carboranyl thymidine derivatives for BNCT	S	[696]
2-[C_6H_4-*p*-NHC(O)Me]	S (Pd-catalyzed cross-coupling), H, B, C	[646]
2-$NHC(O)CH_2NHEt_2$ lidocaine analogues local anesthetics	S, H, B, IR, MS, analgesic activity	[881]
Azides		
1-N(boc)NH(boc)-12-C(O)OH boc = *tert*-butyloxycarbonyl] hydrazino	S, X, H, B, C, MS	[268]
1-$NHNH_2CF_3C(O)OH$-12-C(O)OH	S, H, B, C, MS	[268]
Nitriles and isonitriles		
$(HOCH_2)HC_2B_{10}HMe_9$-2-CN (FF)	S, H, B, C, MS	[663]
$[NC(CH_2)_3]HC_2B_{10}Me_{10}$ (FF)	S, H, B, C, MS	[106]
1-C_6H_4CN-12-CH_2OH androgen receptor antagonist	S, X, H, docking study with hAR LBD	[912]
Phosphorus derivatives		
1-P(O)Me(OMe)-12-R R = H, CMe═CH_2	S	[697]
1-PMe(OEt)-12-R R = H, Me, CH_2═CMe, Ph	S	[297]
1-[PMe(OEt) = N-C_6H_4-*p*-NO_2]-12-R R = H, Me, CH_2═CMe, Ph	S	[297]
1-PMe(OEt)R• R = $OCMe_3$, Me phosphoranyl radicals	ESR	[298]
1-P(O)(OEt)OCH═CCl_2	S	[699]
$HCB_{10}H_{10}C$—PPh_2-CH_2—$(CH_2$—O—$CH_2)_3$—CH_2—PPh_2-$CB_{10}H_{10}CH^{2+}$ $2X^-$ X = Br, I (FF) water-soluble phosphonium salts for BNCT	S, X, H, B, C, P, MS	[701]
1,12-{P(O)[OCH_2-*cyclo*-$C_5H_5(OH)_4O]_2\}_2$ water-soluble glycophosphonates for BNCT	S, H, B, C, P, MS, IR	[305]
Sulfur derivatives		
1-CH_2SH-12-$CH_2CH_2C(O)OH$	S, H, C, IR, MS	[671]
1-CH_2SCMe_3	S, H, C, IR, MS	[671]
1-CH_2SCMe_3-12-R R = $(CH_2)_3OH$, $CH_2CH_2C(O)OH$	S, H, C, IR, MS	[671]
1-SC_4H_9-12-R R = H, $SiPh_3$, $CH_2CHMeEt$	S, H, B, C, IR, MS	[619]

Compound	Information	References
p-$C_6H_4(CB_{10}H_{10}C—C_4H_3S)_2$ thiophene (FF)	S, H, C, MS	[317]
cis/*trans*-1-CH═CH–C_4HBr_2S thiophene	S, H, B, C, MS	[875]
1,12-$[S(O)_2Ph]_2$ sulfone	S, IR	[311]
$[S(O)_2OR]_2C_2B_{10}(OH)_{10}$ R = H, Me (FF)	S, X(H), H, B, C, IR, MS	[702]
$[M^+]_2$ $\{[S(O)_2O]_2C_2B_{10}(OH)_{10}\}^{2-}$ M = Na, K (FF)	S, X, H, B, C, IR, MS	[702]
1-CPhH($OSO_3C_6H_4Me$)-12-C_6H_4R R = H, CF_3, Me, OMe, NMe_2 tosylates	S, rate constants, electronic effects of substituents	[320]
1-benzyl *p*-toluenesulfonates (tosylates)	Hydrolysis kinetics	[322]
1′,3′,5′-{1,12-[Et_2S–$(CH_2)_3$-]$_2$—MeSi]$C_2B_{10}H_{10}\}_3C_6H_3$ (FF)	S, H, B, C, IR, MS	[632]
Chloro derivatives		
1-Cl-12-Me	S, IR (actual)	[600]
1-Cl	Dipole moment	[344]
2,*n*-Cl_2 *n* = 3,4,7,9,10	ESR, dipole moment	[707]
B-Cl_n *n* = 3, 4, 5	S	[601,706]
Bromo derivatives		
1-Br	Dipole moment	[344]
1-Br-12-Me	S	[600,677]
	IR (actual)	[600]
	H (substituent effects)	[22]
2,9-Br_2	S	[601]
Iodo derivatives		
1-I	Dipole moment	[344]
1,12-I_2	S	[600,676,677]
	H (substituent effects)	[22]
	B	[22]
	IR (actual spectrum)	[600]
	IR	[22]
1-I-12-Me	S	[600,677]
	IR (actual)	[600]
	H (substituent effects)	[22]
Exo-Polyhedral Main-Group Metal and Metalloid Element Derivatives		
Silicon		
1-$SiMePh_2$	S, H, B, C, IR, MS	[702]
1-$SiPh_3$-12-R R = *n*-C_5H_{11}, $EtCHMeCH_2$, SC_4H_9, C≡C—C_5H_{11}, C_6H_4—OC_7H_{15}, $CH_2CH_2C_6H_{10}C_6H_4F$	S, H, B, C, IR, MS	[619]
1-$Si(C_6H_{13})_3$-12-$C(CH_2)_3Cl$	S, H, B, C, IR, MS	[713]
1-$OSiMe_3$-12-$CH(OEt)_2$	S	[666]

Continued

Compound	Information	References
$HCB_{10}H_{10}C—(CB_{10}H_{10}C)_2—CB_{10}H_{10}C—SiR_3$ R = *n*-C_6H_{13}, *n*-C_4H_9 (FF)	S, X (*n*-C_4H_9), H, B, C, IR, MS	[714]
B-$CH_2CH_2SiMe_3$	MS (detailed)	[461]
B,B′-$(CH_2CH_2SiMe_3]_2$	MS (detailed)	[461]
B-$CH_2CH_2SiR_3$ R = Cl, Me	S	[462]
B,B′-$(CH_2CH_2SiR_3)_2$ R = Cl, Me	S	[462]
n-$CH_2CH_2SiCl_3$ *n* = 1, B	MS (fragmentation patterns)	[715]
B-$CH_2CH_2SiR_3$ R = Me, Cl	IR (detailed study; inductive effect)	[460]
B,B′-$(CH_2CH_2SiR_3)_2$ R = Me, Cl	IR (detailed study; inductive effect)	[460]
1′,3′,5′-{1,12-[$Et_2S—CH_2)_3$-]$_2$—MeSi]$C_2B_{10}H_{10}$}$_3C_6H_3$ (FF)	S, H, B, C, IR, MS	[632]
1,12-{Co_2C_2[$SiMe_3$](CO)$_4$[$PPh_2CH_2PPh_2$]}$_2$	S, X, H, B, IR, E	[716]
Tin		
1-$SnEt_3$-12-R	^{119}Sn γ-resonance spectra; quadrupole splittings; acceptor properties of cage	[475]
{−$SnMe_2$—[1,7-$CB_{10}H_{10}C$]—SnMe)$_2$—1,12-$CB_{10}H_{10}C$]}$_n$ polymer (FF)	S	[466]
1,12-[$(CH_2)_nC(O)O^-$ $SnMe_3^+$]$_2$ *n* = 0, 1	Mössbauer, pK_a, E (half-neutralization potential)	[226]
Exo-Polyhedral Transition Metal Complexes		
Molybdenum		
1-C≡C-Mo(C_7H_7)[$Ph_2P(CH_2)_2PPh_2$]	S, X, H, B, C, P, IR, UV, E, ESR(cation)	[910]
1-C≡C-Mo(C_7H_7)[$Ph_2P(CH_2)_2PPh_2$]-12-C≡CH	S, X, H, B, C, P, IR, UV, E, ESR(cation)	[910]
1,12-{C≡C-Mo(C_7H_7)[$Ph_2P(CH_2)_2PPh_2]_2$	S, X, H, B, C, P, IR, UV, E	[910]
Iron		
1-(η^6-naphthyl)$FeCp^+$	S, ESR	[510]
1-[C_6H_4—*p*-CH═CHC_6H_4FeCp]	S, UV, E, NLO(β hyperpolarizability)	[513]
Ruthenium		
$(bpy)_2Ru(NC_5H_4$-NC_5H_3—*p*-C_6H_4—$CB_{10}H_{10}C$—*p*-$C_6H_4Br)^{2+}$ bpy = bipyridine (FF)	S, H, B, MS	[649]
$(bpy)_2Ru(NC_5H_4—NC_5H_3—p$-$C_6H_4—CB_{10}H_{10}C—p$-$C_6H_4$-$NC_5H_3—NC_5H_4)Ru(bpy)_2^{4+}$ bpy = bipyridine (FF) photoluminescent complex	S, H, B, MS,UV,E	[649]
Cobalt		
1-Co_2C_2[$SiMe_3$](CO)$_4$[$PPh_2CH_2PPh_2$]	S, X, H, B, IR, E	[720]
1,12-{Co_2C_2[$SiMe_3$](CO)$_4$[$PPh_2CH_2PPh_2]]_2$	S, X, H, B, IR, E	[716,720]
[$Co_4(OH)_2(O_2C$-$CB_{10}H_{10}C$-$CO_2)_3(DMF)_2]_n$ polymers for CO_2 adsorption	S, TGA, variable-temp. X-ray diffraction	[722]
Rhodium and Iridium		
$(N_2C_{12}H_8)Ir(N_2C_{10}H_8-1,12-CB_{10}H_{10}CH)_2^+$ PF_6^- enhances phosphorescence emission	S, H, B, C, MS, UV, phosphorescence	[839]

Compound	Information	References
$(HCB_{10}H_{10}C—C_6H_4$-*p*-2′-$C_5H_4N)_3Ir$ 3 Ir—N, 3 Ir—C *fac*/*mer* isomers (FF)	S, X, H, B, C, MS, UV, photoluminescence, luminescence/ phosphorescence efficiency	[854]
cyclo-{1,12-$(O_2C)_2C_2B_{10}H_8$-2,10-[IrCp*(*cyclo*-NC_4H_4N)IrCp*]$_2$-2,10-$H_8B_{10}C_2(CO_2)_2$} 4 B—Ir	S, X, H, B, MS	[857]
cyclo-[Cp*M(NC_5H_4-CH═N)-R-(N═CH-C_5H_4N)MCp*]$_2${[1,12-$C(O)O]_2C_2B_{10}H_{10}$}$_2$ M = Rh, Ir R = C_6H_4, C_6Me_4, $C_{10}H_6$ naphthyl	S, X, H, B, I	[939]
Platinum		
1-CH_2SPt(terpyridine)$^+$ $OSO_2CF_3^-$	S, H, B, C, MS	[314]
1,12-[$(CH_2)_3$SPt(terpyridyl)]$_2C_2B_{10}H_{10}^{2+}$ [$OSO_3CF_3^-$]$_2$ (FF)	S, H, B, C, Pt, MS, cell toxicity	[536]
1,12-[C≡C—C_5H_4N-*trans*-Pt[PEt_3]$_2OSO_2CF_3$]$_2$	S, H, C, F, IR	[533]
cyclo-[1,8-$C_{14}H_8$]$_2$ $\{Pt[PEt_3]_2-NC_5H_4-C\equiv C-CB_{10}H_{10}C-C\equiv C-C_5H_4N-Pt[PEt_3]_2\}_2^{4+}$ $C_{14}H_8$ = anthracene; rectangular macrocycle (FF)	S, H, C, IR	[533]
cyclo-{$(CH_2)_3$Pt[PEt_3]$_2$]$_4\{C\equiv C-C_5H_4N-Pt[PEt_3]_2-C\equiv C-CB_{10}H_{10}C-C\equiv C-Pt[PEt_3]_2-NC_5H_4-C\equiv C\}_4^{8+}$ square macrocycle (FF)	S, H, C, IR	[533]
cyclo-({C(O)O-Pt[PEt_3]$_2$-1,8-$C_{14}H_8$}$C_2B_{10}H_{10})_2$ $C_{14}H_8$ = anthracene rectangular macrocycle (FF)	S, X, H, P	[534]
cyclo-({C(O)O-Pt[PEt_3]$_2$-2,9-$C_{14}H_8$}$C_2B_{10}H_{10})_2$ $C_{14}H_8$ = phenanthrene; rhomboidal macrocycle (FF)	S, X, H, P	[534]
Gold		
$Au(PPh_2-CB_{10}H_{10}C-PPh_2)_2^+Cl^-$ (FF)	S, H, B, C	[698]
1,12-$(PPh_2AuCl)_2$	S, H, B, C	[698]
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)	[932]
Mercury		
$Hg(CB_{10}H_{10}CMe)_2$ (FF)	MS (detailed)	[547]
$Hg(CB_{10}H_{10}C—Ph)_2$·2,2′-bipyridine (FF)	S, X	[632]
{$Hg(CB_{10}H_{10}C—Ph)_2$}$_2$·2,2′-bipyridine (FF)	S, X	[632]
2-R R = HgOC(O)CF_3, HgCl	S	[548]
Theoretical Studies		
Molecular and electronic structure calculations		
$C_2B_{10}H_{11}^{\bullet}$, $C_2B_{10}H_{10}^{\bullet\bullet}$ radicals	DFT, CASPT2	[587]
1,12-X_2 X = Li, BeH, F, Cl, CN, Me, SiH_3, OH, SH, H_2, BH_2	*Ab initio*; cluster parameters	[703]
n-$SCH_2C(O)OH$ *n* = 1,2	EHMO, NEMO; charge distribution	[176]
1,12-$(SH)_2$/9,12-$(SH)_2$ attached to surface of Au microcrystals	Dipole moments	[704]
$RCB_{10}H_{10}CR^{2-}$ R = $B_{12}H_{11}$, $B_{12}H_{10}$-C_7H_6; R′ = H, C_5H_4, C_7H_6 (FF)	β (first hyperpolarizability); NLO	[589]
1-CH_2X X = Cl, Br, I	Dipole moment	[344]
1-X X = Cl, Br, I	Dipole moment	[344]
$Me_2N—C_6H_4$ *p*-$CB_{10}H_{10}C—p$-$C_6H_4—NO_2$	Dipole moment; electronic effects transmission	[627]

Continued

Compound	Information	References
EtMeCHCH$_2$—CB$_{10}$H$_{10}$C—C(O)O-(C$_6$H$_4$)$_2$—*cyclo*-C$_5$H$_{11}$ optically active mesogenic esters (FF)	Conformational energies	[689]
(18-crown-6)$^+$ [(*p*-C$_6$H$_4$OH)(*p*-C$_6$H$_4$OH)C$_2$B$_{10}$H$_{10}$]$^-$ (FF)	Electron densities	[634]
1-[C(O)OC$_6$H$_4$-*p*-R]CB$_{10}$H$_{10}$C-12-C$_6$H$_{13}$ R = (CH$_2$)$_2$-*bicyclo*-C$_8$H$_{12}$-*p*-C$_5$H$_{13}$, N = N-C$_6$H$_4$-*p*-OC$_6$H$_{13}$, OC(O)C$_8$H$_{17}$ comparison with ionic analogues; effect of coulombic interactions on mesophase stability (FF)	Molecular modeling	[940]
1-[Cp*Ru(Ph$_2$PCH$_2$CH$_2$PPh$_2$)—C≡C]	DFT, electronic structure	[719]
1,12-[Cp*Ru(Ph$_2$PCH$_2$CH$_2$PPh$_2$)—C≡C]$_2$	DFT, electronic structure	[719]
(*cyclo*-O$_2$C$_3$HMe$_2$)Ir(N$_2$C$_{10}$H$_8$—1,12-CB$_{10}$H$_{10}$CH)$_2$	DFT: HOMO-LUMO levels	[839]
(N$_2$C$_{12}$H$_8$)Ir(N$_2$C$_{10}$H$_8$ − 1,12 − CB$_{10}$H$_{10}$CH)$_2^+$ PF$_6^-$	DFT: HOMO-LUMO levels	[839]
1,12-{*cyclo*-[B—N(R)—*o*-C$_6$H$_4$—N(R)—]}$_2$ R = Et, Ph; diazaborolyl	Molecular geometry, GIAO NMR	[847]
Ph-(*p*-C$_6$H$_4$)$_2$—CB$_{10}$H$_{10}$C—R R = Me, C$_6$H$_3$-2′,3′-Cl$_2$ inclusion compounds with tris-*o*-phenylenedioxycyclotriphosphazene (TPP)	DFT: geometry optimization	[929]
n-C$_5$H$_{11}$-CB$_{10}$H$_{10}$C—C$_6$H$_4$—*p*-C$_6$H$_2$FX$_2$ X = H, F (FF)	DFT: molecular structure	[930]
1-C$_5$H$_{11}$—12-C$_6$H$_4$-*p*-R R = C≡C—C$_6$H$_4$-OC$_8$H$_{17}$, N = CH—C$_6$H$_4$—OC$_8$H$_{17}$, N = N—C$_6$H$_4$—C(O)O—C$_5$H$_{11}$*	DFT: dipole moment, polarizability, geometry	[947]
1-C$_5$H$_{11}$—O—C$_6$H$_4$-CB$_{10}$H$_{10}$C—L—C$_6$H$_4$—*p*-OC$_5$H$_{11}$ L = CH$_2$CH$_2$, CH=CH	DFT: dipole moment, polarizability, geometry	[947]
Other calculations		
1-(C$_6$H$_{10}$-*p*-OH)-12-R R = H, CH$_2$OH estrogen receptor-beta ligands	Docking models with ERα and ERβ sites	[893]
1,12-I$_2$	Zero-point vibrational energy and B—X bond length (X = I, Xe) vs. 1,12-C$_2$B$_{10}$H$_{10}$Xe$_2^+$ ion obtained via radioactive decay	[950]

[a]Substituents on the carborane cage. "FF" indicates that the full formula of the compound is given. [b]S, synthesis; X, X-ray diffraction; H, ^{1}H NMR; B, ^{11}B NMR; C, ^{13}C NMR; F, ^{19}F NMR; P, ^{31}P NMR; Pt, ^{195}Pt NMR; IR, infrared data; MS, mass spectroscopic data; UV, UV-visible data; E, electrochemical data; ESR, electron spin resonance; NLO, nonlinear optical properties; DSC, differential scanning calorimetry; BNCT, boron neutron capture therapy; ED, gas phase electron diffraction; STM, scanning tunneling microscopy; XPS, X-ray photoelectron spectroscopy.