Thermodynamic and Kinetic Data for Macrocycle Interaction with Neutral Molecules

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Received April 23, 1992 (Revised Manuscript Received July 13, 1992)

Contents

I. Introduction

This review contains thermodynamic and kinetic data for the interaction of macrocycles with neutral molecules. To the best of our knowledge, the first papers reporting thermodynamic data for the interactions of macrocycles (other than porphyrins) with neutral molecules were published in 1972.[1,2] Since that time, interest has increased particularly in the design of macrocycles with predetermined guest complexation properties and in the determination of thermodynamic and kinetic data for these interactions. The most important part of this review is the compilation of thermodynamic and kinetic data. These data provide a quantitative base for understanding the effect of macrocycle and guest parameters on the thermodynamic and kinetic stabilities of the resulting complexes. In turn, this understanding can lead to the rational design of new macrocycles and to predictions of their effectiveness in forming complexes of desired stabilities with guest species. In addition, the compilation makes apparent areas where data are missing and future work is needed. Particular effort has been made to include literature from the former USSR, Eastern Europe, and the People's Republic of China.

No comprehensive review of data for these interactions has been published. There are several reviews containing compilations of some thermodynamic and kinetic data for neutral molecule-macrocycle interaction. These reviews are now listed together with the major areas of emphasis in each case.

(1) F. Diederich, "Complexation of Neutral Molecules by Cyclophane Hosts", 1988.[3] The review discusses in particular the contribution provided by synthetic cyclophanes as hosts to the understanding of molecular complexation of neutral organic guest molecules in aqueous and organic solvents, the influence of organic solvents and electron donor–acceptor interactions on the stability of complexes, and the role of force field calculations together with computer graphics in the design of the effective hosts. Limited kinetic data and many tables with thermodynamic data are given. There are 252 references, the most recent are from 1987.

(2) F. Diederich, *Cyclophanes*, 1991.[3a] The book containing over 670 references presents the latest developments in cyclophane chemistry. There is a detailed discussion on molecular recognition with emphasis on major driving forces which lead to complexation between cyclophanes and a variety of charged and uncharged organic molecules in water and organic solvents. Numerous tables with thermodynamic data for cyclophane–neutral molecule interaction are included. The book has also chapters on chiral recognition, catalytic processes, and solvents effects in molecular recognition.

(3) C. D. Gutsche, *Calixarenes*, 1989.[4] Comprehensive information is given on calixarenes including background, synthesis, characterization and properties, conformations, introduction of functional groups, complex formation, and applications. In Chapter 6, interaction of calixarenes with neutral molecules is discussed, and some tables with thermodynamic data are given. The book contains numerous references, many of them are from 1988.

(4) A. Collet, "Cyclotriveratrylenes and Cryptophanes", 1987.[5] The article contains 113 references and deals mostly with design, synthesis, geometry, optical activity, and complexation of the title compounds. There are two paragraphs on cryptophane interactions with neutral molecules and one table with thermodynamic data.

(5) F. de Jong and D. N. Reinhoudt, "Stability and Reactivity of Crown-Ether Complexes", 1980.[6] Crown ether complexation with metal cations, protonated

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0009-2665/92/0792-1261$10.00/0

Reed M. Izatt was born in Logan, UT. He received his B.S. degree at Utah State University in 1951 and his Ph.D. degree in 1954 with Professor W. Conard Fernelius in coordination chemistry at The Pennsylvania State University. After two years of postdoctoral work at Carnegie-Mellon University, he joined the Brigham Young University Chemistry Department in 1956. He delivered the Annual Sigma Xi lecture at BYU in 1966 and the Annual BYU Faculty Lecture in 1970. He was BYU Teacher of the Month in October 1974. He received the BYU Karl G. Maeser Research and Creative Arts Award in 1967 and was the recipient of an NIH Career Development Award (1967–1972), the Utah Award (American Chemical Society) in 1971, the Huffman Award (Calorimetry Conference) in 1983, the Willard Gardner Award of the Utah Academy of Sciences, Arts, and Letters in 1985, and the State of Utah Governor's Medal in Science in 1990. He is a Fellow of the American Association for the Advancement of Science and is Chairman of the Organizing Committee for the annual International Symposium on Macrocyclic Chemistry. His research interests include the design of novel molecular recognition systems for the selective separation of cations, anions, and neutral species; calorimetry applied to metal–ligand and nonelectrolyte interactions, particularly at elevated temperatures and pressures; and the compilation of thermodynamic data.

Jerald S. Bradshaw was born in Cedar City, UT, and received a B.A. degree at the University in 1955. After four years as an officer in the U.S. Navy, he enrolled in a Ph.D. program at UCLA. He received the Ph.D. in 1963 with Prof. Donald J. Cram on electrophilic substitution at saturated carbon. He received an NSF postdoctoral fellowship for the 1962–1963 academic year to work with Prof. George S. Hammond at the California Institute of Technology. After three years as a research chemist at Chevron Research in Richmond, CA, he joined the faculty at Brigham Young University in 1966. He was named Professor of the Year at BYU in 1975. He was U.S. National Academy of Sciences Exchange Professor for the academic year of 1972–1973 and the Summer of 1982, working with Prof. Miha Tisler at the University of Ljubljana, Yugoslavia. He also was a visiting professor with Dr. J. F. Stoddart at the University of Sheffield, England, in 1978, and a National Science Foundation Cooperative Research Fellow with Dr. L. F. Lindoy at James Cook University, Townsville, Australia, in 1988. He is a member of the American Chemical Society. He received the 1989 Utah Award from the Salt Lake and Central Utah sections of the American Chemical Society. He received the State of Utah Governor's Medal in Science in 1991. In 1992, he presented the Annual Faculty Lecture at BYU. His research interests include the synthesis and cation complexation properties of macrocyclic multidentate compounds, the photochemical reactions of heterocyclic compounds, and the preparation of new polysiloxanes for chromatography uses.

amines, arenediazonium salts, and racemic salts is discussed, as well as the chemical reactivity of metal–cation complexes. This review contains a short paragraph discussing complexation of crown ethers with H_2O and organic neutral molecules. Two tables which contain thermodynamic data are included.

(6) D. N. Reinhoudt and H. J. den Hertog, Jr., "Complexation of Neutral Molecules by Synthetic Macroheterocyclic Hosts", 1988.[7] This is a short review with 24 references in which the authors discuss selective complex formation of crown ethers and preorganized macrocycles with neutral molecules. The discussion is based on X-ray and NMR analysis. One table gives a limited number of thermodynamic data.

(7) J. Franke and F. Vögtle, "Complexation of Organic Molecules in Water Solution", 1986.[8] The review deals with the complexation of organic molecules, anions, and cations inside cavities, niches, or pockets of macrocyclic hosts. One table contains a limited number of K values. There are 84 references, several of which were published in 1985.

(8) H. J. Schneider, "Mechanisms of Molecular Recognition: Investigations of Organic Host-Guest Complexes", 1991.[9] This recently published review with 197 references indicates the importance of noncovalent interactions in organic host–guest complexes in solution. The text contains numerous thermodynamic data for complexation of macrocycles with organic cations, anions, and neutral molecules.

The compilation of thermodynamic (log K, ΔH, ΔS, ΔC_p) and kinetic (k_f, k_d, $\Delta H^{\ddagger}$, $\Delta S^{\ddagger}$) data is intended to be exhaustive. Included in the tables are data for the interaction of a wide variety of macrocycles with many different neutral molecules. The reactions have been studied in a variety of solvents and under a variety of experimental conditions. The experimental conditions and some supplementary information are provided for each interaction listed. It is important to realize that the data are valid only at the specific conditions given. Few studies have been made at temperatures outside of the 20–30 °C range. The solvents used include H_2O (D_2O), various organic solvents, and various solvent mixtures. The abbreviations used in the tables can be understood by reference to the structures and names given in Charts I–XXXVII (macrocycles) and Charts XXXVIII and XXXIX (neutral molecules). The chart in which each macrocycle is located is indicated in the tables. The nomenclature used is defined in the charts.

This review is intended to be a companion to our earlier reviews[10–12] involving the thermodynamic and kinetic quantities associated with cation and anion interaction with macrocycles. In those reviews, the cation and anion parameters which affect macrocycle–ion complex stability are presented and discussed. Design features which enable one to achieve high selectivity of one ion over other similar ions are also discussed. Many of these same principles apply to the present review.

In this review, the relevant thermodynamic and kinetic data are tabulated, the factors are identified and discussed which enable workers to discriminate selectively among similar molecules, possible practical applications are presented, and opportunities for future work are given.

Krystyna Pawlak was born in Lithuania and received her M.D. degree at the Medical Academy in Gdansk, Poland, in 1964. She obtained her specialization in psychiatry at the Medical Academy in Gdansk and at the Institute of Neurology and Psychiatry in Warsaw. After five years of practicing medicine at the State Psychiatric Hospital, she served as a Director of the Outpatient Clinic for Alcoholics and Drug Addicts in Gdansk where she did research on pharmacodynamics of drugs used in the treatment of alcoholics. From 1973 to 1986, she was a consultant in the Outpatient Psychiatric Clinic in Gdynia and a sworn expert for the court. She was a member of the Polish Psychiatric Society. From 1981 to 1982, she was an observer in The Tower Hospital in Leicester, England. In 1986, she joined the chemistry research group at Brigham Young University. Her recent interests are in researching the known literature on the thermodynamics of macrocycle and cyclodextrin interactions with cations, anions, and neutral molecules and the compilation of thermodynamic data. In 1992 she became a member of Sigma Xi the Scientific Research Society.

Ronald L. Bruening was born in Salt Lake City, UT, and received his B.S. degree in chemical engineering at Brigham Young University in 1985. He obtained his M.S. degree in chemistry in 1986 and his Ph.D. in chemistry with Prof. R. M. Izatt in 1988 at BYU. He received the H. Tracy Hall Award as the outstanding graduating Ph.D. student in 1988 and Sigma Xi Outstanding Ph.D. Dissertation Award for College of Physical and Mathematical Sciences in 1989. From 1986 to 1988 he was a research assistant at BYU. Since 1988, he has been Vice-President of Research, IBC Advanced Technologies, Inc., Provo, UT, and a research associate at BYU. He is a member of the American Chemical Society, Sigma Xi, and Tau Beta Pi Honorary Engineering Society. His scientific interests involve macrocycle-mediated cation transport in membrane systems and cation determinations and separations in silica gel column systems.

II. Thermodynamics of Neutral Molecule–Macrocycle Interaction

Table I contains log K, ΔH, and ΔS data and Table II contains ΔC_p data for the interaction of macrocycles with neutral molecules. The method used to determine the thermodynamic quantities is given in each case together with the temperature of measurement, the conditions (solvent, supporting electrolyte, buffer, pH), some supplementary information (e.g., equations), and the literature reference.

Byron J. Tarbet was born in Chicago, IL, and received his B.S. degree in chemistry at Brigham Young University in 1984. He obtained his Ph.D. in organic chemistry with Prof. J. S. Bradshaw in 1988 at BYU. From 1986 to 1988 he was a research assistant at BYU. Since 1988, he has been Manager of Organic Synthesis, IBC Advanced Technologies, Inc., Provo, UT, and a research associate at BYU. He is a member of the American Chemical Society. His scientific interests involve synthesis of compounds for use in separation systems.

A. Complexation of Neutral Molecules by Various Macrocycles

Studies on neutral molecule–macrocycle interactions have been far fewer in number than those on cation–macrocycle interactions. Although Pedersen[279] discussed the possibility of complexation of thiourea and thiourea-related compounds by crown ethers and presented some results in 1971, only in recent years has this field received substantial attention. The motivation to study neutral molecule–macrocycle interactions is understandable because the function of neutral molecules is as important as that of charged molecules in many chemical and biological processes. In addition, there is increasing interest in the possibility of using macrocycles to separate certain neutral molecules from environmental systems.

1. Coronands and Cryptands

a. Crown Ethers. Crown ethers are capable of interacting with many neutral organic and inorganic guests that have acidic properties by formation of hydrogen bonds between the oxygen atoms of the polyethers and the hydrogen atoms of these guests. The organic guests and water act as proton donors, and the ether oxygen atoms of the macrocyclic ring act as proton acceptors. The formation of complexes of crown ethers with neutral organic compounds that have pronounced acidity (e.g., $CHCl_3$) also leads to a change in the conformation of the macrocyclic ring to one similar to that which it has in complexes with metal salts.[27]

The ability of a crown ether to interact with molecules of proton–donor solvents in complexing reactions with metal ions has an appreciable effect on the thermodynamic parameters of these reactions. A study of the solvation of macrocyclic ethers by water and other organic solvents is therefore of considerable interest.

Golovkova and co-workers measured the abilities of crown ethers to coordinate with water in chloroform using a ^1H NMR method. They found the association constant order to be $N_2$18C6-1 (Chart II) > $Cy_2$18C6-1 (Chart II) > 18C6-1 (Chart II) > $B_2$18C6-1 (Chart II) > $B_2$24C8-1 (Chart III) > 15C5-1 (Chart I) > B15C5-1 (Chart I) > $S_2$18C6-1 (Chart III) > B12C4-1 (Chart I).[19]

The most stable complex with water among the 18-membered oxygen-containing crown ethers was formed by $Cy_2$18C6-1 (Chart II). In this case, the high stability is probably due to a strong retention of water in this macrocycle cavity, resulting from the steric arrangement of cyclohexyl rings.[19] The thermodynamic stability of the 18C6-1 (Chart II)–water complex was higher than that of the $B_2$18C6-1 (Chart II)–water complex in which introduction of benzo units causes withdrawal of the electron density from the neighboring oxygen atoms.[27] Replacement of two oxygen atoms by sulfur to form 1,10-$S_2$18C6 ($S_2$18C6-1, Chart III) resulted in a significant reduction of complex stability in the reaction with water.[19] The participation of sulfur atoms in hydrogen bonding is improbable, due to their weak electron-donor properties. On the other hand, replacement of two oxygen atoms by nitrogen in 1,10-$N_2$18C6 ($N_2$18C6-1, Chart II) enhanced the stability of the complex formed by this macrocycle with water. The greater stability is attributed to the higher electron donor strength of nitrogen compared to that of oxygen. The complex of 1,10-$N_2$18C6 ($N_2$18C6-1, Chart II) with water is formed through hydrogen bonds, N···H–O. The complexes of 18C6-1 (Chart II) and 1,10-$S_2$18C6 ($S_2$18C6-1, Chart III) are formed through oscillating O···H–O bonds.[19] The stabilities of the complexes formed by interaction of either smaller or larger oxygen-containing macrocycles with water were lower than those of the complexes with the 18-membered macrocycles[19,27] which was attributed to the less symmetrical structures of these complexes. This observation was also made by Reinhoudt and his co-workers[55] who examined complexation of 2,6-pyridinium crown ethers with water. However, both groups of workers note that the 18-membered cavity was apparently too small to accommodate a water molecule. The water molecule is situated above the plane of the macrocyclic ring, but the 18-membered ring has the correct number of heteroatoms for a complementary arrangement of donor and acceptor atoms for hydrogen bonding with water. The larger 2,6-pyridinium-21C7 (Py21C7-3, Chart III) macrocycle is suited to encapsulate one water molecule almost at the center of the cavity, but absence of an optimal arrangement of heteroatoms results in a rather asymmetrical conformation of the macroring.[55]

The formation of hydrogen bonds in these complexes was established and confirmed by IR and NMR studies.[19,27,40,44] The existence of water–crown hydrogen bonding has been demonstrated also by X-ray crystallography.[55,280,281]

Formation of hydrogen bonds between host and guest also plays an important part in the complexation of crown ethers with other organic solvents. Reinhoudt and co-workers studied the structures and thermodynamic stabilities of complexes of simple crown ethers with small molecules that have relatively acidic hydrogen atoms, such as nitromethane, acetonitrile, and malononitrile.[39,42] From the X-ray analysis of the 18C6-1 (Chart II) complex with nitromethane, it was concluded that C–H···O hydrogen bonds play an important role in the interaction between host and guest.[42] The 18C6-1 (Chart II)–malononitrile (1:1) complex in C_6D_6 was found to be one of the most stable with $-\Delta G$ = 13.4 kJ mol^{-1}.[60] However, the stability of this complex is relatively low in comparison with the stabilities of the corresponding complexes with charged guests, such as the alkylammonium cations ($-\Delta G$ = 22.2–32.6 kJ mol^{-1} in C_6D_6).[282] The analysis of thermodynamic results indicates the presence of a compensating effect of ΔH and $T\Delta S$: the more negative the enthalpy of binding is; the more negative the entropy contribution. Although a detailed interpretation of all parameters, including (de)solvation is not possible, it is very likely that part of the unfavorable entropy contribution is related to the necessity of attaining the proper organization of the bonding sites of the receptor molecule.[7]

Reinhoudt and co-workers have studied the complexation of urea with macrocyclic polyethers.[43] It was known from a previous study that the association constants of urea with macrocyclic polyethers in water were very low, e.g., for the 18C6-1 (Chart II)–urea complex log $K < 0.1$.[38] These workers found that proton-donating groups, e.g., carboxyl or pyridinium in the cyclic polyethers, facilitated the complexation of urea in water.[43] An X-ray crystal structure of the 2-carboxyl-1,3-xylyl-30C9 ((1,3-B)30C9-2, Chart IV)–urea complex revealed the complete encapsulation of the urea molecule in the macrocyclic cavity.[43] The urea is bound via five hydrogen bonds of which four are formed between the urea NH_2 groups and ether oxygens and one between the urea oxygen and the carboxyl OH group of the crown ether. Although there is no proton transfer in the complex, the strong hydrogen bond between the oxygen atom of urea and the carboxyl group of the ligand plays an important role in stabilizing the complex.[41]

b. Hemispherands. The principle of preorganization is that the log K value for the host–guest complex formation is increased significantly, if the host and guest are organized for optimal interaction prior to binding.[283] This principle is experimentally demonstrated with the synthesis of spherands designed to complex selectively with Li^+ and Na^+ cations.[284] It has been shown that partially preorganized macrocycles such as hemispherands (e.g., see structure of Spher-18C3-1 in Chart V) are also capable of complexing neutral molecules.[61] Reinhoudt and co-workers studied complexation of several hemispherands with malononitrile and found that the complexes formed were thermodynamically stable in organic solvents, $CDCl_3$ and C_6D_6. The binding free energies ($-\Delta G$ = 5.0–11.3 kJ mol^{-1}) were favorable when compared with the stabilities of the corresponding complexes of flexible crown ethers.[60] X-ray studies of free and complexed hemispherands revealed that in the more preorganized hemispherands both the methoxy oxygen atoms and the heteroatoms of the polyether ring are involved in the hydrogen bonding of the guest.[60]

c. Cryptands. Few complexes of cryptands with neutral molecules have been reported. Cryptand [2.2.2]-1 (Chart V) formed a less stable complex with water than either $N_2$18C6-1 (Chart II) or $Cy_2$18C6-1 (Chart II). This result is probably due to the less favorable steric situation which impedes the water molecules from entering into the three-dimensional cryptand [2.2.2]-1 cavity. On the other hand, cryptand [2.2.2]-1 formed more stable complexes with water than either 12-, 15-, or 24-membered macrocyclic polyethers.[19] Complexation of cryptands [2.2.2]-1, [2.2.1]-1, and [2.1.1]-1 (all in Chart V) with bromine and iodine

(X_2) was also studied.[62] The formation of X^+ ion complexes in chloroform was detected ($K = [X^+L]/[X_2][L]$). There was a correlation between cryptand cavity dimension and complex stability in the case of iodine. Cryptand cavity radii are 1.40, 1.15, and 0.80 Å for [2.2.2]-1, [2.2.1]-1, and [2.1.1]-1, respectively. The radius for I^+ is 0.62 Å in the vapor phase and 0.83 Å in solution. The log K values for complexes with I_2 were 6.36, 6.73, and 7.48 for [2.2.2]-1, [2.2.1]-1, and [2.1.1]-1, respectively.[62]

2. Cyclophanes

Water-soluble macrocyclic hosts of the cyclophane type have large cavities with well-defined sizes and shapes and regions of very pronounced hydrophobicity as potential binding sites for apolar guests in aqueous solution.[83] These properties as well as their substrate specificity, due to their intrinsic geometrical requirements for host–guest interactions, give them the potential to be superior enzyme models.[3,285,286]

a. Monocyclic with Oxygen Donor Atoms. Diederich and co-workers synthesized a series of cyclophanes (see Charts VI–VIII) which are soluble in water in the pH = 7 region due to the presence of quaternary ammonium nitrogens and are excellent receptors for apolar aromatic guests. Quaternary ammonium nitrogens were provided by spiropiperidinium rings attached to the paracyclophane frame and were located remote from the cavity of the host to avoid perturbation of the hydrophobicity of its binding sites.[83] These macrocycles bound neutral and anionic aromatic guests more strongly than acyclic guests and aromatic guests bearing cationic (ammonium) residues.[85] Extensive NMR investigation of host complexation with aromatic guests indicated the formation of highly structured cavity inclusion complexes with exclusive 1:1 stoichiometry.[83] Hydrophobic and van der Waals interactions which are based on solvation–desolvation processes were shown to be important forces for the complexation of neutral aromatic guests in water.[83,85] Electron-donor–acceptor interactions which stabilize complexes between electron-rich cyclophane hosts and electron-deficient aromatic substrates appear to be important forces for complexation in organic solvents.[68,78] Dougherty and co-workers found, however, that in the case of macrocycles constructed from electron-rich π systems (e.g., (1,4-B)$_2$32C4-2, Chart VIII), electron-donor–acceptor interactions with neutral molecules are even more important in aqueous solution than hydrophobic effects.[87,88]

Diederich and co-workers also synthesized optically active cyclophanes (e.g., Isoquin28C4-1 and 2, Chart VI) which form diastereomeric complexes with neutral molecules.[71–74,76] So far, the optical resolution of neutral guests has almost exclusively been observed by free or immobilized cyclodextrins in aqueous solution.[72]

Whitlock and co-workers reported the synthesis of monocyclic naphthalenophanes (Nap$_2$24C4-1 and Nap$_2$-28C4-1, Chart VI) which display charge-transfer complexation (a classical π–π interaction with the "face-edge" conformation).[63]

b. Monocyclic with Nitrogen Donor Atoms. In general, this type of hydrophobic cyclophanes contains rigid macrocyclic skeletons containing nitrogen donor atoms. Murakami and co-workers constructed the following five types of cyclophanes: (i) cyclophanes without flexible hydrocarbon chains (no data for the interactions of these cyclophanes with neutral molecules have been reported), (ii) cyclophanes with short or long flexible hydrocarbon chains branched at nitrogen atoms, e.g., K_4(1,4-B)$_4$N$_4$28C4-1 and K_4(1,4-B)$_4$N$_4$28C4-3, respectively, Chart IX, (iii) octopus cyclophanes with four or eight very long hydrocarbon chains, e.g., K_4(1,4-B)$_4$N$_4$-28C4-5, Chart IX, (iv) tetraazacyclotetradecane-capped cyclophane, Cyclophane-30, Chart XIX, and (v) cubic cyclophanes, e.g., Cyclophane-31, Chart XIX.[96]

The substrate-binding behavior of these cyclophane hosts was studied. Results showed that the most important driving force for molecular recognition in aqueous media is the hydrophobic interaction. These host molecules provide cavities that are deep and hydrophobic enough to incorporate hydrophobic substrates of various bulkiness through an induced-fit mechanism which originates from the flexible character of hydrocarbon chains. Moreover, when additional functional sites having noncovalent interactions (electrostatic, charge-transfer, and so on) were introduced into appropriate positions within host molecules, the host–guest interactions were expected to be much more enhanced.[95] Octopus cyclophanes (e.g., (1,4-B)$_4$N$_4$28C4-4, Chart IX) exhibited two different binding modes. For small molecules which can be completely incorporated into the macrocyclic cavity, the charge-transfer interactions contribute much more than hydrophobic interactions to the overall guest-binding process. For guest molecules larger than the macrocyclic cavity, the induced-fit mechanism resulting from the flexible hydrocarbon chains is much more important for guest recognition than charge-transfer interactions.[94]

Koga and co-workers synthesized a series of quaternary ammonium cyclophanes built either with diphenylmethane or naphthylphenylmethane units.[109,110] Cyclophanes with diphenylmethane units (e.g., (1,4-B)$_4$N$_4$30C4-3, Chart X) selectively formed inclusion complexes with aromatic guests while cyclophanes with naphthylphenylmethane units (e.g., Nap(1,4-B)$_2$N$_4$-34C4-2, Chart XI), which have rigidly extended cavities, formed inclusion complexes with bulky aliphatic guests.[109,110] Both kinds of cyclophanes discriminated among the aliphatic and aromatic guests on the basis of the steric fit between the host and guest.[110]

Schneider and co-workers have synthesized several cyclophane-type macrocycles.[108,115,117–119,121] They found that the cyclophane ((1,4-B)$_4$N$_4$34C4-1, Chart X) bearing N^+ charges on the inside of the cavity bound aromatic substrates 60 times stronger than aliphatic substrates of similar shape. Much smaller differences were observed with the same cyclophane bearing no charges in the vicinity of the substrate. NMR spectroscopic studies with aromatic ring current and electric field effect calculations indicated that naphthalene derivatives were encapsulated in the cavity of the charged cyclophane in a pseudoequatorial manner suitable for an $N^+\cdots\pi$ interaction. The analysis of

solvent effects on host–guest equilibrium constants indicated a large van der Waals contribution to the binding of naphthalene with these types of cyclophanes. In the case of aliphatic substrates, the position of the N^+ atom of the host in relation to the plane of the guest π-system is an important factor in this large difference in binding.[119]

c. Monocyclic with Various Donor Atoms. Hamilton and co-workers have developed a new class of biomimetic receptors for nucleotide base substrates by introducing multiple recognition sites into a macrocyclic structure. Their strategy was to assemble hydrogen bonding and hydrophobic groups (and ultimately electrostatic or reactive groups) within a macrocycle that can form a cavity complementary to the nucleotide base structure.[127,128] They found that changing the complementarity of the hydrogen-bonding component allowed them to obtain selective receptors for thymine (NapPy$N_2$20C5-1 to -3, Chart XII),[128,129] guanine (NapNaphthyrN23C7-1 and NapNaphthyrN25C7-1, Chart XII),[134] and adenine (NapPy$_2N_2$23C6-1 and NapPy$_2N_2$25C6-1, Chart XII),[133] while the orientation of the aromatic π-stacking is influenced by the electronic characteristics of the interacting groups.[132]

The guanine selective macrocyclic receptors (NapNaphthyrN23C7-1 and NapNaphthyrN25C7-1, Chart XII) containing naphthyridine and naphthalene units bound the guanine derivative, 2′,3′,5′-tri-*O*-pentanoylguanosine, by both hydrogen bonding and hydrophobic stacking interactions. Hamilton and co-workers found that the association constants for the formation of these complexes were more than 4-fold larger than that for the complex of 2′,3′,5′-tri-*O*-pentanoylguanosine with the simple naphthyridine which lacks the stacking component.[134] Similar binding enhancements have been observed in related ditopic receptors for thymine and adenine.[134]

In addition to nucleotide base receptors, Shinkai and Hamilton and co-workers synthesized a macrocyclic receptor (NapPy$N_2$20C5-1, Chart XII) for flavins whose design also follows the multisite strategy. This receptor design is based on hydrophobic interaction (aromatic stacking) with the phenyl moieties and hydrogen-bonding interaction with the pteridine moieties of guest molecules.[130] Other receptors for biologically interesting substrates synthesized by this group include one (Nap(1,3-B)Py$_2N_2$32C8-1, Chart XIII) with two separated hydrogen-bonding regions for longer dicarboxylic acids[139] and several with six inwardly facing hydrogen bonds for barbiturates (e.g., (1,3-B)(1,4-B)$_2$Py$_2N_4$34C8-1, Chart XIII).[141] Diederich and co-workers synthesized flavin cyclophanes (Flavinophane-1 and 2, Chart XIV) which mimic the active sites of flavoenzymes and in their oxidized forms demonstrate efficient binding of aromatic substrates via hydrophobic π–π stacking.[81,144,145]

New water-soluble cyclophanes incorporating the Tröger's base structural unit ((1,4-B)$_4N_4$28C6-1, (1,4-B)$_4N_4$30C6-1 to -4, all in Chart XII) were prepared by Wilcox and co-workers.[135–137] These chiral compounds had relatively rigid frames compared to those of other cyclophanes and were found to form inclusion complexes with benzene derivatives in aqueous solution.[137]

d. Mono- and Bicyclic without Heteroatoms. Mono- and bicyclic macrocycles without heteroatoms (see Chart XV) have been synthesized by Mourad and co-workers, and their complexation abilities with neutral molecules have been studied in organic solvents.[146–154] The electron-donor cyclophanes (π-bases) formed charge-transfer π–π molecular complexes with electron acceptors (π-acids) such as tetracyanoethylene, dichlorodicyano-*p*-quinone, and chloranil. Stability constants for the formation of the molecular complexes in CH_2Cl_2 increased as the difference in the acidic character of the electron acceptor and the basic character of the electron donor grew larger.[148,149,154] With iodine, a weak δ-electron acceptor, the cyclophanes formed π–δ molecular complexes, but the interactions were weaker than those derived from complexation with strong π-acids.[147]

e. Polycyclic with Various Donor Atoms. Following the general scheme established by Lehn for the synthesis of cryptands,[287] Diederich and co-workers prepared several spherical, suitably sized macrobicyclic cyclophanes (Cyclophane-1 to -4, Chart XVI) for the binding of larger arenes.[82,155–157] The same group of scientists synthesized an optically active host ((20C6)(29C4)-1, Chart XVI) which has two, almost independent recognition sites, one being a cyclic polyether and the other a cyclophane. A change in solvent switched this ditopic macrobicycle from a good cation binder to an efficient receptor for neutral naphthalene derivatives.[67,75,76]

Still and co-workers prepared enantioselective macrobicyclic hosts with large solvent-filled cavities. The hosts (Cyclophane-7 and -8, Chart XVII) have an amide binding site and additional functionality which distinguishes guest chiral substituents based on steric and hydrogen-bond-donating properties.[160,161] Their complexation abilities in organic solvents were studied. Still and co-workers also synthesized two chiral macrotricyclic receptors (Cyclophane-9 and -10, Chart XVII), having only limited conformational flexibility and deep basketlike binding sites.[162] The high selectivity of these hosts for certain L-amino acid derivatives over D-amino acid derivatives ($\Delta\Delta G$ = 12.6 kJ mol^{-1}, $CDCl_3$) is reminiscent of that of certain naturally occurring enzymes for enantiomers.[162]

Whitlock and co-workers reported the synthesis of bicyclic cyclophane-type macrocycles (Cyclophane-11 to -19, Chart XVII) possessing "phenol sticky cavities".[163–166] These "phenol sticky" macrocycles bound acidic para-substituted phenols in nonpolar organic solvents with a high degree of electronic and chemical specificity. These properties are due to a combination of a concave oriented pyridine functional group capable of serving as a hydrogen-bond acceptor and a rigid cavity.[165] Ortho- and meta-substituted phenols did not fit into the cavities of these macrocycles.[164] Whitlock and co-workers also synthesized macrobicycles (Cyclophane-24 to -27, Chart XVIII) with incorporated concave-oriented and sterically encumbered phosphine oxide functional groups which are strong hydrogen-bond acceptors.[168,169] The complexation ability of these macrocycles with neutral organic guests was examined.

Vögtle and co-workers, by means of modular donor spacer strategy, were able to obtain macrobicyclic tris-(pyridine) hosts (e.g., Cyclophane-29, Chart XIX) with successively larger conically shaped cavities which exhibit remarkable selectivities for trihydroxyben-

zenes.[171] Using the same techniques, they synthesized large macrobicyclic tris(catechol) hosts (e.g., Cyclophane-28, Chart XIX) for molecular recognition and transport of nucleobases.[170] The complexation study supports the existence of multiple hydrogen bonding between given guests and these hosts in a suitably sized cagelike cavity.[170,171]

Tetraazacyclotetradecane-capped (Cyclophane-30, Chart XIX) and cubic (Cyclophane-31, Chart XIX) cyclophanes were designed by Murakami and co-workers.[172,173] The cubic cyclophane behaved as a polycationic host in acidic aqueous media and exhibited size-sensitive and regioselective molecular discrimination that originates from the rigid geometry of its hydrophobic cavity.[173]

3. Calixarenes

The term "calixarene" was introduced by Gutsche[288] for a homologous series of macrocyclic phenol–formaldehyde condensates. It originated from the observation that the molecular models of the tetrameric members of the series have a chalicelike or cuplike appearance. Calixarenes (see Charts XX–XXII) are mainly receptors for small neutral molecules, although in deprotonated form they also bind cations.[289,290]

Calixarene complexes with neutral molecules in the solid state were observed even before the basic structures of the calixarenes were established.[291-293] The data indicated that the extent of complexation depended on the para substituent of the calixarene, e.g., *p-tert*-butyl- and *p-tert*-amylcalix[4]arene appeared to form tighter complexes with toluene than did the *p*-hydro- and *p-tert*-octylcalix[4]arenes.[183] This correlated with X-ray crystallographic studies of Andreetti which showed that the unsubstituted calix[4]arene failed to form an *endo*-calix complex, possibly because its cavity was too shallow. The *p-tert*-octyl-substituted calix[4]arene failed to form an *endo*-calix complex because the para substituent folds back into the calix. On the other hand, the *p-tert*-butyl-substituted calix[4]arene formed a tight endo-complex with toluene because *tert*-butyl groups extended the depth of the cavity but were not able to fold back into it.[183]

Studies of the interaction, in both aqueous and organic solutions, between calixarenes and guest molecules, were reported only recently[180,183,198,199] Water soluble calixarenes are most interesting because of their potential as enzyme mimics.

There exist only a few cases of the inclusion of guest molecules by calixarenes in organic media.[4,180,183] This lack of examples is because host–guest-type complexation in organic media always involves competition between complexation and solvation of guests by solvent molecules.[180,183] The driving force for inclusion of aliphatic amines by calix[4]arenes in polar solvents (acetone and acetonitrile) is postulated to be a combination of proton transfer and electrostatic attraction.[183] Among the most stable of the complexes formed by calixarene-neutral molecule interaction are those formed by "double cavity" calixarenes.[4,177] The "double cavity" calixarenes (Double Cavity Calix-1 to -3, Chart XXII) are unusual in that they possess both an enforced cavity on the "lower rim" and a semiflexible cavity on the "upper rim". These macrocycles appear to behave both as hydrogen-bond donors, forming complexes with amines, and hydrogen bond acceptors, forming complexes with acids and phenols.[4,177]

Recently, Arimura and Shinkai synthesized calix[4 and 6]arenes bearing on the "lower rim" (*S*)-2-pyrrolidone units which have hydrogen-bonding sites as well as a chiral center. The formation of a molecular complex between calix[6]arene (Calix6-24C-18, Chart XXI) and ferrocenecarboxylic acid in chloroform, through hydrogen-bond interaction, was detected by induced circular dichroism.[180]

The majority of host–guest chemistry of calixarenes, however, has been studied in aqueous solutions. The first-water soluble calixarene was prepared by Ungaro and co-workers[294] by affixing carboxymethyl groups to the phenolic oxygen atoms at the "lower rim" of the calixarene; Shinkai and co-workers[199] introduced sulfonic acid groups in the para positions at the "upper rim"; Gutsche and co-workers[184] attached amino and carboxyl functions on the "upper rim". Studies of complexation in water gave some evidence that there is some size–shape complementarity between the guest molecules and the cavity of the calixarenes.[184,186,196]

Resorcinol cyclotetramers (Calix4-16C-21 to -23, Chart XX), synthesized and examined by Schneider,[189,190] Aoyama,[191-193] and Shinkai,[194] and their co-workers, are structurally related to calixarenes. These compounds have four independent binding sites composed of a pair of hydrogen-bonded OH groups on adjacent benzene rings.[191] One of them, cyclotetramer "Calix4-16C-22", displayed a significant selectivity toward certain dicarboxylic acids in $CDCl_3$. This selectivty is due in part to its ability to interact with guests via two-point hydrogen bonding.[192]

4. Cryptophanes

Cryptophanes, a new family of cavitands, were synthesized by Collet and co-workers. Cryptophanes (see Charts XXIII and XXIV), constructed from two cyclotriveratrylene caps connected to one another by three bridges, have an enforced, roughly spherical or ellipsoidal hydrophobic cavity and three windows in the equatorial region which allow guests to enter.[203,204,208] The first member of the cryptophane family, the anti isomer cryptophane-A type (Cryptophane-2, Chart XXIII), was designed in the early 1980s to complex tetrahedral halomethanes and was followed by the preparation of a series of related cryptophane (B, C, D, etc.) types.[5,295]

In general, two main stereoisomeric types (anti and syn) of cryptophanes have been synthesized. These cryptophanes contain three identical bridges of structure O–(Z)–O (where Z may be $(CH)_n$, $CH_2CH{=}CHCH_2$, or $CH_2C{\equiv}CCH_2$), and the R and R′ substituents on the caps display either an anti or a syn relationship. In most cryptophanes, R = R′, and the D3-anti and C3h-syn isomers have been identified. There also exist a pair of C3-anti and C3-syn isomers, with R = CH_3 and R′ = H, and a pair with unsymmetrical bridges of structure $O(CH_2)_3S$.[203]

Collet and co-workers also studied the ability of cryptophanes to bind neutral halomethanes and hydrocarbons in lipophilic as well as in aqueous solvents. Cryptophanes showed selectivity among these guests, according to their shape, size,[202,205,206,208] and even chirality (CHFClBr).[202]

In organic solvents, the apparent stability of the complexes depends on the intrinsic stability of the host–guest supermolecules as well as encompassed *solvent–guest* and *solvent–host* interactions.[5,206,211] Cryptophane-4 (Chart XXIII, cryptophane-E type) formed stable complexes in tetrachloroethane with chloroform and other halomethanes that are 70–80 Å^3 in size and with isobutane.[209] The study showed that formation of these complexes was enthalpy driven and entropy disfavored, so their stability should be ascribed to attractive host–guest interactions provided by dispersion forces. The strength of complexes was enhanced by a good or almost ideal (e.g., for isobutane) complementarity between the host and the guests. By contrast, the complexation of smaller (CH_2Cl_2) or larger (>$CHClBr_2$) substrates is not enthalpy driven. These complexes therefore owe their stability to the operation of external factors. These factors may include solvophobic effects, as well as more subtle thermodynamic contributions such as specific heat and/or volume differences between the complexes and their separated components.[209]

In water or other hydrophilic solvents, the contribution of hydrophobic forces is expected to enhance the stability of the complexes between cryptophanes and neutral, lipophilic guests. In fact, isobutane appeared to be more than 500 times better bound by Cryptophane-6 (Chart XXIII, cryptophane-E type) in water than by Cryptophane-4 (Chart XXIII, cryptophane-E type) in tetrachloroethane. The hydrophobic contribution in this case (−15.9 kJ mol^{-1}) is close to that reported for $CHCl_3$ (−12.6 kJ mol^{-1}) regarding its complexation by Cryptophane-3 (Chart XXIII, cryptophane-A type) in tetrachloroethane and Cryptophane-5 (Chart XXIII, cryptophane-A type) in water.[204]

5. Miscellaneous

a. Cavitands and Carcerands. Cram[214,215,217] and Dalcanale[216] and their co-workers have reported a series of highly preorganized synthetic organic compounds with enforced concave surfaces of molecular dimensions which they refer to as cavitands. The cavitands prepared by Cram and co-workers contained cylindrical wells of varying depths whose limited diameters allowed inclusion only of slim and linear guests. These workers studied complexation by these hosts (Cavitand-1 to -3, Chart XXV) of CS_2 in chloroform and benzene.[214] They also designed cavitands (Cavitand-4 and -5, Chart XXV) containing two binding cavities, one shaped like a box and the other like a bowl.[215] It was suggested that varying the substituents of the cavity rims could lead to bifunctional hosts having even stronger binding and dramatically different guest selectivities for each cavity.[215] Complexation of CD_3CN by each cavity of these cavitands in CCl_4 was examined. Shell closure of two cavitands created carcerands, a new family of large, rigidly hollow hosts.[219]

The efforts of Dalcanale and co-workers resulted in a cavitand (Cavitand-6, Chart XXV) which, in organic solvents, selectively bound neutral aromatic compounds, such as benzene, toluene, chlorobenzene, fluorobenzene, and benzonitrile, but did not bind benzaldehyde, anisole, benzoic acid, and phenol. In addition, this macrocycle showed a solvation–temperature-driven equilibrium between extended (dominant at $T \leq -60$ °C) and vessellike (dominant at $T \geq +5$ °C) forms. This equilibrium could be intentionally switched using temperature.[216] Two forms of a temperature-dependent cavitand, kite and vase, were also observed by Cram and co-workers.[296,297]

b. Porphyrins and Porphyrin Derivatives. Thermodynamic data have been reported for complexation of neutral molecules by porphyrins and macrocycles with porphyrin subunits built into their rings. Kano and co-workers compared the complexation of tetraarylporphyrins with quinones in organic solvents and water. They found that the stability of the complexes was much larger in water than in organic solvents. The thermodynamic parameters indicated that complexation in water was an enthalpically favorable process, suggesting that the van der Waals interactions were the main binding forces and that hydrophobic interaction did not play an important role in complex formation in water.[220]

Macrocyclic porphyrin dimers (Porphyrin-79 to -86, Chart XXXII)[256,258,261] and trimers (Porphyrin-87 to -89, Chart XXXIII)[224,245] have been synthesized and their complexation properties have been studied. A strong π–π interaction between the two porphyrin moieties in the dimer makes the existence of the cavity possible and controls the geometry adopted by these systems. Porphyrin trimers, obtained by Sanders and co-workers, have a semi-preorganized cavity which can accommodate more than one organic guest and is flexible enough to bind guest molecules even when they do not fit the relaxed cavity.[244] These conformational properties allow the trimeric porphyrins to mimic some aspects of enzymatic binding.[244]

Chiral doubly steroid-capped porphyrin (Porphyrin-95, Chart XXXV) bound a variety of functionalizied amines via a combination of metal–amine and hydrogen-bonding interactions. This material demonstrated both cooperative multipoint binding and metalloporphyrin-directed catalysis of a selective acylation of a single hydroxy group in the cap.[242]

Recently, Diederich and co-workers designed porphyrin-bridged cyclophanes (Porphyrin-90 to -94, Charts XXXIII and XXXIV) which complex neutral guests such as aromatic hydrocarbons or pyridine derivatives.[262,263] Porphyrin-93 (Chart XXXIV) bound arenes more strongly than similar cyclophanes that are not bridged by a porphyrin.[263] The possible explanation is that aromatic substrates are exposed not only to the shielding cyclophane cavity but also to the strongly shielding region of the porphyrin ring. The porphyrin-bridged cyclophanes can serve well as a synthetic model of cytochrome P-450 enzymes.[263]

c. Other. Among other macrocycles are those synthesized by Nolte and Reinhoudt and co-workers which have synthetic molecular clefts[264,265] or metallo clefts.[266,298] Macrocycles with synthetic clefts (Other-1 to -5, Chart XXXVI) bound dihydroxybenzenes in organic solvents. The guests were sandwiched between the *o*-xylylene walls of the host and form hydrogen bonds with the receptor. Dihydroxybenzenes, which have not only hydroxy groups but also electron-withdrawing groups, formed stronger hydrogen bonds and more stable complexes than those of the unsubstituted dihydroxybenzenes, e.g., $K = 70$ M^{-1} and 3×10^5 M^{-1} for catechol and 2,3-dicyanohydroquinone

complexes with Other-4 (Chart XXXVI) in $CDCl_3$, respectively.[264] One of the macrocycles with a molecular cleft (Other-5, Chart XXXVI)[265] showed allosteric binding properties, and in organic solvents, bound 1,3-dinitrobenzene more strongly by a factor of 6 in the presence of potassium thiocyanate. The enhancement is caused by the conversion of the macrocycle into the anti-anti conformer, and not by an ionic strength effect, as was verified in a control experiment. In the case of macrocycles with a metallo cleft (Other-6 to -12, Chart XXXVI), neutral guests may be coordinated in addition to an immobilized electrophilic metal cation provided the geometry for coordination of the cation is consistent with the geometry necessary for complexation of the neutral guest.[298]

Cyclotetrachromotropylene (Other-22, Chart XXXVII) was designed by Poh and co-workers.[274,276] This macrocycle resembles the calixarenes. A complexation study in water showed that hydrophobic interactions, as expected, are the driving forces for the complexation of cyclotetrachromotropylene with aromatic hydrocarbons, and the stability of the complexes is influenced by the size and polarizability of the guests.

Unsaturated tetraazamacrocyclic metal complexes that coordinate amine bases (Other-17 to -21, Chart XXXVII)[271-273] and vaulted macrobicyclic ligand-transition metal complexes (Other-13 to -16, Chart XXXVI) that act as hosts of alcohols and phenols[269,270] have also been reported.

B. Selectivities

Achieving selective complexation between receptors and substrates of biochemical interest has been a driving force for the design of macrocycles capable of the selective binding of cations, anions, and neutral molecules. As in the case of cations and anions,[11,12] selectivities of macrocycles toward neutral molecules are governed by many parameters.

Size-based selectivity is quite common among complexes of macrocycles with neutral molecules. Reinhoudt and co-workers studied complexation of malononitrile with the series of 15–33-membered 2,6-pyridino crown ethers in organic solvents ($CDCl_3$ and C_6D_6) and found that the most stable complex was formed with the 18-membered macrocycle. This complex was isolated as a crystalline compound. For either smaller or larger ring sizes, the enthalpy change upon complexation becomes less favorable.[39] In the case of urea, good efficiencies for its extraction into chloroform required ring sizes ≥ 27.[43] Cyclophanes designed with two diphenylmethane units and two oligomethylene bridges via four nitrogens formed, in water, inclusion complexes with aromatic guests but not with aliphatic guests.[106,109] X-ray analysis showed that the cavity of (1,4-B)$_4$N$_4$30C4-2 (Chart X) in its crystalline complexes has rectangularly shaped open ends (about 3.5×7.9 Å) with a depth of 6.5 Å.[109,299] By CPK molecular model studies, selective complexation of the macrocycle with aromatic guests seems to be reasonable because the shorter side of this rectangle fits well with the thickness of the aromatic ring (3.4 Å).[109] A cubic cyclophane exhibited size-sensitive and regioselective molecular discrimination that originates from the rigid geometry of its hydrophobic cavity. Evaluation of the binding constants in acidic aqueous media showed that *N*-phenyl-1-naphthylamine fit the host cavity most tightly among the guest molecules examined, even though pyrene and perylene are more hydrophobic than *N*-phenyl-1-naphthylamine.[173]

Selectivity based on the shape of host and neutral guests has been shown. Cavitands with a cylindrical cavity for linear guests like CS_2 were produced by Cram and co-workers.[214] Recently, very stable complexes of spherical cryptophane hosts with the halomethanes in $(CDCl_2)_2$ have been described by Collet and co-workers.[207,210] Cryptophane-4 (Chart XXIII, cryptophane-E type) not only displayed a size recognition of $CHCl_3$ over $CHCl_2Br$ by 1.3 kJ mol^{-1}, although the difference in volume of these two molecules is only 5%, but also efficiently recognized tetrahedral (sp^3) vs flat (sp^2) molecules.[209] This cryptophane did not discriminate between isobutane and $CHBr_2Cl$, which have the same van der Waals volume, but formed more stable complex with $CHCl_3$ (tetrahedral) than with acetone (flat), although they have the same size.[204,209] 2,4,6-Tri(4-pyridyl)-1,3,5-triazine has a good size and shape complementarity with the cavity of porphyrin trimers.[244] Its binding constant to Porphyrin-87 (Chart XXXIII) in CH_2Cl_2 was greater than the square of its binding constant to Porphyrin-32 (Chart XXIX) and its 1:1 complex with Porphyrin-88 (Chart XXXIII) was so stable that it could be observed directly by fast atom bombardment mass spectroscopy (FABMS) (log K was about 10). In the Porphyrin-88 complex, analysis of ring-current-induced chemical shift changes showed the pyridyl groups were lying flat in the plane of the three zinc atoms.[244] Vögtle and co-workers produced macrobicycles with a conical-shaped cavity which complexed in CH_2Cl_2 only certain trihydroxybenzenes e.g., 1,3,5- and 1,3,4-trihydroxybenzenes, but not structurally related compounds or 1,2,3-trihydroxybenzene.[171]

Study of macrocycle interaction with neutral molecules shows that complementary positioning of recognition sites (particularly hydrogen bonding, π–π interactive and hydrophobic groups) and other active groups into the macrocycle structure can lead to very strong and specific complexation.[127] According to this observation, the number, kind, and arrangement of donor atoms in macrocycle frameworks should play a role in the selectivity they show toward guests. For example, malononitrile formed in organic solvents ($CDCl_3$ and C_6D_6) the most stable complexes with 18-membered macrocycles because the orientation of their binding sites is the most favorable compared with smaller or larger macrocycles.[39] The presence of a nitrogen atom in the macrocyclic ligand reduced the enthalpy of complexation with malononitrile from −59.4 kJ mol^{-1} for 18C6-1 (Chart II) to −34.7 and −23.8 kJ mol^{-1} for the complexation by 2,6-pyridino-18C6 (Py18C6-1, Chart II) and N18C6-1 (Chart II), respectively. These decreases can be due to stronger intraannular interactions in the uncomplexed 2,6-pyridino-18C6 (Py18C6-1, Chart II) (CH···N) and N18C6-1 (Chart II) (NH···O).[39] Amino acid-containing macrocycles bind water molecules additionally via two amide NHs acting as hydrogen-bond donors. The structural arrangement of these amide groups is important because the large distance between them decreases the possibility of forming hydrogen bonds with water.[40]

Incorporation of benzene, cyclohexane, and pyridine rings into macrocyclic skeletons causes the macrocycles to become more rigid and may alter the binding strength and selectivity of the ligands. B18C6-1 (Chart II) formed a weaker complex than its nonaromatic analogues with malononitrile in $CDCl_3$ because of the electron-withdrawing properties of the benzo unit.[39] Among the 18-membered oxygen-containing macrocyclic polyethers, $Cy_2$18C6-1 (Chart II) formed the most stable complex with water in $CHCl_3$. Probably, the steric arrangement of the cyclohexyl rings in this isomer enhances the strong retention of water in the cavity of the crown ether.[19]

Chiral macrotricyclic receptors (see Cyclophane-8 to -10, Chart XVII) constructed by Still and co-workers[161,162] bound diamides of certain amino acids in $CDCl_3$ with high selectivity which is dependent upon the nature of the amino acid side chain (~8.4 kJ mol^{-1} for serine vs alanine) and the type of *N*-alkyl substituent (>12.6 kJ mol^{-1} for methyl vs *tert*-butyl). In addition, chiral groups incorporated into the correct location on the macrocyclic framework allowed the separation of optically active enantiomeric molecules. With Boc-protected (Boc = butoxycarbonyl), *N*-methylamide derivatives of the amino acids, enantioselectivity ranged from 7.1 to 12.6 kJ mol^{-1} (ΔG) in $CDCl_3$ with the L isomer always being bound preferentially.[162] Another chiral macrocycle, Cyclophane-7 (Chart XVII), produced by Still's group distinguished energetically and spectrally between certain enantiomeric amides in C_6D_6.[160] Collet and co-workers achieved analytical optical resolution of CHFClBr in $CDCl_3$, as determined by ^1H NMR spectroscopy, by inclusion of the haloform within the cavity of chiral, suitably-sized Cryptophane-1 (Chart XXIII, cryptophane-C type).[202] The NMR chemical shifts of the (+) and (−) enantiomers of the guest were separated, allowing for an easy determination of the guest enantiomeric composition.[202]

Hamilton and co-workers, by varying the hydrogen bonding regions and electronic characteristics of the $\pi-\pi$ stacking groups in the macrocyclic structure, prepared selective receptors for nucleotide bases in $CDCl_3$,[128,129,133,134] flavins in $CHCl_3$,[130] barbiturates in $CDCl_3$ and CH_2Cl_2,[141] and dicarboxylic acids in $CDCl_3$.[139]

Incorporation of alkyl groups into the "lower rim" of calixarenes synthesized by Shinkai and co-workers results in strong but nonselective binding sites. On the other hand, incorporation of alkyl groups into the "upper rim" results in relatively weak but selective binding sites.[178]

The face-to-face zinc porphyrin complex (Porphyrin-85, Chart XXXII) displayed better selectivity toward 4,4′-bipyridine over diamines $H_2N(CH_2)_nNH_2$ in CH_2Cl_2.[260,261] This selectivity is attributed to the separation and relative orientation of the two functional groups in the guest and also to the rigidity of the host molecules.

Selectivities of macrocycles toward charged and neutral species are influenced by many parameters. However, in order to optimize neutral molecule–macrocycle interaction, it is important that the binding sites of the macrocycle be preorganized and be of the correct nature to interact with substrate binding sites.

C. Solvent Effects

The influence of the solvent on macrocycle interaction with neutral molecules is pronounced. The large difference in binding strength in various solvents results mainly from solvation–desolvation phenomena.[64,67,82,84] Water is an exceptional medium because it provides the strongest solvophobic driving forces for complexation and shows specific substituent solvation effects.[64] Complexation in organic solvents is dependent on the ability of the solvent molecules to compete effectively with the guest for the cavity of the host.[67,180]

Cryptophane-1 (Chart XXIII, cryptophane-C type) designed by Collet and co-workers bound CH_2Cl_2 with the apparent stability constant, K = 2.6 M^{-1} in $CDCl_3$ at 310–330 K,[202] and with apparent stability constant, K = 325 M^{-1} in $(CDCl_2)_2$ at 300 K.[204] The reason for this significant difference in binding constants is that the first solvent, $CDCl_3$, is a strong competitor with the guest for the host cavity binding sites. On the other hand, the second, bulky $(CDCl_2)_2$ cannot easily enter the host cavity.[5,204] Chapman and Still also observed that the binding cavity is sensitive to the size and shape of the solvent molecules and that large solvents do not penetrate and solvate the cavity as well as smaller ones. By using properly sized solvents, a binding site need not be extensively desolvated to accept and bind a smaller or more appropriately shaped substrate.[159]

The influence of the solvent on complexation of macrocyclic polyethers with malononitrile was studied by comparing complexation in $CDCl_3$ and C_6D_6.[39] For example, in the interaction of 18C6-1 (Chart II) with malononitrile, ΔH (kJ mol^{-1}) and ΔS (J K^{-1} mol^{-1}) are, respectively, for $CDCl_3$ −22 and −46 and for C_6D_6 −59 and −154. The larger enthalpy and entropy changes upon complexation in $CDCl_3$ reflect the greater polarity of $CDCl_3$, which means stronger solvation of both malononitrile and crown ether. These solvent interactions must be broken before complexation can occur, resulting in a less favorable enthalpy change. Desolvation of both the crown ether and malononitrile prior to complexation results in a positive entropy change.

Diederich and co-workers have studied the complexation of a macrobicyclic cyclophane (Cyclophane-3, Chart XVI) with pyrene in water and 17 organic solvents covering the entire polarity range.[156] They found that complexation strength decreased steadily from water (ΔG = −39.3 kJ mol^{-1}) to nonaqueous polar protic solvents, to dipolar aprotic solvents, and to apolar solvents like carbon disulfide (ΔG = −5.4 kJ mol^{-1}). Binding was strongest in solvents with low molecular polarizability and with high cohesive interactions such as water.[156] Recently, this group of scientists measured calorimetrically the enthalpy changes for the above cyclophane interaction with pyrene in 12 solvents over a wide range of solvent polarities and observed that complexation is enthalpy driven in all media.[79] The reaction exothermicity generally increased from apolar solvents, to dipolar aprotic solvents, to protic solvents. The study showed that reactions having similar ΔG values in two solvents, e.g., acetone and *N*,*N*-dimethylacetamide, can differ dramatically in their enthalpic and entropic terms.[79] For example, in the reaction of Cyclophane-3 (Chart XVI) with pyrene, ΔG (kJ mol^{-1}), ΔH (kJ mol^{-1}), and ΔS (J K^{-1} mol^{-1}), respectively, were in acetone −18.0, −27.6, and −31.8 and in *N*,*N*-dimethylacetamide −18.4, −8.4, and +33.1.[79]

Two types of guest-binding behavior were observed in octopus cyclophanes ((1,4-B)$_4$N$_4$28C4-2 and -3, Chart

IX) having L-aspartate residues. The type of behavior was determined by the nature of the media used for preparation of cyclophane stock solutions.[98] First, when an aqueous stock solution of the macrocycle was injected into an aqueous buffer containing a guest, the host–guest complexation immediately reached an equilibrium state as monitored by fluorescence spectroscopy. Concurrently, the chiral L-aspartate residues of the host underwent conformational changes so as to attain effective guest incorporation. ^{1}H NMR spectroscopy indicated that the guest molecule was incorporated into the three-dimensional cavity provided intramolecularly by the macrocyclic ring and the eight hydrocarbon chains. When, in turn, an organic stock solution of the macrocycle was injected into an aqueous buffer containing a guest, time-dependent and biphasic complexation behavior was observed. This behavior is consistent with fast incorporation of a guest molecule into the hydrophobic host cavity followed by slow and long-range conformational changes of the host, as induced by the incorporated guest.[98]

D. Heat Capacities, ΔC_p

The availability of heat capacity changes for neutral molecule–macrocycle interaction should be helpful in better understanding the nature of the interactions between the solvent and the macrocycle, neutral molecule, and resulting host–guest complex. In addition, information may be derived concerning the internal modifications of the guest and host upon complexation. Unfortunately, few ΔC_p values are available.

Dougherty and co-workers performed variable-temperature NMR studies on the interaction of macrocyclic cyclophanes with a variety of guests and found significant heat capacity effects.[89] The origin of the binding forces changed from entropic at lower (21 °C) to enthalpic at higher (61 °C) temperatures. The magnitude of ΔC_p in this study reflected a dependence on solvent and on the electronic and structural properties of the guests. ΔC_p was larger in water than in chloroform, and methylated guests in aqueous media had much higher values for ΔC_p compared with non-methylated guests.[89]

Diederich and co-workers in their calorimetric studies found that all inclusion reactions between a macrocyclic cyclophane, (1,4-B)$_4$30C4-3 (Chart VII), and various benzene derivatives displayed negative heat capacity values in both water and methanol.[79] The largest negative ΔC_p values were measured for the complexation of benzene derivatives that possess a molecular dipole and hydroxy substituents, e.g., *p*-nitrophenol and *p*-cresol, and therefore interact strongly with their solvent cages.[79]

E. Applications

Macrocycle complexation with neutral molecules is a relative young area in macrocyclic chemistry. Interest in this research area is strongly stimulated by the possibility of applications in separation processes; conversion of chemical reactions into optical or electronic signals; the mimicking of enzymes in their capability to bind substrates rapidly, selectively, and reversibly; and the catalyzing of chemical reactions.

The following are examples of possible applications. Hamilton and co-workers have developed a new class of biomimetic receptors for nucleotide base substrates.[128] The understanding of the key features of nucleotide recognition could lead to the design of "synthetic repressor" molecules that might artificially activate or control genes.[127] The hydrophobic cage provided by octopus cyclophanes is highly apolar and acts to repress the molecular motion of guests. The results imply that octopus cyclophanes can be used as effective apoenzyme models for simulation of enzymatic functions.[102,103] Chiral recognition in diastereomeric host–guest complexes has great potential as an efficient, nondestructive method to separate optical isomers in crystallization, distribution, transport, and chromatographic experiments. So far, the resolution of neutral guests has almost exclusively been observed by free or immobilized cyclodextrins in aqueous solution.[71,72,74,76]

III. Kinetics of Neutral Molecule–Macrocycle Interaction

Studies on the thermodynamics of neutral molecule–macrocycle interaction, although many fewer in number than in the case of cation–macrocycle interaction, are much more numerous than those on the kinetics of neutral molecule–macrocycle interaction. Few mechanistic studies of the reactions between neutral molecules and macrocycles have been reported. Kinetic and activation parameters for neutral molecule–macrocycle interactions are given in Table III, together with the method, temperature, and solvent used in their determination. When necessary, relevant equations are also given under the conditions heading.

Muchova and Holba studied the kinetics of reaction of several crown ethers with iodine[301] and KI[300] in chloroform. They found that, in the case of iodine, rate constants and their temperature dependence indicated formation of molecular complexes (crown ether···I_2) and (crown ether···I^+)I^- according to the scheme:

$$\text{crown} + I_2 \rightleftarrows (\text{crown}\cdots I_2) \rightarrow (\text{crown}\cdots I^+)I^- \overset{I_2}{\rightleftarrows} (\text{crown}\cdots I^+)I_3^- \rightarrow (\text{crown}\cdots I^+) + I_3^- \quad (1)$$

With increasing temperature, the equilibrium concentration of one or the other complex, or both, decreased. This effect is ascribed to the decomposition of an unstable complex. The most likely species to decompose is the complex (crown···I_2) in which iodine is coordinated to the crown by a weak van der Waals bond. As the rate-determining step, the authors propose either the slow decomposition of the complex (crown···I_2) or the slow dissociation of the complex (crown···I^+)I_3^-.[301]

Pizer examined the dynamics of cryptand protonation in aqueous solution according to the reaction: [2.2.2]-1 + $H_2O \rightleftarrows H^+$[2.2.2]-1 + OH^- by temperature-jump techniques and found that the achieved rate constants can permit the determination of the extent to which the ligand imposes dynamic constraints on the complexation process and is significant in understanding previously observed slow rates of metal cryptate formation.[302]

Using cavitand structures, Cram and co-workers synthesized carcerands which have large enough dimensions to sterically inhibit dissociation of their complexes with neutral molecules and permit isolation

and characterization of these complexes. The term "constrictive binding" was suggested for this phenomenon.[305]

Kinetics of neutral molecule coordination to macrocycle–metal complexes has been studied. Chung and Chang[23] examined the complexation reactions of the aqua(*rac*-5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane)copper(II), $CuL(H_2O)^{2+}$ blue isomer, with neutral monodentate molecules. The first step of the reaction is a diffusion-controlled interaction by the neutral molecule to form an outer-sphere complex. The second step is the associative interchange of H_2O and neutral molecule within the outer-sphere complex.[23] Sanders and co-workers have studied complexation of zinc–porphyrin dimers with triethylenediamine and found the large variation of behavior (uni- or bimolecular exchange processes) to be due to isomeric forms of dimers and the concentration of triethylenediamine.[256]

IV. Suggestions for Future Work

Several needs become apparent upon reviewing the work compiled in this review. First, there are few kinetic data for the interaction of neutral guests with macrocyclic hosts. These data would be useful for the characterization of these systems. For example, it would be of interest to compare rate data for these systems with those for cation–macrocycle interaction.[11,12] Second, few log K and ΔH values have been reported as a function of temperature. A knowledge of these quantities over a wide temperature range would be useful in identifying and understanding reaction driving forces and solvent-solute interactions. Third, few ΔC_p values are available. These values obtained in a variety of solvent media could provide valuable information concerning solvent effects in host–guest interactions. Finally, there is a need for greater involvement of modern analytical chemistry techniques in the study of promising systems and in finding uses for them. For example, the demonstrated selectivities could lead to development of sensing agents, separation systems, and recovery systems.

The design and synthesis of macrocycles which are selective toward specific neutral organic molecules have been demonstrated with many examples. Use of the design principles provided in these studies could lead to the preparation of hosts targeted toward specific guests of environmental and industrial interest. Application of such systems to practical problems could provide innovative solutions to many difficult problems.

Examination of the log K data in this review reveals that few workers check their experimental procedure by using a standard chemical system. In most cases, this is understandable because few log K values for neutral molecule–macrocycle interactions have been determined in more than one laboratory. An important need is for one or more standard reactions to be studied in multiple laboratories. This has been done for metal–ligand interaction.[306] The desirability of standard reactions is evident when one considers the large number of log K values being determined and the value of accurate data in providing information which will serve as a basis for future ligand design. Calibration of equipment by using such reactions would insure that many errors would not go undetected.

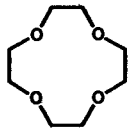
Similar comments can be made concerning the determination of ΔH and ΔS values. A careful study by us[307] compared log K and ΔH values determined by ^1H NMR and calorimetry. The results showed that log K values determined by the two methods were in good agreement, but the corresponding ΔH values were not. Values of ΔH determined from the variation of log K with temperature differed appreciably from those determined calorimetrically. There is concern that ΔH values of low accuracy may be produced from temperature variation studies. Conclusions drawn from these data could lead to incorrect models. Thus, it would be desirable to have and use standard systems to calibrate procedures.

Acknowledgments. Appreciation is expressed to Mrs, Daria J. Zamecka-Krakowiak for the preparation of the charts and to Dr. Krzysztof E. Krakowiak and Dr. Zenon Pawlak for valuable comments. Partial financial support is acknowledged from the Office of Naval Research and IBC Advanced Technologies, Inc.

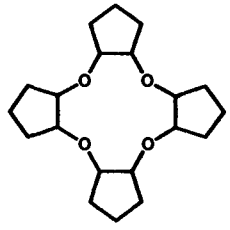
CHART I

1. Coronands and Cryptands

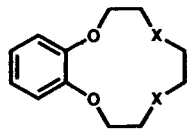
a. Crown Ethers



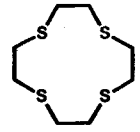
12C4-1



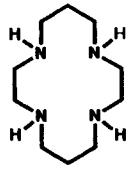
12C4-2



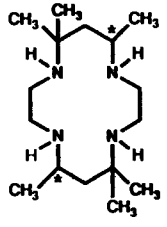
B12C4-1
X = O
$BS_2$12C4-1
X = S



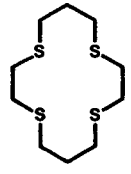
$S_4$12C4-1



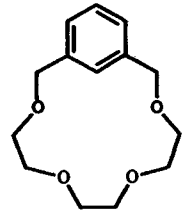
$N_4$14C4-1



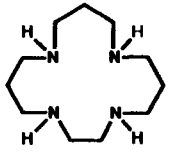
$N_4$14C4-2
(racemic)
$N_4$14C4-3
(meso)



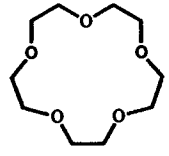
$S_4$14C4-1



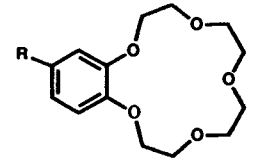
(1,3-B)15C4-1



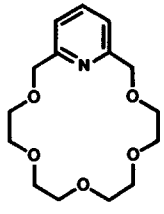
$N_4$15C4-1



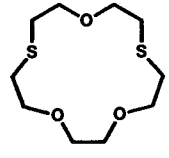
15C5-1



B15C5-1 R = H	B15C5-7 R = C(O)C_2H_5
B15C5-2 R = Br	B15C5-8 R = C(O)OCH_3
B15C5-3 R = I	B15C5-9 R = C(O)OC_2H_5
B15C5-4 R = C_2H_5	B15C5-10 R = n-C(O)OC_3H_7
B15C5-5 R = C(O)H	B15C5-11 R = NH_2
B15C5-6 R = $C(O)CH_3$	B15C5-12 R = N=CH-[2-HOC_6H_4]



Py15C5-1

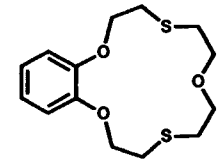


$S_2$15C5-1

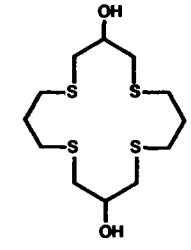
CHART II

1. Coronands and Cryptands (cont.)

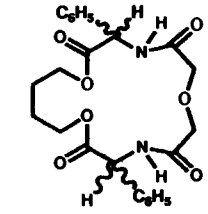
a. Crown Ethers (cont.)



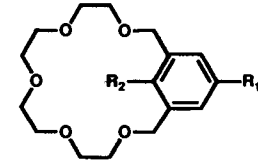
$BS_2$15C5-1



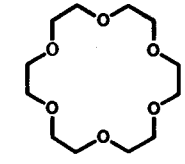
$S_4$16C4-1



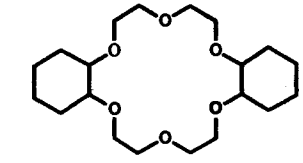
$K_4N_2$17C5-1



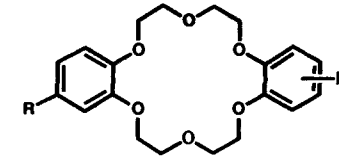
(1,3-B)18C5-1
R_1, R_2 = H
(1,3-B)18C5-2
R_1 = H; R_2 = CO_2H
(1,3-B)18C5-3
R_1 = H; R_2 = CO_2CH_3
(1,3-B)18C5-4
R_1 = Cl; R_2 = OH
(1,3-B)18C5-5
R_1 = Cl; R_2 = $OCH_2CH{=}CH_2$



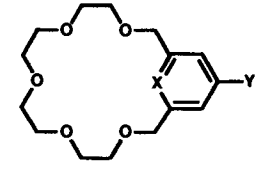
18C6-1



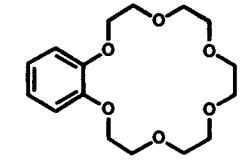
$Cy_2$18C6-1
(mixture of isomers)



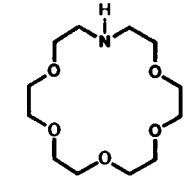
$B_2$18C6-1
R = H
$B_2$18C6-2
R = Br



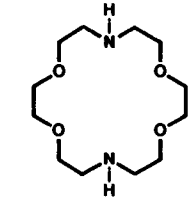
Py18C6-1
X = N; Y = H
Py18C6-2
X = N; Y = C_6H_5
Py18C6-3
X = NH^+; Y = H



B18C6-1



N18C6-1

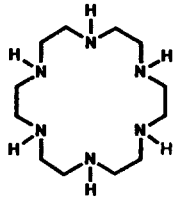


$N_2$18C6-1

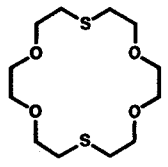
CHART III

1. Coronands and Cryptands (cont.)

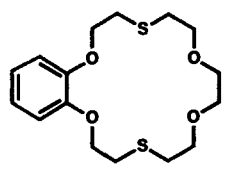
a. Crown Ethers (cont.)



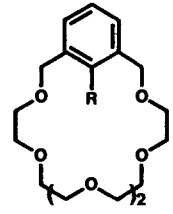
$N_6$18C6-1



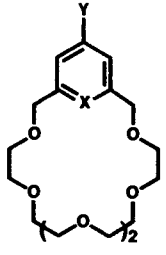
$S_2$18C6-1



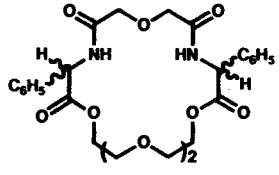
$BS_2$18C6-1



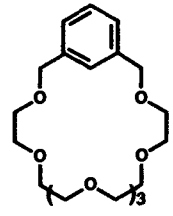
(1,3-B)21C6-1
R = H
(1,3-B)21C6-2
R = CO_2H



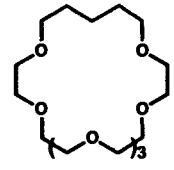
Py21C7-1
X = N; Y = H
Py21C7-2
X = N; Y = C_6H_5
Py21C7-3
X = NH^+; Y = H



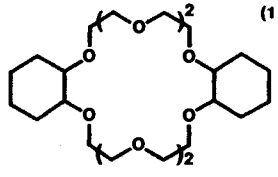
$K_4N_221C7-1$ (±)
$K_4N_221C7-2$ (meso)



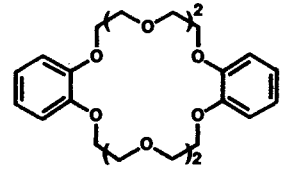
(1,3-B)24C7-1



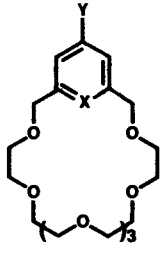
24C8-1



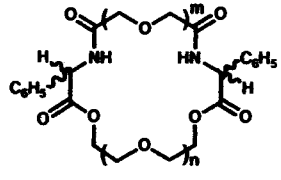
$Cy_224C8-1$



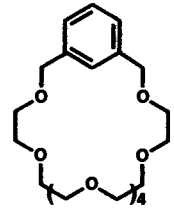
$B_224C8-1$



Py24C8-1
X = N; Y = H
Py24C8-2
X = N; Y = C_6H_5
Py24C8-3
X = NH^+; Y = H



$K_4N_224C8-1$
m = 1; n = 3 (±)
$K_4N_224C8-2$
m = 1; n = 3 (meso)
$K_4N_224C8-3$
m, n = 2

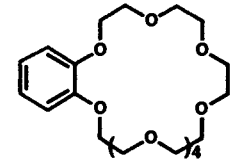


(1,3-B)27C8-1

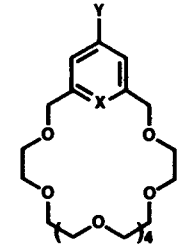
CHART IV

1. Coronands and Cryptands (cont.)

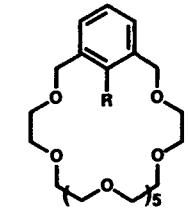
a. Crown Cthers (cont.)



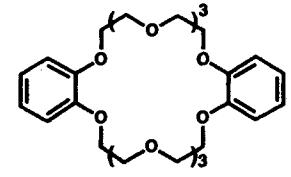
B27C9-1



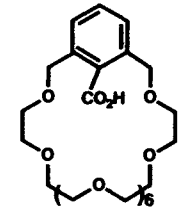
Py27C9-1
X = N; Y = H
Py27C9-2
X = N; Y = C_6H_5
Py27C9-3
X = NH^+; Y = H



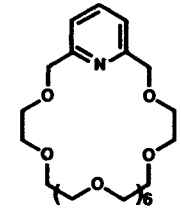
(1,3-B)30C9-1
R = H
(1,3-B)30C9-2
R = CO_2H



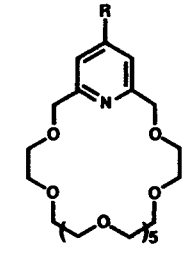
$B_230C10-1$



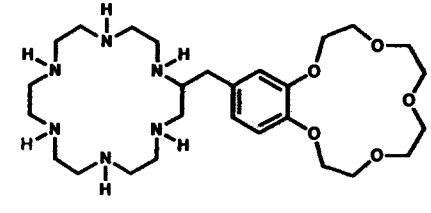
(1,3-B)33C10-1



Py33C11-1



Py30C10-1
R = H
Py30C10-2
R = C_6H_5

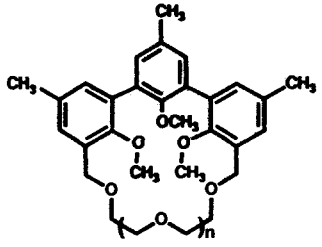


$(N_6$18C6)(B15C5)-1

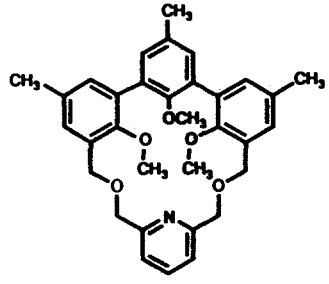
CHART V

1. Coronands and Cryptands (cont.)

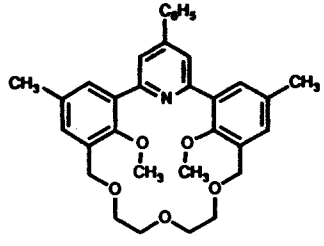
b. Hemispherands



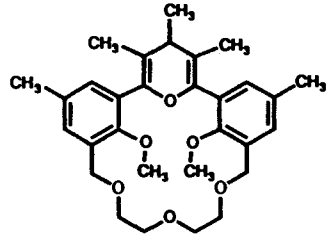
Spher-18C3-1
n = 1
Spher-24C4-1
n = 2



Spher-Py18C3-1



Spher-Py18C4-1



Spher-Pyrano18C4-1

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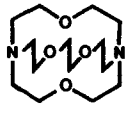
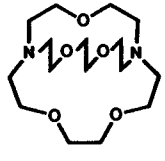
1. Coronands and Cryptands (cont.)

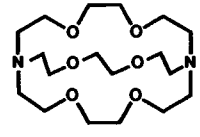
c. Cryptands



[2.1.1]-1



[2.2.1]-1

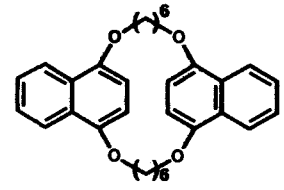


[2.2.2]-1

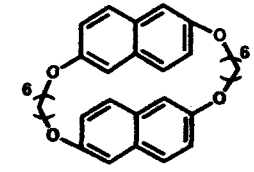
CHART VI

2. Cyclophanes

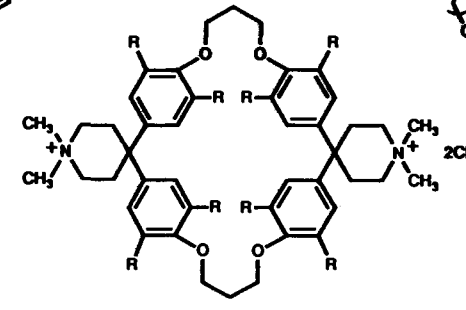
a. Monocyclic with Oxygen Donor Atoms



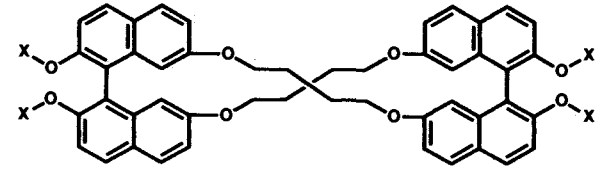
$Nap_2$24C4-1



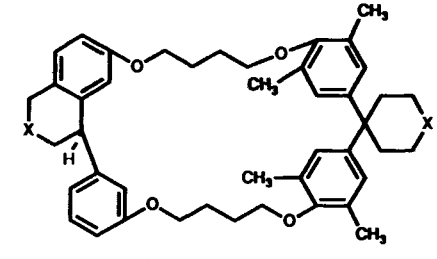
$Nap_2$28C4-1



$(1,4\text{-B})_4$28C4-1
R = H
$(1,4\text{-B})_4$28C4-2
R = OCH_3

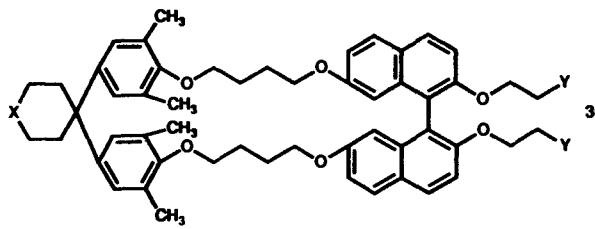


$Nap_4$28C4-1
X = $CH_2CH_2N(C_2H_5)_3^+$ Cl^-
(RR)

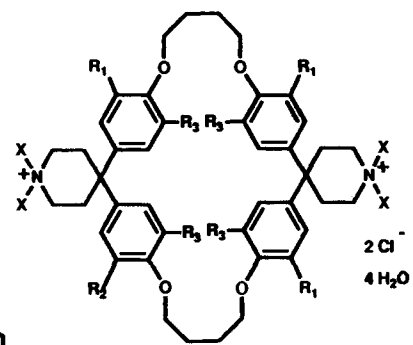


Isoquin28C4-1
X = NC_2H_5 (+)
Isoquin28C4-2
X = $N(C_2H_5)_2^+$ Cl^- (+)

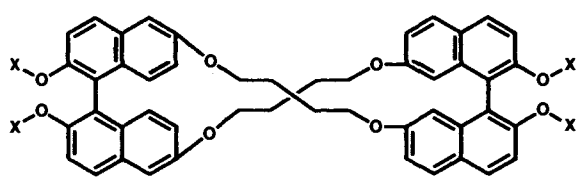
CHART VII
2. Cyclophanes (cont.)
a. Monocyclic with Oxygen Donor Atoms (cont.)



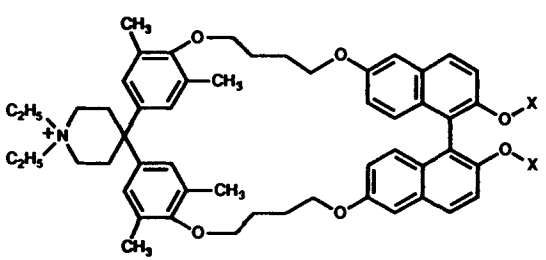
$Nap_2(1,4\text{-}B)_2$29C4-1
X = $N(C_2H_5)_2^+$;
Y = $N(C_2H_5)_3^+$ (S)
$Nap_2(1,4\text{-}B)_2$29C4-2
X = $N(C_2H_5)_2^+$;
Y = $N(C_2H_5)_3^+$ (R)
$Nap_2(1,4\text{-}B)_2$29C4-3
X = $N(C_2H_5)_2^+$;
Y = $N(C_2H_5)_3^+$
(racemic)



$(1,4\text{-}B)_4$30C4-1
R_1, R_2, R_3 = H; X = CH_3
$(1,4\text{-}B)_4$30C4-2
R_1, R_2, R_3 = CH_3; X = CH_3
$(1,4\text{-}B)_4$30C4-3
R_1, R_2, R_3 = OCH_3; X = CH_3
$(1,4\text{-}B)_4$30C4-4
R_1, R_3 = CH_3; R_2 = H; X = C_2H_5
$(1,4\text{-}B)_4$30C4-5
R_1, R_3 = CH_3; X = C_2H_5

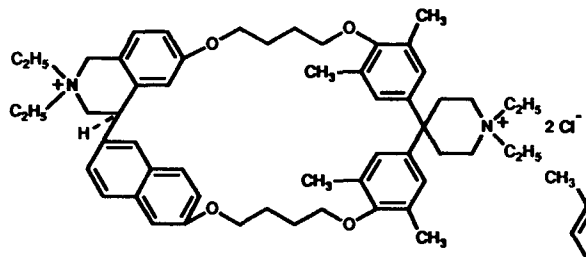


$Nap_4$30C4-1
X = $CH_2CH_2N(C_2H_5)_3^+$ Cl^-
(RR)

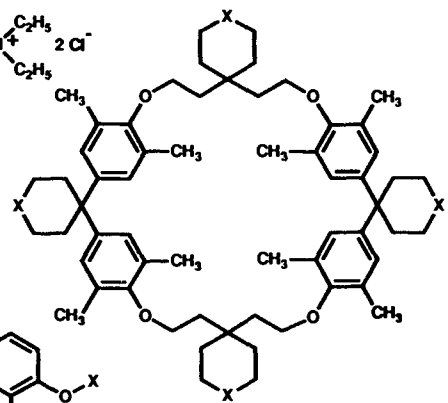


$Nap_2(1,4\text{-}B)_2$31C4-1
X = $CH_2CH_2N(C_2H_5)_3^+$ Cl^-
(R)

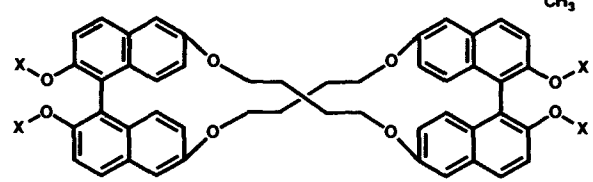
CHART VIII
2. Cyclophanes (cont.)
a. Monocyclic with Oxygen Donor Atoms (cont.)



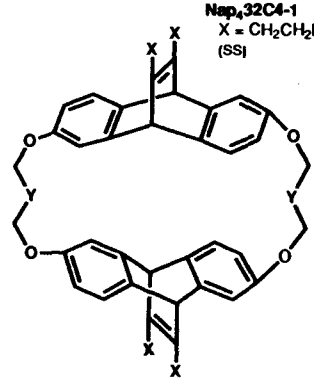
IsoquinNap31C4-1
isomer (S)
IsoquinNap31C4-2
isomer (R)



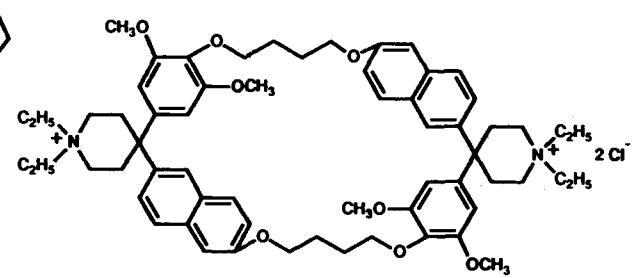
$(1,4\text{-}B)_4$32C4-1
X = NCH_3
$(1,4\text{-}B)_4$32C4-2
X = $N(CH_3)_2^+$ Cl^-



$Nap_4$32C4-1
X = $CH_2CH_2N(C_2H_5)_3^+$ Cl^-
(SS)

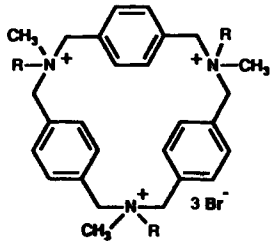


$(1,4\text{-}B)_2$32C4-1
X = CO_2CH_3; Y = 1,4-C_6H_4
$(1,4\text{-}B)_2$32C4-2
X = $CO_2^-Cs^+$; Y = 1,4-C_6H_4
$(1,4\text{-}Cy)_2$32C4-1
X = $CO_2^-Cs^+$;
Y = 1,4-cyclohexane

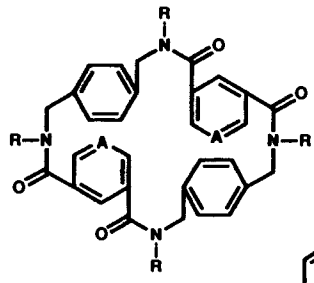


$Nap_2(1,4\text{-}B)_2$34C4-1

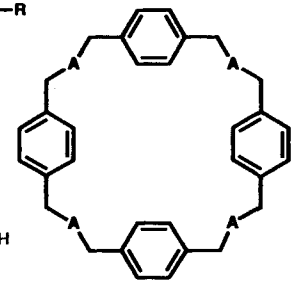
CHART IX
2. Cyclophanes (cont.)
b. Monocyclic with Nitrogen Donor Atoms



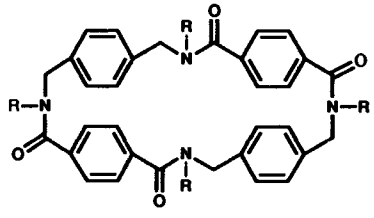
(1,4-B)$_3$N$_3$21C3-1
R = CH_2-[2,3-$(OH)_2$-4-CH_2N^+-$(CH_3)(C_{14}H_{29})_2C_6H_2$]
(1,4-B)$_3$N$_3$21C3-2
(1,4-B)$_3$N$_3$21C3-1 with coordinated Fe^{3+}



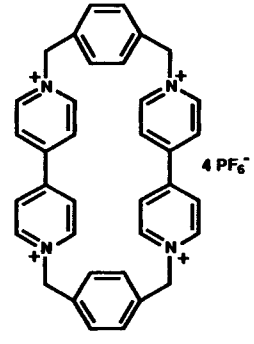
K$_4$Py$_2$(1,4-B)$_2$N$_4$28C4-1
A = N; R = $(CH_2)_{10}CO_2H$
K$_4$Py$_2$(1,4-B)$_2$N$_4$28C4-2
A = $NCH_3^+ I^-$; R = $(CH_2)_{10}CO_2H$



(1,4-B)$_4$N$_4$28C4-1
A = N-C(O)-[4-$CO_2HC_6H_4$]
(1,4-B)$_4$N$_4$28C4-2
A = N—C(O)CH_2
$(CH_3)_3N^+CH_2C(O)NHCHC(O)N(C_{14}H_{29})_2$ Br^-
(1,4-B)$_4$N$_4$28C4-3
A = N—C(O)
$(CH_3)_3N^+CH_2C(O)NHCHCH_2C(O)N(C_{14}H_{29})_2$ Br^-
(1,4-B)$_4$N$_4$28C4-4
A = NCH_2-[1,4-C_6H_4]-CH_2-$N(CH_3)CH_2C_6H_5$

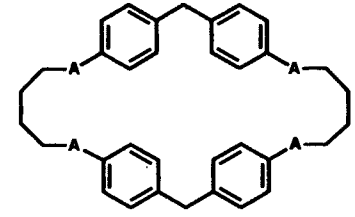


K$_4$(1,4-B)$_4$N$_4$28C4-1
R = $(CH_2)_2CO_2H$
K$_4$(1,4-B)$_4$N$_4$28C4-2
R = $(CH_2)_{10}CO_2H$
K$_4$(1,4-B)$_4$N$_4$28C4-3
R = $(CH_2)_{10}N(CH_3)_3^+$ Br^-
K$_4$(1,4-B)$_4$N$_4$28C4-4
R = $(CH_2)_{10}N(CH_3)_2^+$ I^-
K$_4$(1,4-B)$_4$N$_4$28C4-5
R = $(CH_2)_2C(O)NHCH[(CH_2)_4NH_3^+$ Cl^- $]$-$C(O)N(C_{14}H_{29})_2$
K$_4$(1,4-B)$_4$N$_4$28C4-6
R = $(CH_2)_2C(O)NH(CH_2)_4CH[NHC(O)$-$(CH_2)_5N(CH_3)_3^+$ Br^- $]C(O)N(C_{14}H_{29})_2$

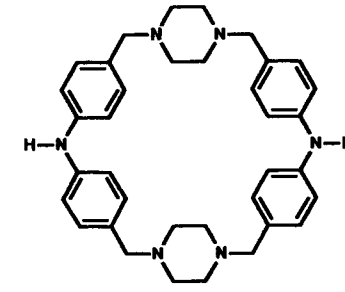


Py$_4$(1,4-B)$_2$28C4-1

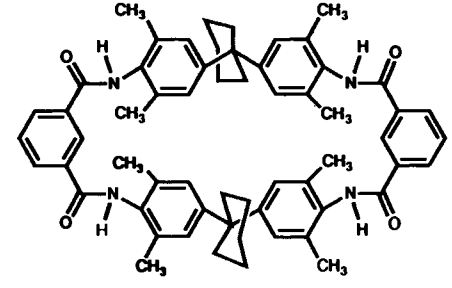
CHART X
2. Cyclophanes (cont.)
b. Monocyclic with Nitrogen Donor Atoms (cont.)



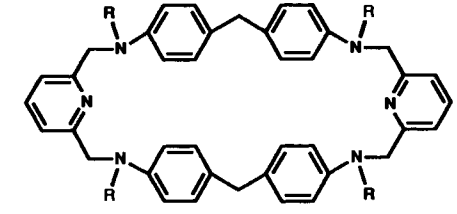
(1,4-B)$_4$N$_4$30C4-1
A = NH
(1,4-B)$_4$N$_4$30C4-2
A = $NH_2^+Cl^-$
(1,4-B)$_4$N$_4$30C4-3
A = $N(CH_3)_2^+Cl^-$



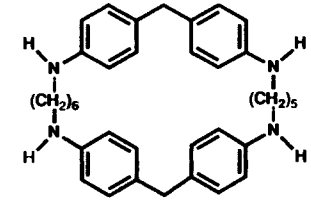
(1,4-B)$_4$N$_6$30C6-1



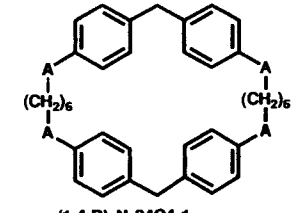
(1,4-B)$_4$(1,3-B)$_2$N$_4$32C4-1



Py$_2$(1,4-B)$_4$N$_4$32C6-1
R = $C(O)CH_2N(CH_3)_3^+$ Cl^-

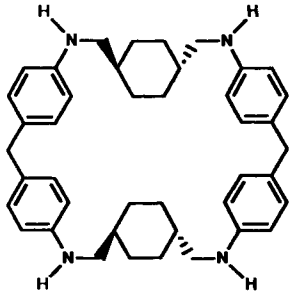


(1,4-B)$_4$N$_4$33C4-1

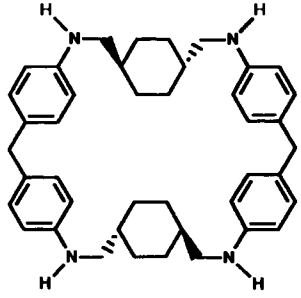


(1,4-B)$_4$N$_4$34C4-1
A = $N(CH_3)_2^+Cl^-$
(1,4-B)$_4$N$_4$34C4-2
A = N-SO_2-[3-SO_3^- C_6H_4]
(1,4-B)$_4$N$_4$34C4-3
A = N-CO-[2-CO_2^- C_6H_4]
(1,4-B)$_4$N$_4$34C4-4
A = NH or
A = N-[4-$SO_2C_6H_4CH_3$] or
A = $N(CH_3)_2^+Cl^-$

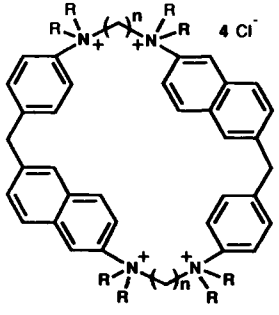
CHART XI
2. Cyclophanes (cont.)
b. Monocyclic with Nitrogen Donor Atoms (cont.)



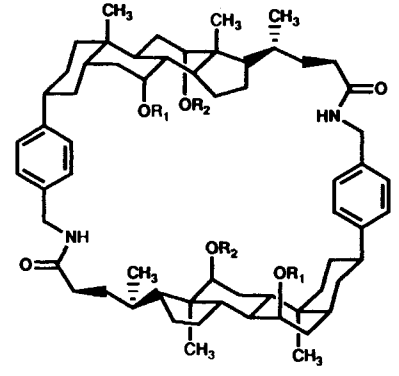
$Cy_2(1,4\text{-}B)_4N_434C4\text{-}1$



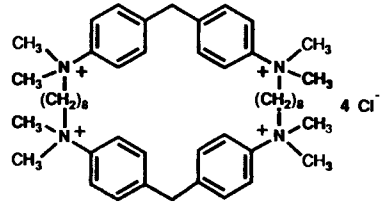
$Cy_2(1,4\text{-}B)_4N_434C4\text{-}2$



$Nap_2(1,4\text{-}B)_2N_434C4\text{-}1$
n = 4; R = H
$Nap_2(1,4\text{-}B)_2N_434C4\text{-}2$
n = 4; R = CH_3
$Nap_2(1,4\text{-}B)_2N_436C4\text{-}1$
n = 5; R = CH_3
$Nap_2(1,4\text{-}B)_2N_438C4\text{-}1$
n = 6; R = CH_3

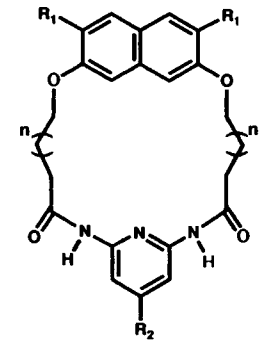


Cholaphane-1
R_1, R_2 = H
Cholaphane-2
R_1, R_2 = C(O)CH_3
Cholaphane-3
R_1 = C(O)CH_3; R_2 = $CH_2C_6H_5$
Cholaphane-4
R_1 = C(O)CH_3; R_2 = H
Cholaphane-5
R_1 = H; R_2 = $CH_2C_6H_5$

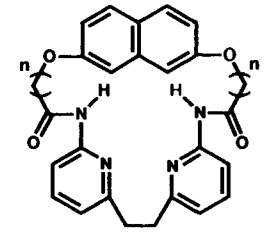


$(1,4\text{-}B)_4N_438C4\text{-}1$

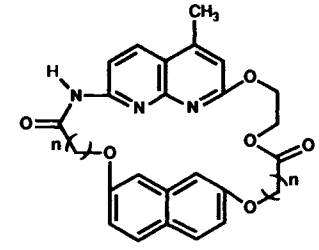
CHART XII
2. Cyclophanes (cont.)
c. Monocyclic with Various Donor Atoms



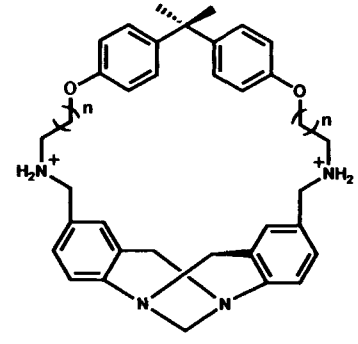
NapPyN20C5-1
n = 1; R_1, R_2 = H
NapPyN20C5-2
n = 1; R_1 = $CO_2C_3H_7$; R_2 = H
NapPyN20C5-3
n = 1; R_1 = OC_4H_9; R_2 = H
NapPyN20C5-4
n = 1; R_1 = H; R_2 = $OCH_2C{\equiv}CH$
NapPyN22C5-1
n = 2; R_1, R_2 = H



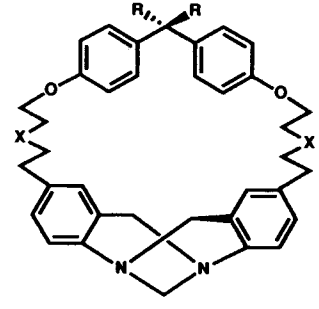
$NapPy_2N_223C6\text{-}1$
n = 2
$NapPy_2N_225C6\text{-}1$
n = 3



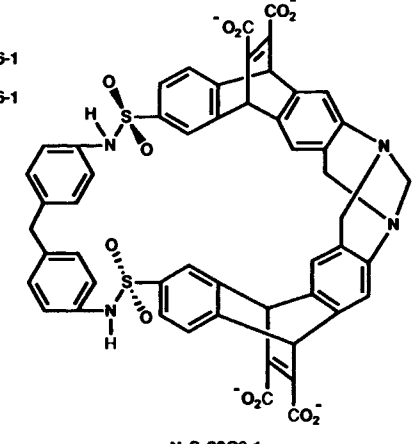
NapNaphthyrN23C7-1
n = 2
NapNaphthyrN25C7-1
n = 3



$(1,4\text{-}B)_4N_428C6\text{-}1$
n = 1
$(1,4\text{-}B)_4N_430C6\text{-}1$
n = 2

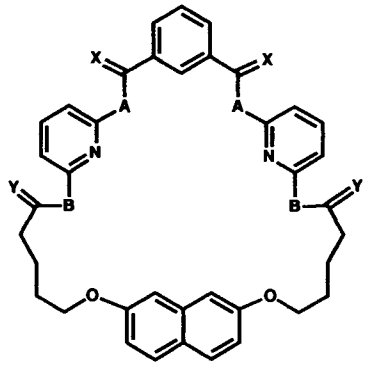


$(1,4\text{-}B)_4N_430C6\text{-}2$
R = H; X = NH
$(1,4\text{-}B)_4N_430C6\text{-}3$
R = CH_3; X = NH
$(1,4\text{-}B)_4N_430C6\text{-}4$
R = CH_3; X = NH_2^+

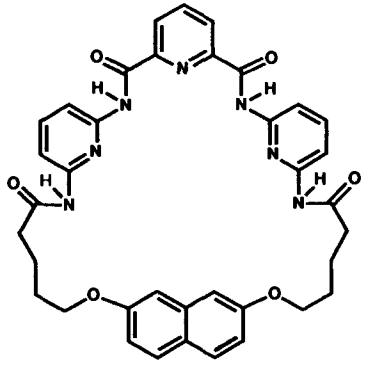


$N_4S_230C6\text{-}1$

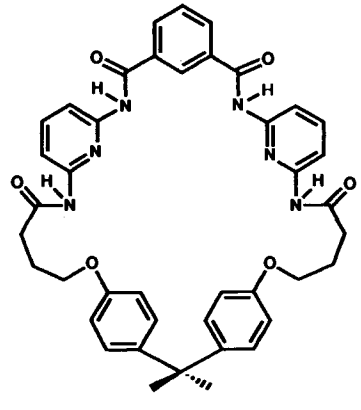
CHART XIII
2. Cyclophanes (cont.)
c. Monocyclic with Various Donor Atoms (cont.)



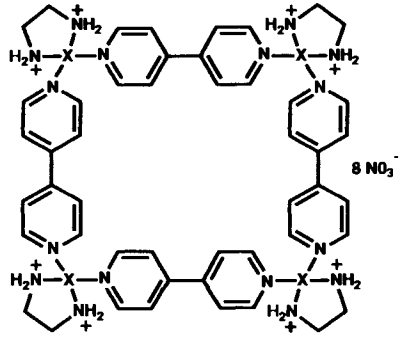
Nap(1,3-B)$Py_2N_2$32C8-1
A, Y = O; B = NH; X = H_2
Nap(1,3-B)$Py_2N_2$32C8-2
A = NH; B, X = O; Y = H_2
Nap(1,3-B)$Py_2N_4$32C8-1
A, B = NH; X, Y = O



$NapPy_3N_4$32C8-1

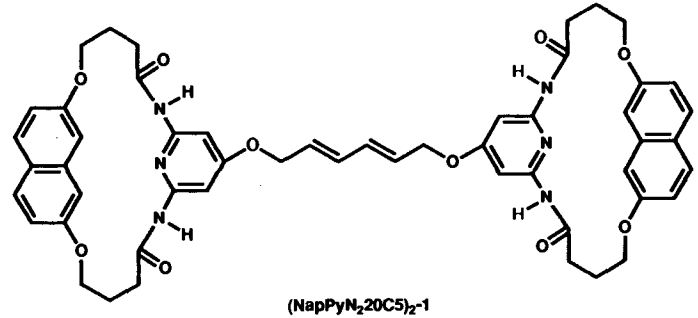


(1,3-B)(1,4-B)$_2Py_2N_4$34C8-1

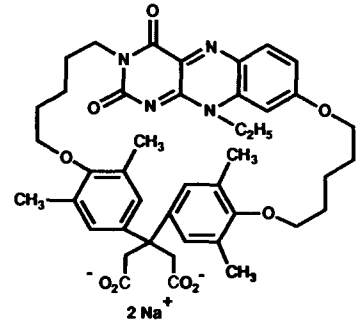


$Py_6Pd_4$36C4-1
X = Pd (III)
$Py_6Pt_4$36C4-1
X = Pt (II)

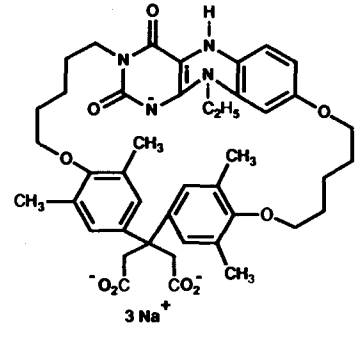
CHART XIV
2. Cyclophanes (cont.)
c. Monocyclic with Various Donor Atoms (cont.)



(NapPy$N_2$20C5)$_2$-1

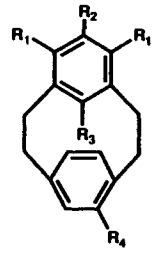


Flavinophane-1
(oxidized)

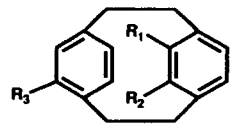


Flavinophane-2
(reduced)

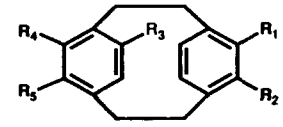
CHART XV
2. Cyclophanes (cont.)
d. Mono and Bicyclic without Heteroatoms



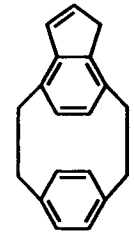
(1,3-B)(1,4-B)11C-1
R_1, R_4 = H; R_2, R_3 = t-C_4H_9
(1,3-B)(1,4-B)11C-2
R_1 = t-C_4H_9; R_2, R_3, R_4 = H
(1,3-B)(1,4-B)11C-3
R_1, R_3 = H; R_2, R_4 = t-C_4H_9



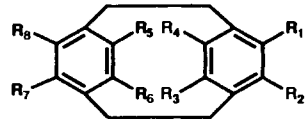
$(1,4\text{-B})_2$12C-1
R_1, R_2, R_3 = H
$(1,4\text{-B})_2$12C-2
R_1 = H; R_2, R_3 = i-C_3H_7
$(1,4\text{-B})_2$12C-3
R_1, R_3 = i-C_3H_7; R_2 = H
$(1,4\text{-B})_2$12C-4
R_1, R_2 = H; R_3 = t-C_4H_9
$(1,4\text{-B})_2$12C-5
R_1, R_2 = H; R_3 = $Si(CH_3)_3$



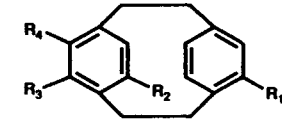
$(1,4\text{-B})_2$12C-6
R_1, R_5 = CH_3; R_2, R_3, R_4 = H
$(1,4\text{-B})_2$12C-7
R_1, R_2, R_4, R_5 = CH_3; R_3 = H
$(1,4\text{-B})_2$12C-8
R_1, R_2, R_4, R_5 = CH_3; R_3 = CHO
$(1,4\text{-B})_2$12C-9
R_1 = CHO; R_2, R_3, R_4, R_5 = H
$(1,4\text{-B})_2$12C-10
R_1, R_5 = CO_2CH_3; R_2, R_3, R_4 = H



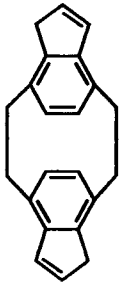
$(1,4\text{-B})_2$12C-32



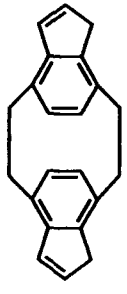
$(1,4\text{-B})_2$12C-11
R_1, R_3, R_6, R_8 = H;
R_2, R_4, R_5, R_7 = CH_3
$(1,4\text{-B})_2$12C-12
R_1, R_3, R_6 = H;
R_2, R_4, R_5, R_7, R_8 = CH_3
$(1,4\text{-B})_2$12C-13
R_1, R_2, R_5, R_7, R_8 = CH_3;
R_3, R_4, R_6 = H
$(1,4\text{-B})_2$12C-14
R_1, R_2, R_3, R_5, R_6, R_7,
R_8 = CH_3; R_4 = H
$(1,4\text{-B})_2$12C-15
R_1 = CHO; R_2, R_7, R_8 = H;
R_3, R_4, R_5, R_6 = CH_3



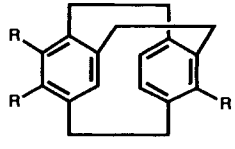
$(1,4\text{-B})_2$12C-16
R_1 = $CH{=}NC_6H_5$; R_2, R_3, R_4 = H
$(1,4\text{-B})_2$12C-17
R_1 = CH=N-[4-ClC_6H_4]; R_2, R_3, R_4 = H
$(1,4\text{-B})_2$12C-18
R_1 = CH=N-[4-$CH_3C_6H_4$]; R_2, R_3, R_4 = H
$(1,4\text{-B})_2$12C-19
R_1 = CH=N-[4-$OCH_3C_6H_4$]; R_2, R_3, R_4 = H
$(1,4\text{-B})_2$12C-20
R_1, R_2 = $CH{=}NC_6H_5$; R_3, R_4 = H
$(1,4\text{-B})_2$12C-21
R_1, R_2 = CH=N-[4-ClC_6H_4]; R_3, R_4 = H
$(1,4\text{-B})_2$12C-22
R_1, R_2 = CH=N-[4-$CH_3C_6H_4$]; R_3, R_4 = H
$(1,4\text{-B})_2$12C-23
R_1, R_2 = CH=N-[4-$OCH_3C_6H_4$]; R_3, R_4 = H
$(1,4\text{-B})_2$12C-24
R_1, R_3 = $CH{=}NC_6H_5$; R_2, R_4 = H
$(1,4\text{-B})_2$12C-25
R_1, R_3 = CH=N-[4-ClC_6H_4]; R_2, R_4 = H
$(1,4\text{-B})_2$12C-26
R_1, R_3 = CH=N-[4-$CH_3C_6H_4$]; R_2, R_4 = H
$(1,4\text{-B})_2$12C-27
R_1, R_3 = CH=N-[4-$OCH_3C_6H_4$]; R_2, R_4 = H
$(1,4\text{-B})_2$12C-28
R_1, R_4 = $CH{=}NC_6H_5$; R_2, R_3 = H
$(1,4\text{-B})_2$12C-29
R_1, R_4 = CH=N-[4-ClC_6H_4]; R_2, R_3 = H
$(1,4\text{-B})_2$12C-30
R_1, R_4 = CH=N-[4-$CH_3C_6H_4$]; R_2, R_3 = H
$(1,4\text{-B})_2$12C-31
R_1, R_4 = CH=N-[4-$OCH_3C_6H_4$]; R_2, R_3 = H



$(1,4\text{-B})_2$12C-33

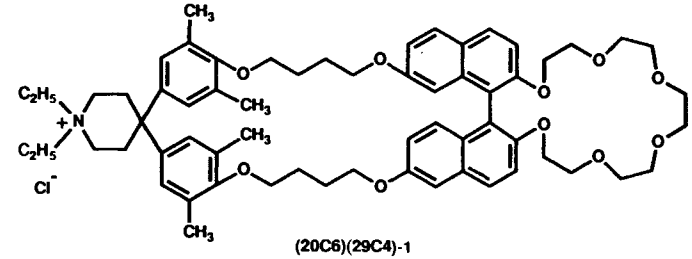


$(1,4\text{-B})_2$12C-34

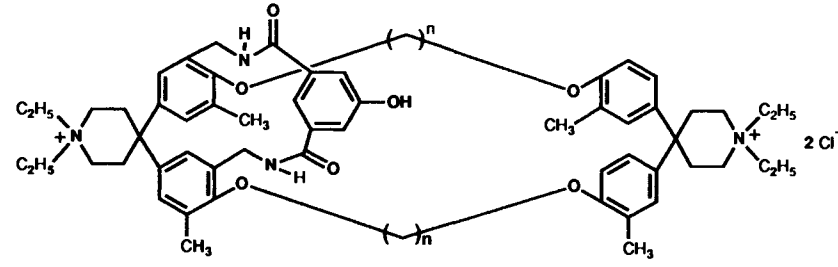


$(1,4\text{-B})_2$12C-35
R = H
$(1,4\text{-B})_2$12C-36
R = CH_3

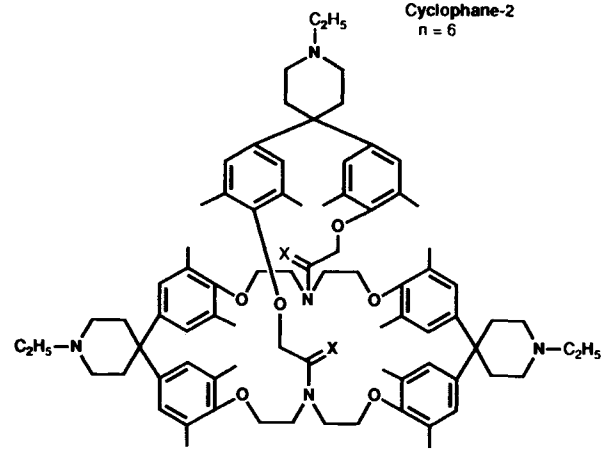
CHART XVI
2. Cyclophanes (cont.)
e. Polycyclic with Various Donor Atoms



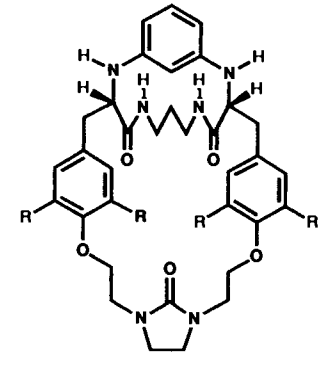
(20C6)(29C4)-1



Cyclophane-1
n = 4
Cyclophane-2
n = 6

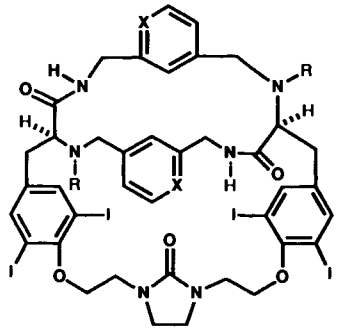


Cyclophane-3
$X = H_2$
Cyclophane-4
X = O

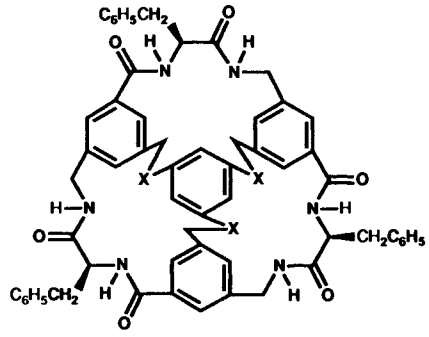


Cyclophane-5
R = I
Cyclophane-6
$R = NO_2$

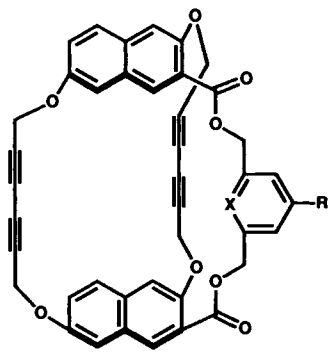
CHART XVII
2. Cyclophanes (cont.)
e. Polycyclic with Various Donor Atoms (cont.)



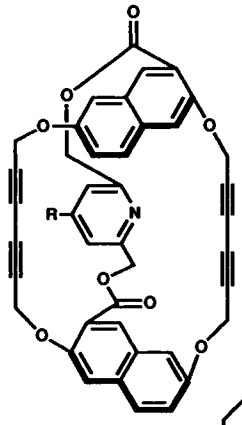
Cyclophane-7
R = $CH_2C_6H_5$; X = CH
Cyclophane-8
R = $CH_2C_6H_5$; X = N



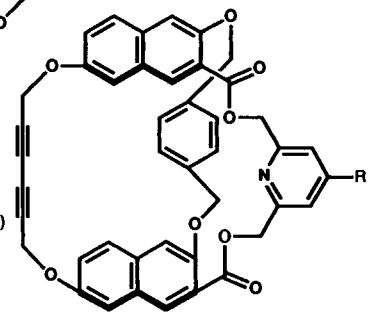
Cyclophane-9
X = O
Cyclophane-10
X = S



Cyclophane-11
X = N; R = H (meso)
Cyclophane-12
X = N; R = Cl (meso)
Cyclophane-13
X = N; R = $N(CH_3)_2$ (meso)
Cyclophane-14
X = N-oxide; R = H (meso)

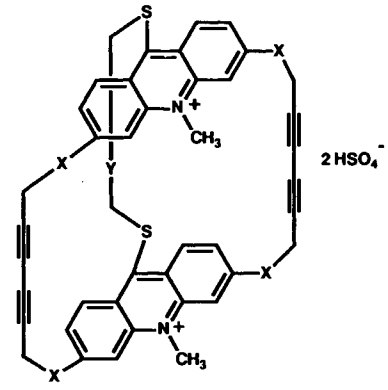


Cyclophane-15
R = H (dl)
Cyclophane-16
R = Cl (dl)
Cyclophane-17
R = $N(CH_3)_2$ (dl)

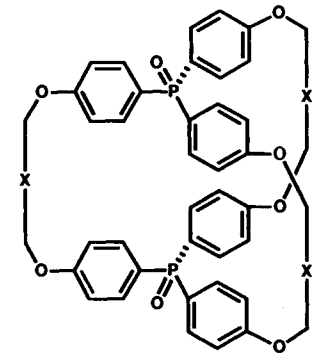


Cyclophane-18
R = H
Cyclophane-19
R = $N(CH_3)_2$

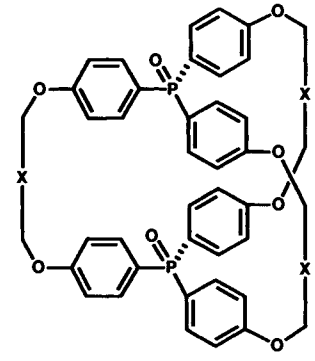
CHART XVIII
2. Cyclophanes (cont.)
e. Polycyclic with Various Donor Atoms (cont.)



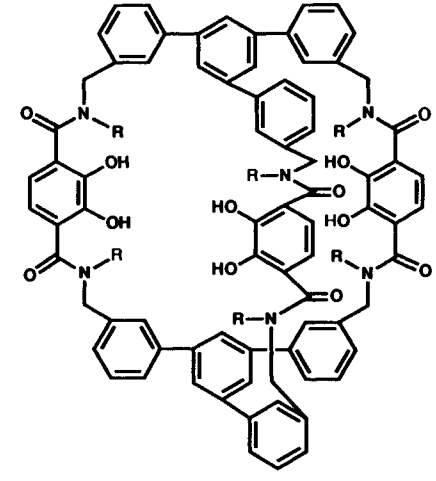
Cyclophane-20
X = O; Y = $(CH_2)_4$
Cyclophane-21
X = O; Y = CH_2OCH_2
Cyclophane-22
X = O; Y = $CH_2O(CH_2)_2OCH_2$
Cyclophane-23
X = NH; Y = CH_2OCH_2



Cyclophane-24
X = C≡C–C≡C
Cyclophane-25
X = $(CH_2)_4$

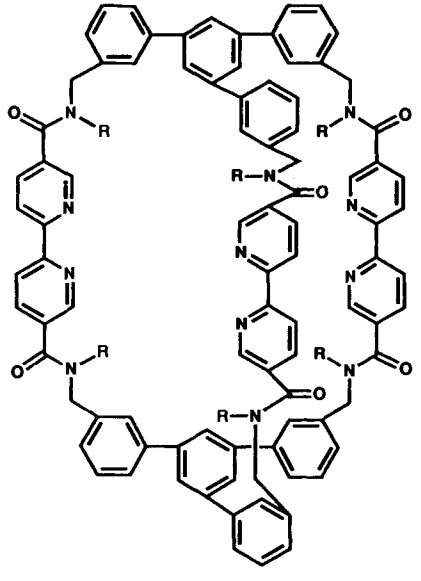


Cyclophane-26
X = C≡C–C≡C
Cyclophane-27
X = $(CH_2)_4$

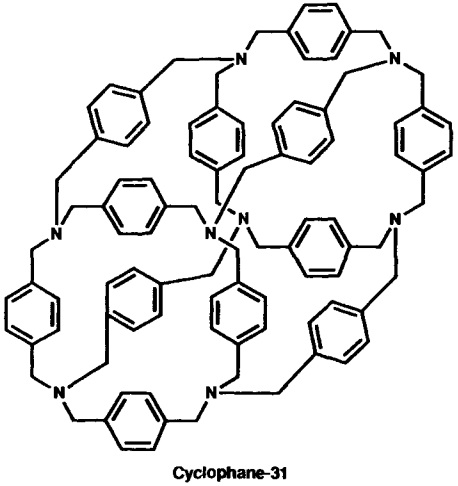


Cyclophane-28
R = $CH_2C_6H_5$

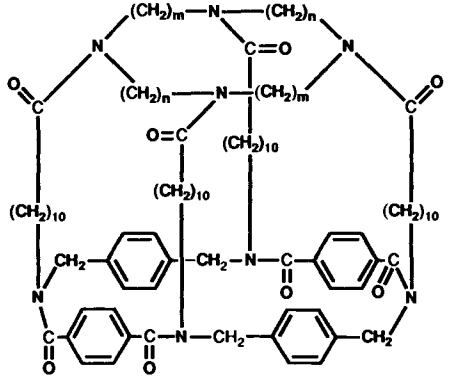
CHART XIX
2. Cyclophanes (cont.)
e. Polycyclic with Various Donor Atoms (cont.)



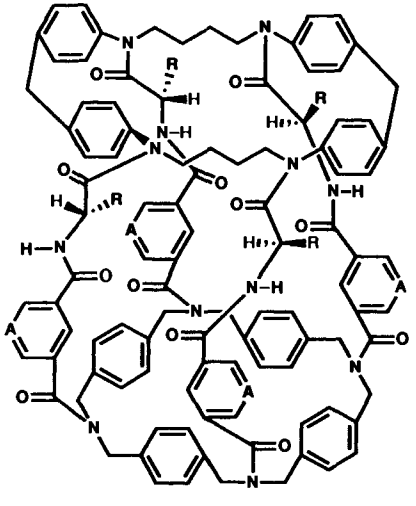
Cyclophane-29
R = $CH_2C_6H_5$



Cyclophane-31

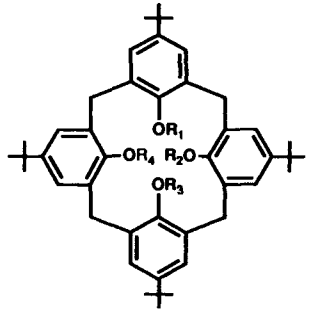


Cyclophane-30
m = 3; n = 2 or
m = 2; n = 3

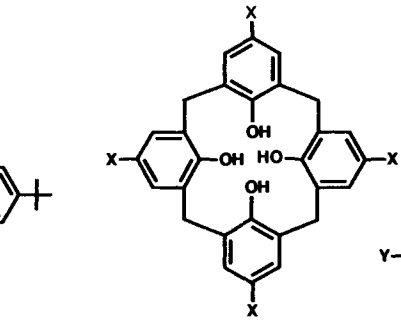


Cyclophane-32
A = N; R = $CH(CH_3)_2$
Cyclophane-33
A = NCH_3^+; R = $CH(CH_3)_2$

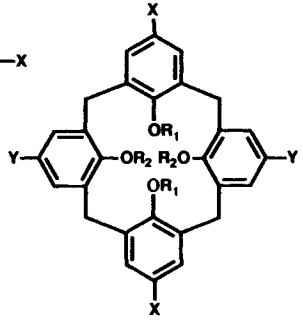
CHART XX
3. Calixarenes



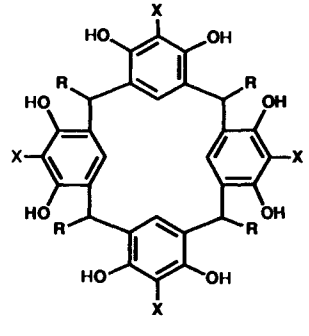
Calix4-16C-1
R_1, R_3 = H; R_2, R_4 = CH_3
Calix4-16C-2
R_1, R_2, R_3, R_4 = $(CH_2)_3SO_3Na$
Calix4-16C-3
R_1, R_2, R_3 = H;
R_4 = C(O)-[3,5-$(NO_2)_2C_6H_3$]
Calix4-16C-4
R_1, R_3 = H;
R_2, R_4 = C(O)-[3,5-$(NO_2)_2C_6H_3$]
Calix4-16C-5
R_1, R_3 = H;
R_2 = C(O)-[3,5-$(NO_2)_2C_6H_3$]
R_4 = CH_2-[3,5-$(NO_2)_2C_6H_3$]
Calix4-16C-6
R_1, R_3 = CH_3;
R_2, R_4 = $CH_2C(O)OCH_2$-[1-Pyrene]
Calix4-16C-7
R_1, R_3 = C_3H_7;
R_2, R_4 = $CH_2C(O)OCH_2$-[1-Pyrene]
Calix4-16C-8
R_1, R_3 = H;
R_2, R_4 =



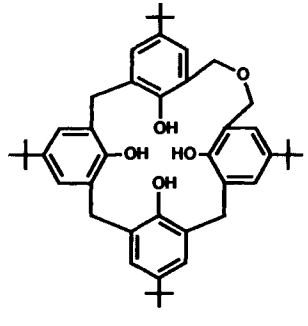
Calix4-16C-9
X = t-C_4H_9
Calix4-16C-10
X = $CH_2CH{=}CH_2$
Calix4-16C-11
4-toluenesulfonate of
Calix4-16C-10
Calix4-16C-12
X = $(CH_2)_2OH$
Calix4-16C-13
4-toluenesulfonate of
Calix4-16C-12
Calix4-16C-14
X = $(CH_2)_2CO_2H$
Calix4-16C-15
X = $CH_2N(CH_2CH{=}CH_2)_2$
Calix4-16C-16
X = —CH_2-N O



Calix4-16C-17
R_1 = H; R_2 = CH_3; X, Y = H
Calix4-16C-18
R_1 = H; R_2 = CH_3;
X = H; Y = t-C_4H_9
Calix4-16C-19
R_1, R_2 = C_4H_9;
X,Y = SO_3Na
Calix4-16C-20
R_1 = H;
R_2 = C(O)-[3,5-$(NO_2)_2C_6H_3$];
X = H; Y = t-C_4H_9

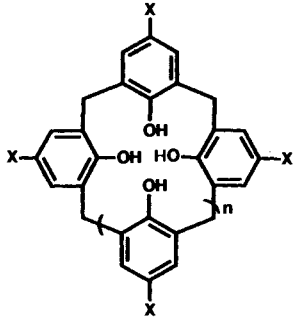


Calix4-16C-21
R = CH_3; X = H
Calix4-16C-22
R = $(CH_2)_{10}CH_3$; X = H
Calix4-16C-23
R = CH_3; X = N=N-[4-SO_3^- C_6H_4]

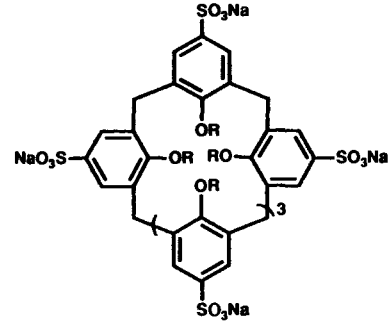


Calix4-18C-1

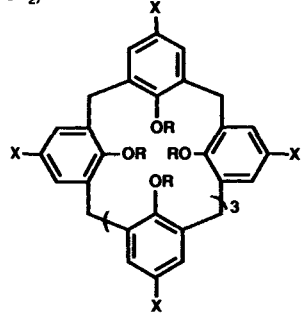
CHART XXI
3. Calixarenes (cont.)

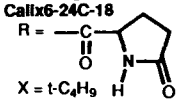


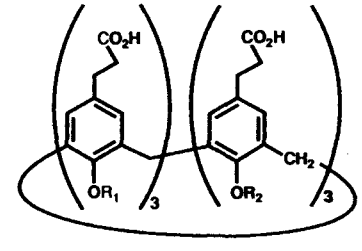
Calix5-20C-1
n = 2; X = $(CH_2)_2CO_2H$
Calix5-20C-2
n = 2; X = $CH_2N(CH_2CH{=}CH_2)_2$
Calix6-24C-1
n = 3; X = $(CH_2)_2CO_2H$
Calix6-24C-2
n = 3; X = $CH_2N(CH_2CH{=}CH_2)$
Calix6-24C-3
n = 3; X = SO_3Na
Calix6-24C-4
n = 3; X = SO_3^- M^+
(M^+ = H^+,Na^+, or NH_4^+)
Calix6-24C-5
n = 3; X = t-C_4H_9



Calix6-24C-6
R = CH_2CO_2H
Calix6-24C-7
R = CH_3
Calix6-24C-8
R = C_4H_9
Calix6-24C-9
R = C_6H_{13}
Calix6-24C-10
R = $C_{12}H_{25}$
Calix6-24C-11
R = $CH_2\underset{*}{C}H(CH_3)C_2H_5$

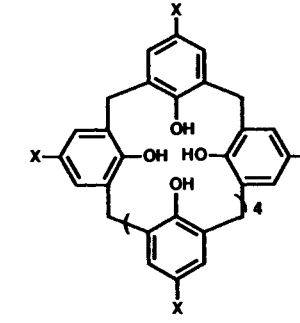


Calix6-24C-12
R = C_6H_{13}; X = SO_3^- M^+
(M^+ = H^+,Na^+, or NH_4^+)
Calix6-24C-13
R = $C_{12}H_{25}$; X = SO_3^- M^+
(M^+ = H^+,Na^+, or NH_4^+)
Calix6-24C-14
R = $(CH_2)_3SO_3Na$; X = C_4H_9
Calix6-24C-15
R = $(CH_2)_3SO_3Na$; X = t-C_4H_9
Calix6-24C-16
R = CH_2CO_2H; X = H
Calix6-24C-17
R = CH_2CO_2H; X = t-C_4H_9
Calix6-24C-18
R = 
X = t-C_4H_9

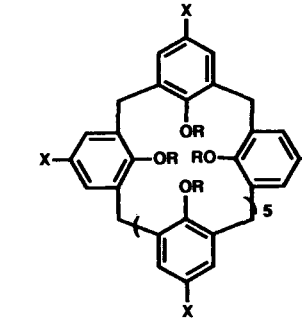


Calix6-24C-19
R_1, R_2 = CH_3
Calix6-24C-20
R_1 = H; R_2 = C_6H_{13}
Calix6-24C-21
R_1 = H; R_2 = CH_2CO_2H

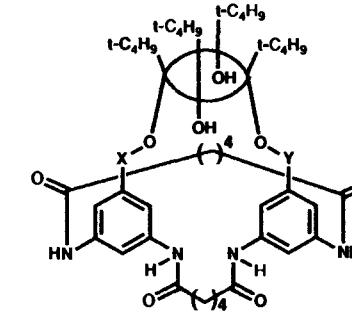
CHART XXII
3. Calixarenes (cont.)



Calix7-28C-1
X = $(CH_2)_2CO_2H$
Calix7-28C-2
X = $CH_2N(CH_2CH{=}CH_2)_2$

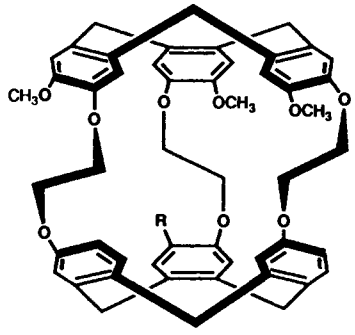


Calix8-32C-1
R = H; X = $(CH_2)_2CO_2H$
Calix8-32C-2
R = H; X = $CH_2N(CH_2CH{=}CH_2)_2$
Calix8-32C-3
R = CH_2CO_2H; X = H
Calix8-32C-4
R = C_4H_9; X = SO_3Na
Calix8-32C-5
R = $(CH_2)_3SO_3Na$; X = t-C_4H_9
Calix8-32C-6
R = $CH_2\underset{*}{C}H(CH_3)C_2H_5$; X = SO_3Na

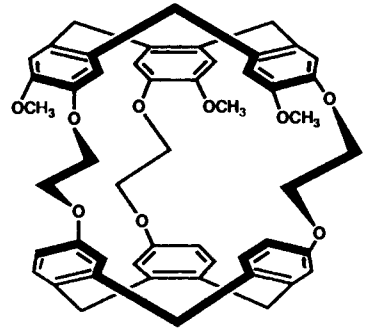


Double Calix-1
X, Y = CH_2
Double Calix-2
X, Y = C(O)
Double Calix-3
X = CH_2; Y = C(O)

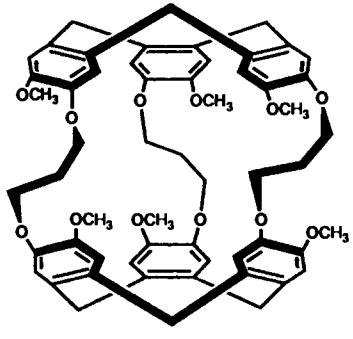
CHART XXIII
4. Cryptophanes



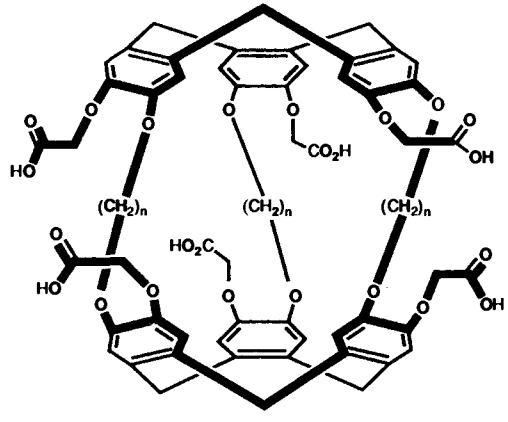
Cryptophane-1
R = H
Cryptophane-2
R = OCH_3



Cryptophane-3

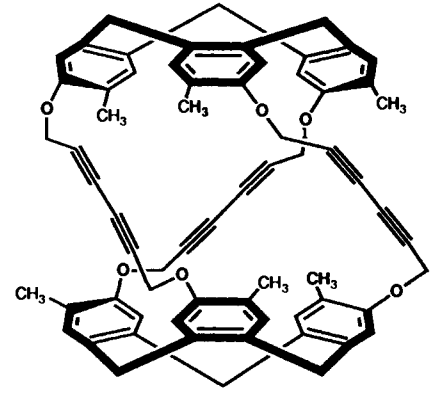


Cryptophane-4

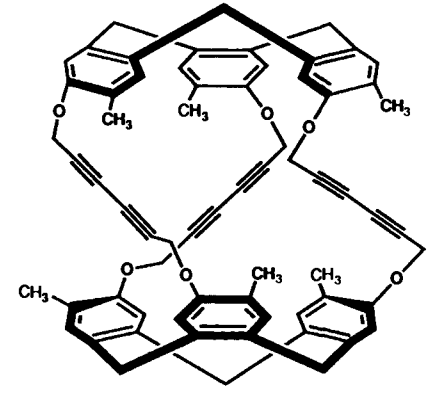


Cryptophane-5
n = 2
Cryptophane-6
n = 3

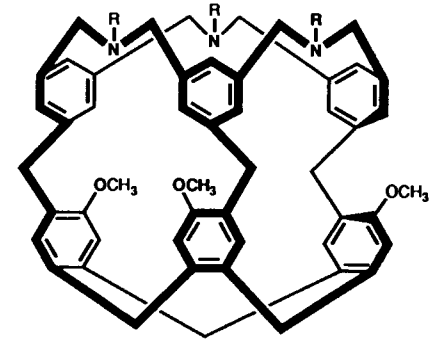
CHART XXIV
4.Cryptophanes (cont.)



Cryptophane-7
(±)

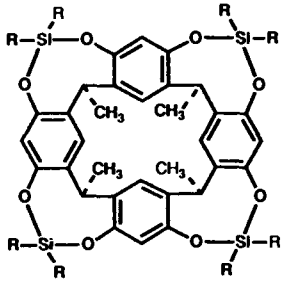


Cryptophane-8
(meso)

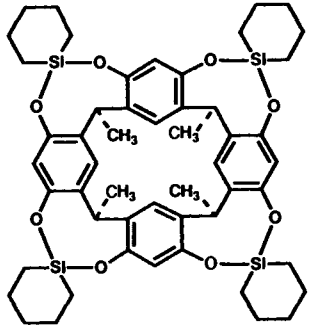


Cryptophane-9
R = H
Cryptophane-10
R = OTosyl

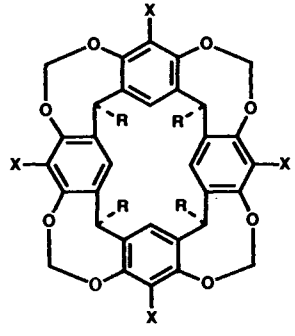
CHART XXV
5. Miscellaneous
a. Cavitands and Carcerands



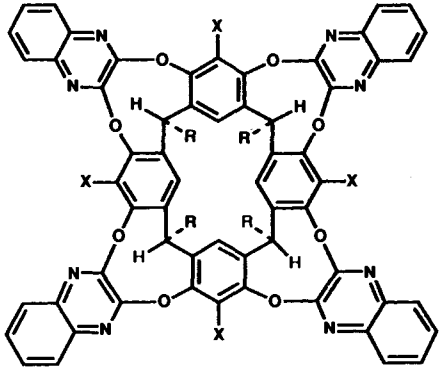
Cavitand-1
R = CH_3
Cavitand-2
R = C_2H_5



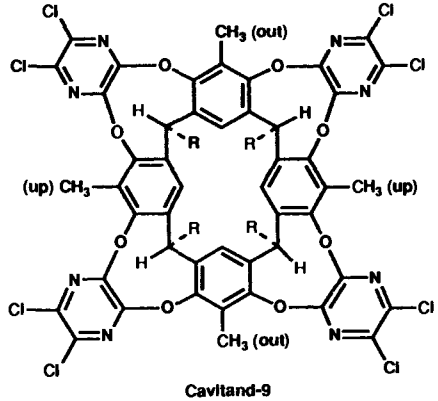
Cavitand-3



Cavitand-4
R = 4-$C_2H_5C_6H_4$;
X = $CH_2OC_4H_9$
(box-like cavity)
Cavitand-5
R = 4-$C_2H_5C_6H_4$;
X = $CH_2OC_4H_9$
(bowl-like cavity)

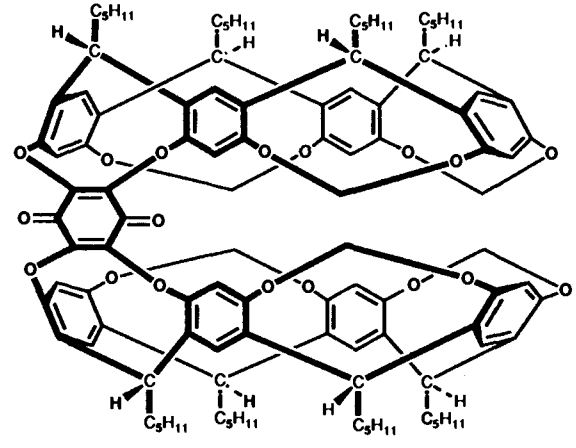


Cavitand-6
R = C_6H_{13}; X = H
Cavitand-7
R = C_5H_{11}; X = CH_3
Cavitand-8
R = C_5H_{11}; X = C_2H_5

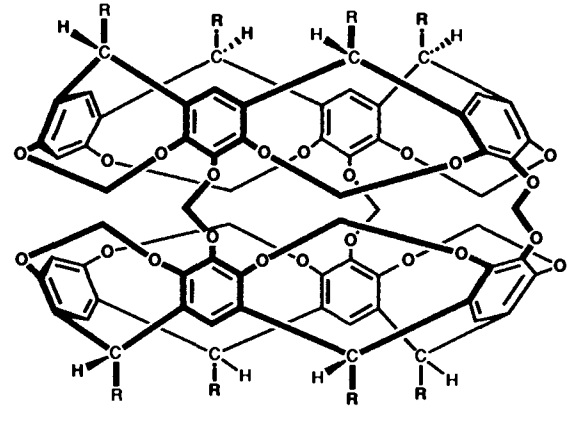


Cavitand-9
R = C_5H_{11}

CHART XXVI
5. Miscelaneous (cont.)
a. Cavitands and Carcerands (cont.)

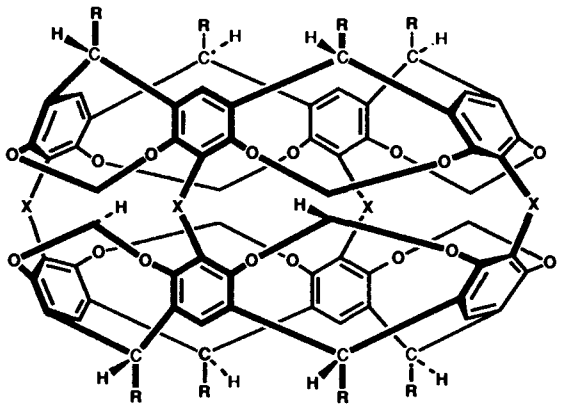


Cavitand-10



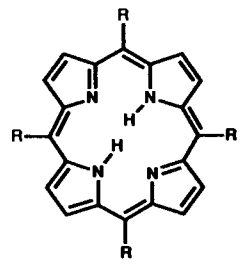
Carcerand-1
R = $(CH_2)_2C_6H_5$

CHART XXVII
5. Miscelaneous (cont.)
a. Cavitands and Carcerands (cont.)

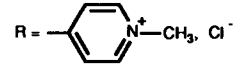


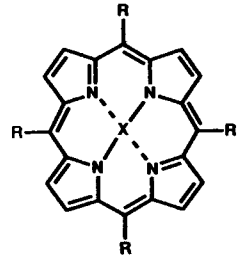
Carcerand-2
R = $CH_2CH_2C_6H_5$
X = CH_2SCH_2
Carcerand-3
R = $CH_2CH_2C_6H_5$
X = CH=N-[1,3-C_6H_4]-N=CH

CHART XXVIII
5. Miscelaneous (cont.)
b. Porphyrines and Porphyrin Derivatives

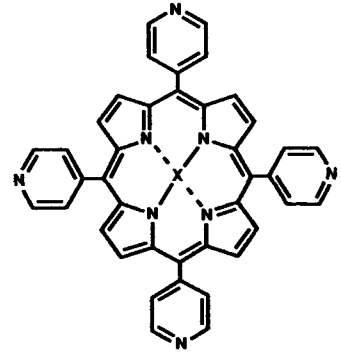


Porphyrin-1
R = C_6H_5
Porphyrin-2
R = 2-HOC_6H_4
Porphyrin-3
R = 3-HOC_6H_4
Porphyrin-4
R = 4-$CH_3C_6H_4$
Porphyrin-5
R = 2-$NH_2C_6H_4$
Porphyrin-6
R = 2-$NHCOCH_3C_6H_4$
Porphyrin-7
R = 4-$N^+(CH_3)_3C_6H_4$, Cl^-
Porphyrin-8



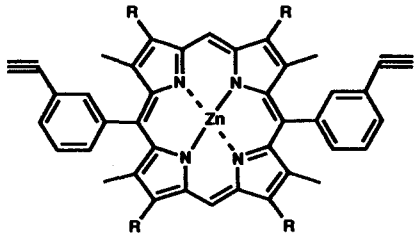


Porphyrin-9
R = C_6H_5; X = Mg(II)
Porphyrin-10
R = C_6H_5; X = Co(II)
Porphyrin-11
R = C_6H_5; X = Ni(II)
Porphyrin-12
R = C_6H_5; X = Cu(II)
Porphyrin-13
R = C_6H_5; X = Zn(II)
Porphyrin-14
R = C_6H_5; X = Cd(II)
Porphyrin-15
R = C_6H_5; X = Hg(II)
Porphyrin-16
R = 3-$CH_3C_6H_4$; X = Zn(II)
Porphyrin-17
R = 4-$CH_3C_6H_4$; X = Zn(II)
Porphyrin-18
R = 3-$OCH_3C_6H_4$; X = Zn(II)
Porphyrin-19
R = 4-$OCH_3C_6H_4$; X = Zn(II)
Porphyrin-20
R = 3-$CO_2CH_3C_6H_4$;
X = Zn(II)
Porphyrin-21
R = 3-FC_6H_4; X = Zn(II)
Porphyrin-22
R = 4-FC_6H_4; X = Zn(II)
Porphyrin-23
R = 3-ClC_6H_4; X = Zn(II)
Porphyrin-24
R = 4-ClC_6H_4; X = Zn(II)
Porphyrin-25
R = 3-BrC_6H_4; X = Zn(II)

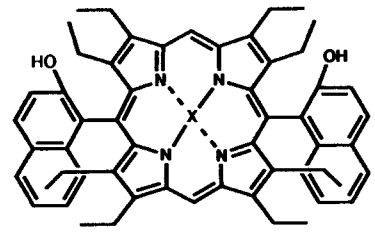


Porphyrin-26
X = VO(II)
Porphyrin-27
X = Mn(III)Cl
Porphyrin-28
X = Fe(III)Cl
Porphyrin-29
X = Ni(II)
Porphyrin-30
X = Cu(II)
Porphyrin-31
X = Zn(II)

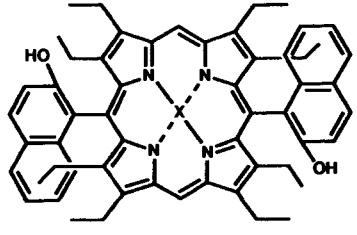
CHART XXIX
5. Miscelaneous (cont.)
b. Porphyrines and Porphyrin Derivatives (cont.)



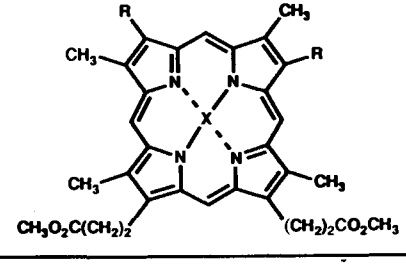
Porphyrin-32
R = C_2H_5
Porphyrin-33
R = $(CH_2)_2CO_2CH_3$



Porphyrin-34
X = 2H
Porphyrin-35
X = Rh(III)CH_2COCH_3

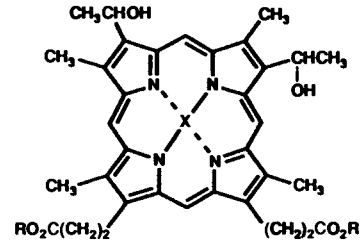


Porphyrin-36
X = 2H
Porphyrin-37
X = Rh(III)CH_2COCH_3

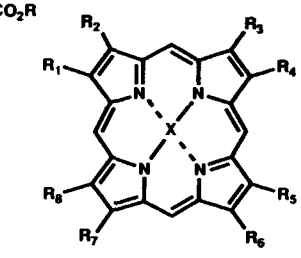


Porphyrin-38
R = H; X = Mg(II)
Porphyrin-39
R = H; X = Fe(II)
Porphyrin-40
R = H; X = Ni(II)
Porphyrin-41
R = $C(O)CH_3$; X = Fe(II)
Porphyrin-42
R = $C(O)CH_3$; X = Ni(II)
Porphyrin-43
R = CH_2=CH_2 ; X = Fe(II)
Porphyrin-44
R = CH=CH_2 ; X = Fe(II)
Porphyrin-45
R = CH=CH_2 ; X = Ni(II)
Porphyrin-46
R = C(O)OH; X = Ni(II)
Porphyrin-47
R = $C_2H_5OCO_2$-CH
X = Ni(II)
Porphyrin-48
R = Cl; X = Mg(II)
Porphyrin-49
R = NO_2; X = Mg(II)

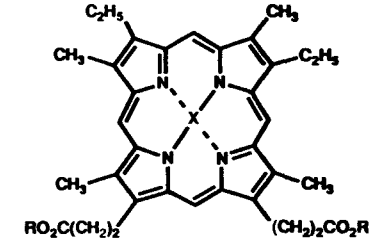
CHART XXX
5. Miscelaneous (cont.)
b. Porphyrines and Porphyrin Derivatives (cont.)



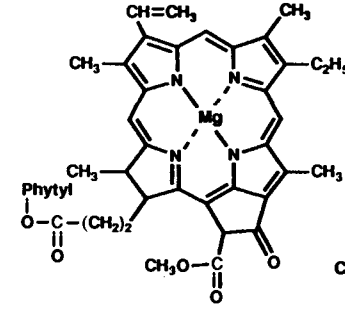
Porphyrin-50
R = H; X = Mn(III)Cl
Porphyrin-51
R = H; X = Fe(III)Cl
Porphyrin-52
R = H; X = Co(III)Cl
Porphyrin-53
R = CH_3; X =VO(II)
Porphyrin-54
R = CH_3; X = Ni(II)
Porphyrin-55
R = CH_3; X = Cu(II)
Porphyrin-56
R = CH_3; X = Zn(II)



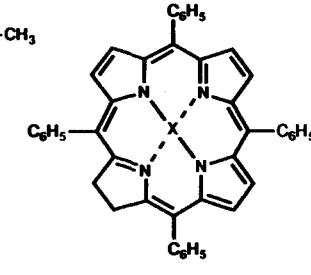
Porphyrin-66
R_1, R_3, R_5, R_7 = CH_3
R_2, R_4, R_6, R_8 = C_2H_5
X = VO(II)
Porphyrin-67
R_1, R_4, R_5, R_8 = CH_3
R_2, R_3, R_6, R_7 = C_2H_5
X = Mg(II)
Porphyrin-68
R_1, R_3, R_5, R_7 = CH_3
R_2, R_6 = C_2H_5
R_4, R_8 = $(CH_2)_2CO_2CH_3$
X = Zn(II)



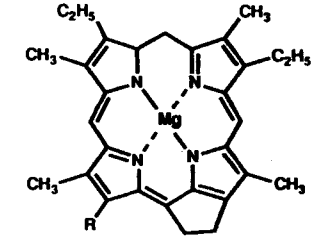
Porphyrin-57
R = H; X = Mn(II)
Porphyrin-58
R = H; X = Mn(III)
Porphyrin-59
R = H; X = Mn(III)Cl
Porphyrin-60
R = H; X = Zn(II)
Porphyrin-61
R = CH_3; X = Mg(II)
Porphyrin-62
R = CH_3; X = Fe(II)
Porphyrin-63
R = CH_3; X = Ni(II)
Porphyrin-64
R = CH_3; X = Cu(II)
Porphyrin-65
R = cholesteryl; X = Mg(II)



Porphyrin-69

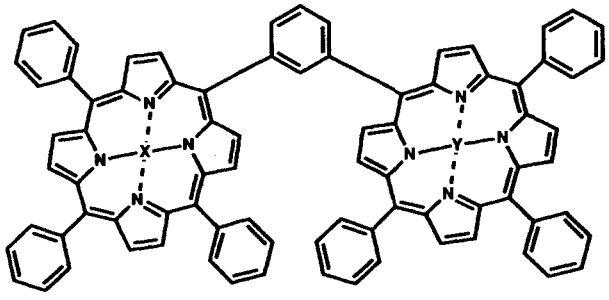


Porphyrin-71
X = Mg(II)
Porphyrin-72
X = Zn(II)

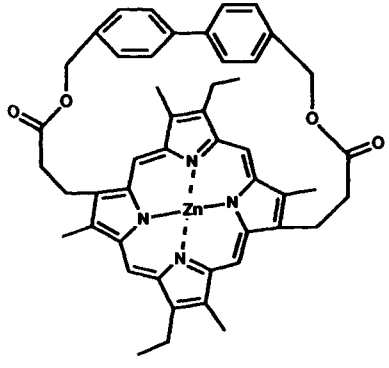


Porphyrin-70
R = $(CH_2)_2CO_2CH_3$

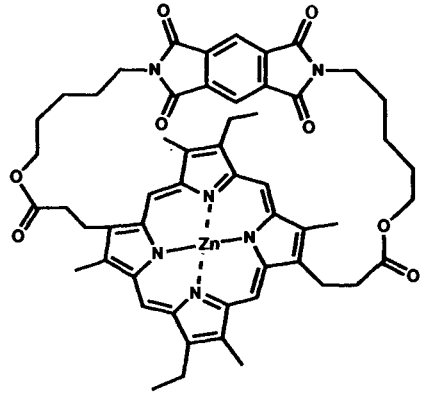
CHART XXXI
5. Miscelaneous (cont.)
b. Porphyrines and Porphyrin Derivatives (cont.)



Porphyrin-73
X, Y = Fe(II)
Porphyrin-74
X, Y = Co(II)
Porphyrin-75
X = 2H; Y = Zn(II)
Porphyrin-76
X, Y = Zn(II)

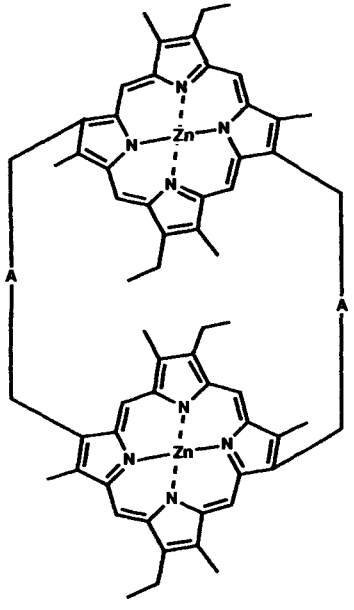


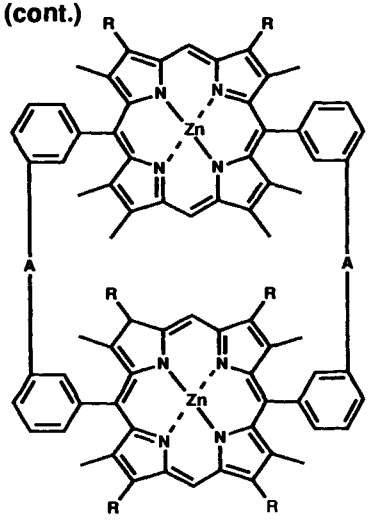
Porphyrin-77



Porphyrin-78

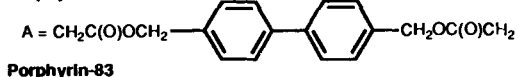
CHART XXXII
5. Miscelaneous (cont.)
b. Porphyrines and Porphyrin Derivatives (cont.)



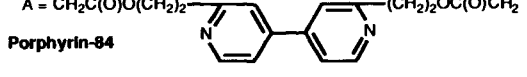


Porphyrin-85
R = C_2H_5
A = $OCH_2[1.3\text{-}C_6H_4]CH_2O$
Porphyrin-86
R = $(CH_2)_2CO_2CH_3$
A = C≡C—C≡C

Porphyrin-79
A = $CH_2C(O)O(CH_2)_2$
(isomer 1; syn or anti)
Porphyrin-80
A = $CH_2C(O)O(CH_2)_2$
(isomer 2; anti or syn)
Porphyrin-81
A = $CH_2C(O)O(CH_2)_2OC(O)CH_2$
(mixture of meso + racemic)
Porphyrin-82



Porphyrin-83



Porphyrin-84

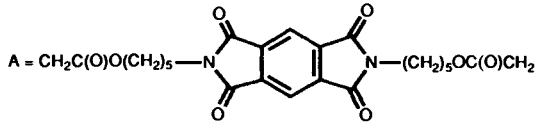
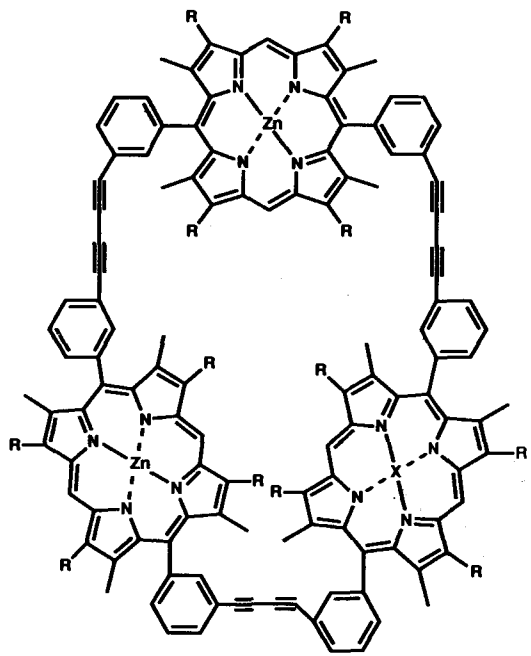
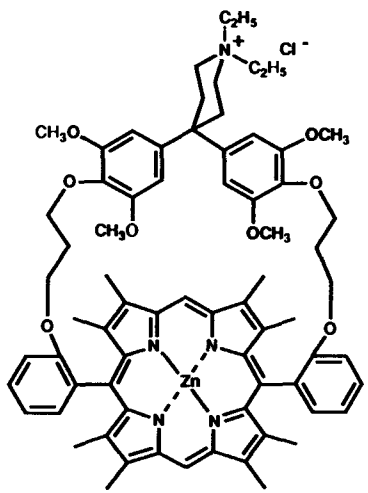


CHART XXXIII
5. Miscellaneous (cont.)
b. Porphyrin and Porphyrin Derivatives (cont.)

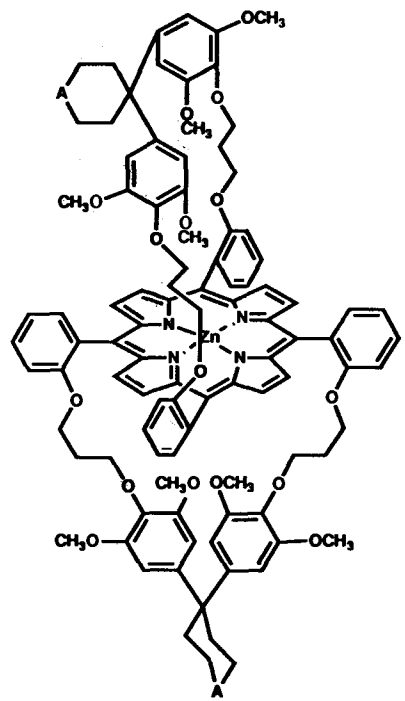


Porphyrin-87
R = C_2H_5; X = 2H
Porphyrin-88
R = C_2H_5; X = Zn(II)
Porphyrin-89
R = $(CH_2)_2CO_2CH_3$; X = Zn(II)

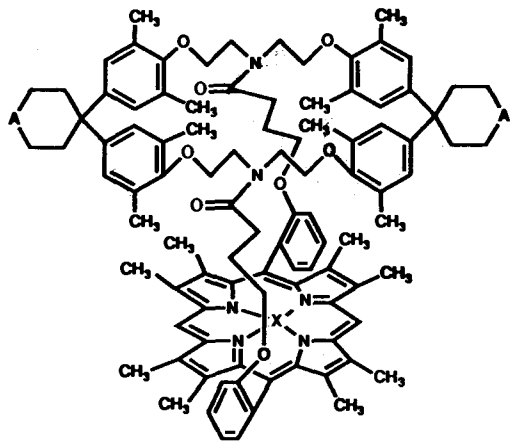


Porphyrin-90

CHART XXXIV
5. Miscellaneous (cont.)
b. Porphyrin and Porphyrin Derivatives (cont.)

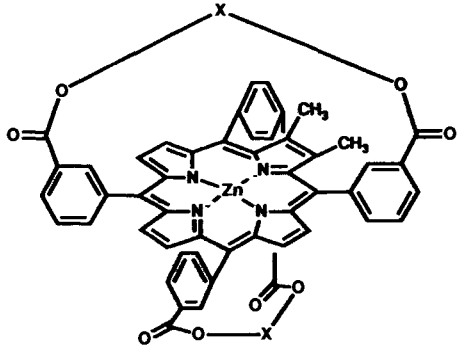


Porphyrin-91
A = $NC(O)CH_3$
Porphyrin-92
A = $N(C_2H_5)_2^+ Cl^-$



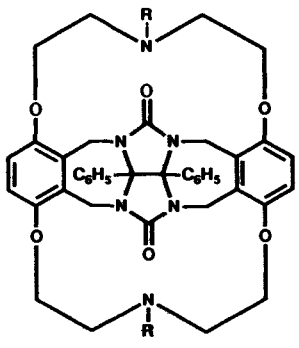
Porphyrin-93
A = NC_2H_5; X = 2H
Porphyrin-94
A = $NC_2H_5^+ Br^-$;
X = Fe-Br

CHART XXXV
5. Miscellaneous (cont.)
b. Porphyrin and Porphyrin Derivatives (cont.)

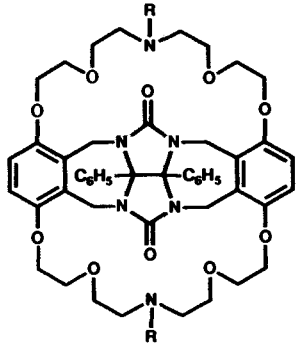


Porphyrin-95

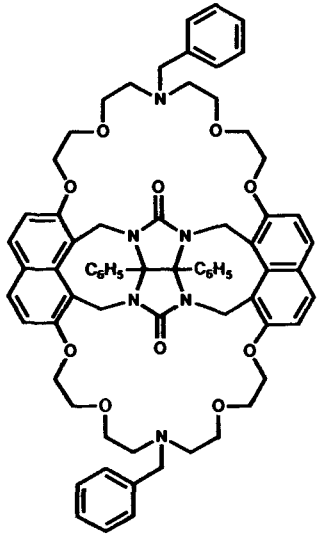
CHART XXXVI
5. Miscellaneous (cont.)
c. Other



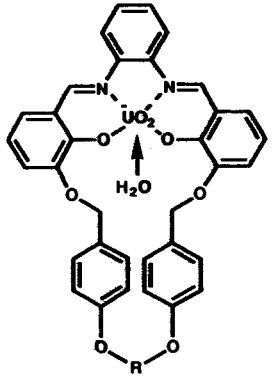
Other-1
R = H
Other-2
R = $CH_2C_6H_5$



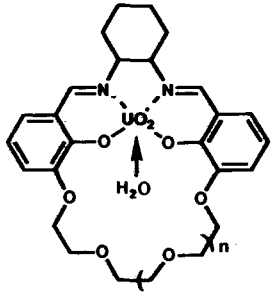
Other-3
R = H
Other-4
R = $CH_2C_6H_5$



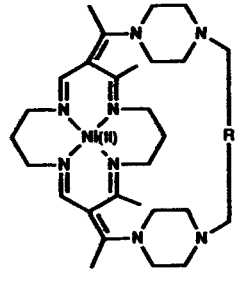
Other-5



Other-6
R = $(CH_2)_3$
Other-7
R = $(CH_2)_4$
Other-8
R = $(CH_2)_2O(CH_2)_2$

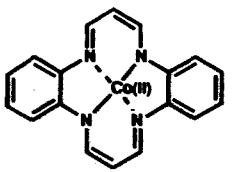


Other-9
n = 2
Other-10
n = 3
Other-11
n = 4
Other-12
n = 5

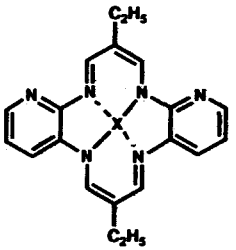


Other-13
R = 1,3-C_6H_4
Other-14
R = 1,4-C_6H_4
Other-15
R = 3,6-Durene
Other-16
R = 9,10-Anthracene

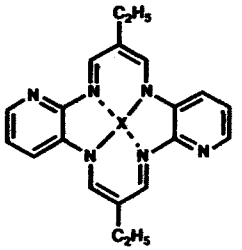
CHART XXXVII
5. Miscellaneous (cont.)
c. Other (cont.)



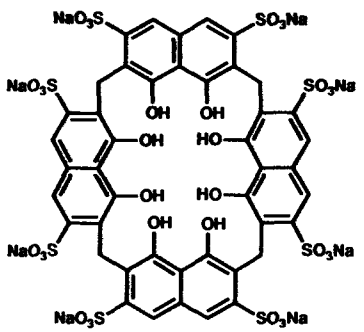
Other-17



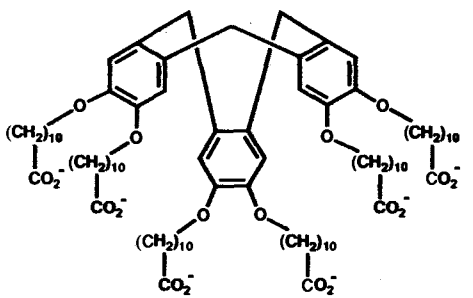
Other-18
X = Co(II)
Other-19
X = Co(III)CN



Other-20
X = Co(II)
Other-21
X = Co(III)CN

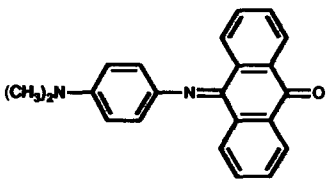


Other-22

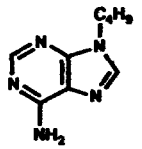


Other-23

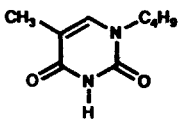
CHART XXXVIII
Organic Guests



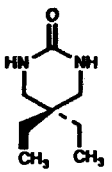
anthrol blue



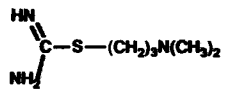
9-butyladednine



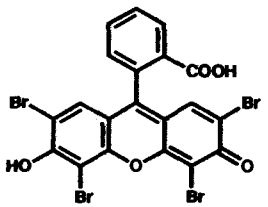
N-butylthymine



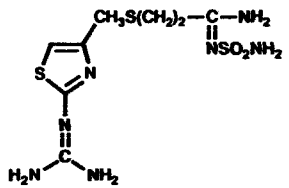
cyclic urea



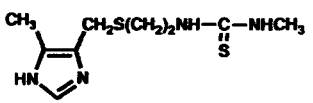
dimaprit



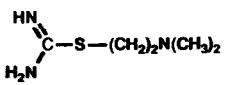
eosin



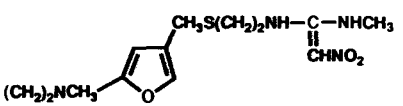
famotidine
(YM-11170)



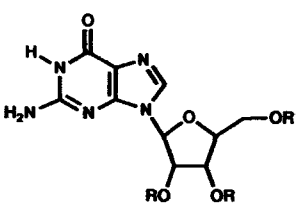
metiamide



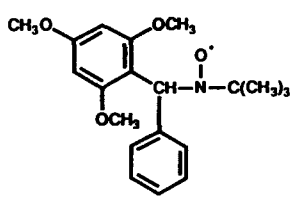
nordimaprit



ranitidine

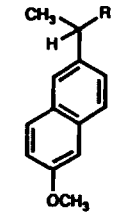


2',3',5'-tri-*O*-pentanoylguanosine
R = pentanoyl

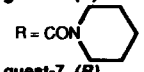


guest-1

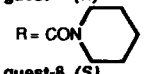
CHART XXXIX
Organic Guests (cont.)



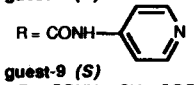
guest-2 *(S)*
R = COOH
guest-3 *(S)*
R = $COOCH_3$
guest-4 *(R)*
R = $COOCH_3$
guest-5 *(S)*
R = $CONH_2$
guest-6 *(S)*



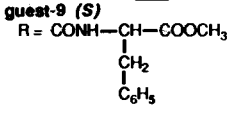
guest-7 *(R)*

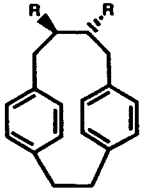


guest-8 *(S)*

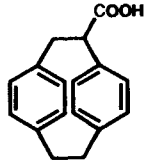


guest-9 *(S)*

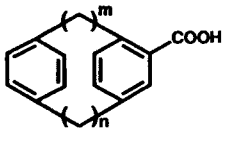




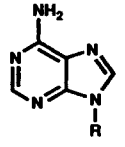
guest-10
R = COOH
guest-11
R = OH



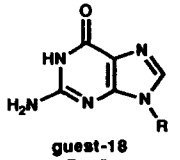
guest-12



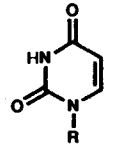
guest-13
m = n = 2
guest-14
m = n = 3
guest-15
m = 3; n = 4
guest-16
m = n = 4



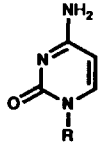
guest-17
R = ribose



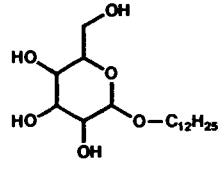
guest-18
R = ribose



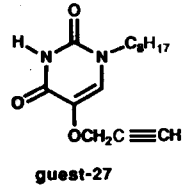
guest-19
R = ribose



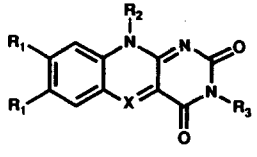
guest-20
R = ribose



guest-21

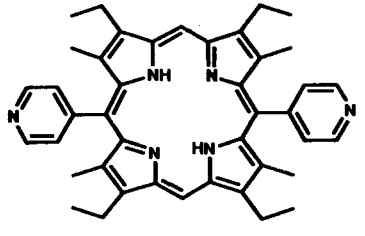


guest-27



guest-22
X = CH; R_1, R_3 = H; R_2 = C_6H_{13}
guest-23
X = CH; R_1 = H; R_2 = C_6H_{13}; R_3 = CH_3
guest-24
X = N; R_1, R_3 = H; R_2 = C_6H_{13}
guest-25
X = N; R_1 = H; R_2 = C_6H_{13}; R_3 = CH_3
guest-26
X = N; R_1 = CH_3;
R_2 = $CH_2(CHOH)_3CH_2(OH)$; R_3 = H

guest-28



guest-29

Nomenclature for CHARTS I-XXXIX

B - benzo, 18C6-1 - 18-crown-6, Calix - calixarene, Cy - cyclohexano, Isoquin - isoquinoline, K - keto, N - nitrogen (heteroatom), Nap - naphthalene, Naphthyr - naphthyridine, Py - pyridine, S - sulphur (heteroatom), Spher - spherand

VI. Tables I–III

Table I. Log K, ΔH, and ΔS Values for Neutral Molecule–Macrocycle Interaction in Solution

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
			Coronands and Cryptands					
			a. Crown Ethers					
12C4-1 (I)	Br_2	0.34	NMR			22	CCl_4/C_2H_5Br (3:1 v/v) (Br_2 competes with $CHCl_3$)	13, 1 (for conditions)
	I_2	0.36	Spec			25	CCl_4	14
	I_2	0.73	Spec	-17.4		25	cyclohexane	15
	I_2	0.68	Spec			30	cyclohexane	15
	ICl	ppt	Spec			25	CCl_4	14
	ICl	2.25	Cal	-26	-147	25	C_6H_6	16
	ICl	1.11(M_2L)	Cal	-26		25	C_6H_6 (M + ML <-> M_2L)	16
	Xe	-1.09	^{129}Xe NMR		53.7	31	$CDCl_3$	17
	tetrachloro-1,4-benzoquinone	0.06	Spec			25	CCl_4	18
	tetrafluoro-1,4-benzoquinone	0.76	Spec			25	CCl_4	18
12C4-2 (I)	ICl	2.45	Cal	-24	-115	25	C_6H_6	16
	ICl	1.76(M_2L)	Cal	-23		25	C_6H_6 (M + ML <-> M_2L)	16
B12C4-1 (I)	H_2O	0.35	NMR			30	$CHCl_3$	19
>$BS_2$12C4-1 (I)	I_2	1.89	Spec	-25	-29	25	CCl_4	20
$S_4$12C4-1 (I)	I_2	1.48	Spec			24	$CHCl_3$	21
$N_4$14C 4-1 (I)	I_2	5.01	Spec			24	CCl_4 ($2I_2$ + L -> $LI^+{\cdot}I_3^-$)	22
	I_2	4.51	Spec			24	$CHCl_3$ ($2I_2$ + L -> $LI^+{\cdot}I_3^-$)	22
	I_2	5.15	Spec			24	CH_2Cl_2 ($2I_2$ + L -> $LI^+{\cdot}I_3^-$)	22
	I_2	4.88	Spec			24	DCE ($2I_2$ + L -> $LI^+{\cdot}I_3^-$)	22
$N_4$14C4-2 (I)	ammonia	1.95	Kin			25	H_2O, 0.2 M $NaClO_4$ [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	ammonia	1.92	Spec			25	H_2O, 0.2 M $NaClO_4$ [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	aniline	0.73	Kin			25	H_2O, 0.2 M $NaClO_4$ [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	aniline	0.73	Spec			25	H_2O, 0.2 M $NaClO_4$ [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	dimethylamine	2.69	Kin			25	H_2O, 0.2 M $NaClO_4$ [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	dimethylamine	2.71	Spec			25	H_2O, 0.2 M $NaClO_4$ [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	ethylamine	2.62	Kin			25	H_2O, 0.2 M $NaClO_4$ [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	ethylamine	2.62	Spec			25	H_2O, 0.2 M $NaClO_4$ [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	methylamine	2.60	Kin			25	H_2O, 0.2 M $NaClO_4$ [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	methylamine	2.61	Spec			25	H_2O, 0.2 M $NaClO_4$ [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	piperidine	3.10	Kin			25	H_2O, 0.2 M $NaClO_4$ [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	piperidine	3.09	Spec			25	H_2O, 0.2 M $NaClO_4$ [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	pyridine	-0.10	Kin			25	H_2O, 0.2 M $NaClO_4$ [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	pyridine	-0.10	Spec			25	H_2O, 0.2 M $NaClO_4$ [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	trimethylamine	1.81	Kin			25	H_2O, 0.2 M $NaClO_4$ [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	trimethylamine	1.82	Spec			25	H_2O, 0.2 M $NaClO_4$ [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
$N_4$14C4-3 (I)	I_2	4.16	Spec			22	$CHCl_3$ ($2I_2$ + L -> $LI^+I_3^-$)	24
$S_4$14C4-1 (I)	I_2	1.92	Spec			24	$CHCl_3$	21
(1,3-B)15C4-1(I)	H_2O	0.90	NMR			22	$CDCl_3$	25
$N_4$15C4-1 (I)	I_2	3.78	Spec			22	$CHCl_3$ ($2I_2$ + L -> $LI^+I_3^-$)	24
15C5-1 (I)	H_2O		IR	-11.7		25	CCl_4	26
	H_2O	0.70	NMR			30	$CHCl_3$	27
	Br_2	-0.10	NMR			22	CCl_4/C_2H_5Br (3:1 v/v), (Br_2 competes with $CHCl_3$)	13, 1 (for conditions)
	I_2	0.34	Spec			25	CCl_4	14
	I_2	0.68	Spec			25	cyclohexane	15
	I_2	0.59	Spec	-12.4	-28.9	35	cyclohexane	15
	I_2	0.54	Spec			45	cyclohexane	15
	ICl	2.03	Spec			25	CCl_4	14
	ICl	2.04	Cal	-27	-176	25	C_6H_6	16
	ICl	1.69(M_2L)	Cal	-26		25	C_6H_6 (M + ML <-> M_2L)	16
	ICl	1.20(M_3L)	Cal	-17		25	C_6H_6 (M + M_2L <-> M_3L)	16
	Xe	-1.09	^{129}Xe NMR		53.7	31	$CDCl_3$	17
	eosin[e]	0.43	Spec			25	H_2O	28
	eosin[e]	2.50	Spec			25	MeOH	28
	methanol		IR	-15.1		25	CCl_4	26
	phenol	1.96	IR	-23.8	-42.3	25	CCl_4	26
	tetrachloro-1,4-benzoquinone	0.10	Spec			25	CCl_4	18
	2,3,5,6-tetracyanopyrazine	~-1.0	Spec			25	CH_2Cl_2	29
	tetrafluoro-1,4-benzoquinone	0.77	Spec			25	CCl_4	18
	tetrafluoro-1,4-benzoquinone	-0.538	NMR			31.6	$CDCl_3$	30
B15C5-1 (I)	H_2O	0.46	NMR			30	$CHCl_3$	19
	ICl	1.56	Cal	-25	-183	25	C_6H_6	16
	ICl	1.18(M_2L)	Cal	-24		25	C_6H_6 (M + ML <-> M_2L)	16
	2,3-dichloro-5,6-dicyano-1,4-benzoquinone	0.81	Spec			11.5	CH_2Cl_2	31
	2,3-dichloro-5,6-dicyano-1,4-benzoquinone	0.61	Spec	-26.8	-82.0	17	CH_2Cl_2	31
	2,3-dichloro-5,6-dicyano-1,4-benzoquinone	0.41	Spec			25	CH_2Cl_2	31
	2-dicyanoethylene-1,3-indandione	0.20	Spec			3	CH_2Cl_2	32
	2-dicyanoethylene-1,3-indandione	-0.14	Spec	-16.4	-69.0	12	CH_2Cl_2	32
	2-dicyanoethylene-1,3-indandione	-0.30	Spec			25	CH_2Cl_2	32
	9-dicyanomethylene-2,4,7-trinitro-fluorene	0.18	Spec			4	CH_2Cl_2	33
	9-dicyanomethylene-2,4,7-trinitro-fluorene	-0.10	Spec			11	CH_2Cl_2	33
	9-dicyanomethylene-2,4,7-trinitro-fluorene	-0.40	Spec	-16.68	-63.4	25	CH_2Cl_2	33
	picric acid	0.211	NMR			21	$CDCl_3$	34
	tetracyanoethylene	-0.040	Spec			10	CH_2Cl_2	35
	tetracyanoethylene	0.123	Spec			22	CH_2Cl_2	35
	tetracyanoethylene	0.170	Spec			32	CH_2Cl_2	35
	tetracyanoethylene		Spec	8.46	26.3	10-32	CH_2Cl_2	35
	2,3,5,6-tetracyanopyrazine	0.63	Spec			1	CH_2Cl_2	29
	2,3,5,6-tetracyanopyrazine	0.48	Spec			11.5	CH_2Cl_2	29
	2,3,5,6-tetracyanopyrazine	0.18	Spec	-21.3	-68.1	25	CH_2Cl_2	29

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	tetrafluoro-1,4-benzoquinone	-0.208	NMR			31.6	$CDCl_3$	30
	2,4,5,7-tetranitro-9-fluorenone	0.46	Spec			4	CH_2Cl_2	33
	2,4,5,7-tetranitro-9-fluorenone	0.39	Spec			11	CH_2Cl_2	33
	2,4,5,7-tetranitro-9-fluorenone	0.20	Spec	-12.1	-36.6	25	CH_2Cl_2	33
	1,3,5-trinitro-benzene	-0.199	NMR	-12.1	-43.5	31.5	$CDCl_3$	36
	1,3,5-trinitro-benzene	-0.289	NMR			50	$CDCl_3$	36
	2,4,7-trinitro-9-fluorenone	0.37	Spec			4	CH_2Cl_2	33
	2,4,7-trinitro-9-fluorenone	0.30	Spec			11	CH_2Cl_2	33
	2,4,7-trinitro-9-fluorenone	-0.22	Spec	-14.8	-54	25	CH_2Cl_2	33
	2,4,6-trinitro-toluene	-0.585	NMR	-13.17	-42.1	30	DCE	37
	urea	none	Polg			25	MeOH, 0.1 M Et_4NI (Rb as indicator)	38
B15C5-2 (I)	picric acid	0.211	NMR			21	$CDCl_3$	34
B15C5-3 (I)	picric acid	0.128	NMR			21	$CDCl_3$	34
B15C5-4 (I)	picric acid	0.232	NMR			21	$CDCl_3$	34
B15C5-5 (I)	picric acid	0.045	NMR			21	$CDCl_3$	34
B15C5-6 (I)	picric acid	0.034	NMR			21	$CDCl_3$	34
B15C5-7 (I)	picric acid	0.176	NMR			21	$CDCl_3$	34
B15C5-8 (I)	picric acid	0.127	NMR			21	$CDCl_3$	34
B15C5-9 (I)	picric acid	0.069	NMR			21	$CDCl_3$	34
B15C5-10 (I)	picric acid	0.208	NMR			21	$CDCl_3$	34
B15C5-11 (I)	picric acid	1.30	NMR			21	$CDCl_3$	34
B15C5-12 (I)	picric acid	1.61	NMR			21	$CDCl_3$	34
Py15C5-1 (I)	malononitrile	1.20	NMR	-26.4	-66.0	25	C_6D_6	7, 39
	malononitrile	1.04	NMR	-6.69	-2.81	25	$CDCl_3$	7, 39
$S_2$15C5-1 (I)	I_2	2.24	Spec	-30.5	-40	25	CCl_4	20
$BS_2$15C5-1 (II)	I_2	1.93	Spec	-22	-18	25	CCl_4	20
$S_4$16C4-1 (II)	I_2	1.51	Spec			24	$CHCl_3$	21
$K_4N_2$17C5-1 (II)	H_2O	1.30	NMR			22	$CDCl_3$	40
(1,3-B)18C5-1 (II)	H_2O	1.15	NMR			22	$CDCl_3$	25
	malononitrile	1.04	NMR	-21.8	-53.4	25	$CDCl_3$	39, 41
	malononitrile	1.00	NMR	-19.7	-46.3	25	C_6D_6	39, 41
	nitromethane	-0.03	NMR			9	C_6D_6	42
	nitromethane	-0.12	NMR			17	C_6D_6	42
	nitromethane	-0.21	NMR			27	C_6D_6	42
	nitromethane	-0.28	NMR			36	C_6D_6	42
	nitromethane	(ML)	NMR	-15.1	-54.4	9-36	C_6D_6	42
(1,3-B)18C5-2 (II)	malononitrile	1.04	NMR	-7.95	-7.02	25	C_6D_6	7, 39, 41
	urea	-0.39	Pot			25	H_2O	43
(1,3-B)18C5-3 (II)	malononitrile	1.59	NMR	-50.2	-139	25	C_6D_6	7, 39, 41
(1,3-B)18C5-4 (II)	malononitrile	0.70	NMR	-18.4	-47.7	25	C_6D_6	39, 41
	malononitrile	0.70	NMR	-18.8	-50.5	25	$CDCl_3$	39, 41
(1,3-B)18C5-5 (II)	malononitrile	1.04	NMR	-19.2	-44.9	25	C_6D_6	39, 41
	malononitrile	nm	NMR			25	$CDCl_3$	39, 41
18C6-1 (II)	H_2O	1.19	IR			25	CCl_4	44
	H_2O		IR	-11.3		25	CCl_4	26
	H_2O	0.70	NMR			30	CD_2Cl_2	27
	H_2O	1.88	NMR			-5	$CHCl_3$	27
	H_2O	1.51	NMR			10	$CHCl_3$	27
	H_2O	1.04	NMR	-35.8	-98	30	$CHCl_3$	27
	Br_2	0	NMR			22	CCl_4/C_2H_5Br (3:1 v/v), (Br_2 competes with $CHCl_3$)	13, 1 (for conditions)
	I_2	0.45	Spec			25	CCl_4	14
	I_2	0.55	Spec	-14	-16	25	CCl_4	20
	I_2	0.69	Spec			25	cyclohexane	15
	I_2	0.59	Spec	-13.7	-32.6	35	cyclohexane	15
	I_2	0.55	Spec			40	cyclohexane	15
	I_2	0.53	Spec			45	cyclohexane	15
	I_2	0.41	UV	-34.3		20	C_6H_5Cl(external complex)	45

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	I_2	0.08	UV	-35.1		20	DCE (external complex)	45
	I_2		UV	~0		20	DCE (internal complex)	45
	ICl	2.10	Spec			25	CCl_4	14
	ICl	1.56	Cal	-29	-225	25	C_6H_6	16
	ICl	1.26(M_2L)	Cal	-29		25	C_6H_6 (M + ML <-> M_2L)	16
	ICl	0.85(M_3L)	Cal	-31		25	C_6H_6 (M + M_2L <-> M_3L)	16
	acetonitrile	0.32	NMR			25	CCl_4	46
	acetonitrile	-0.10	NMR			9	C_6D_6	42
	acetonitrile	0.23(M_2L)	NMR			9	C_6D_6 (M + ML <-> M_2L)	42
	acetonitrile	-0.22	NMR			17	C_6D_6	42
	acetonitrile	-0.05(M_2L)	NMR			17	C_6D_6 (M + ML <-> M_2L)	42
	acetonitrile	-0.32	NMR			27	C_6D_6	42
	acetonitrile	-0.44	NMR			36	C_6D_6	42
	acetonitrile	(ML)	NMR	-25.1	-92.1	9-36	C_6D_6	42
	acetonitrile	0	Spec			25	C_6H_6	47
	acetonitrile	-0.59(M_2L)	Spec			25	C_6H_6 (M + ML <-> M_2L)	47
	acetonitrile	<-0.40	Spec			25	$CHCl_3$	47
	acetonitrile	-0.24	Spec			25	Me_2CO	47
	N^4-acetylsulfadimethoxine	none	UV			25	$CHCl_3$	48
	N^4-acetylsulfamethoxazole	none	UV			25	$CHCl_3$	48
	N^4-acetylsulfamethoxypyridazine	none	UV			25	$CHCl_3$	48
	N^1-acetylsulfisoxazole	0.80	NMR			24.5	$CDCl_3$	48
	N^1-acetylsulfisoxazole	0.83	UV			25	$CHCl_3$	48
	4-aminobenzoic acid	0.33	NMR			24.5	$CDCl_3$	48
	4-aminobenzoic acid	0.91	UV			25	$CHCl_3$	48
	4-chloroaniline	-0.33	NMR			24.5	$CDCl_3$	48
	4-chloroaniline	none	UV			25	$CHCl_3$	48
	chloroform	2.18	Polg			25	H_2O, 0.1 M KCl (apparent K)	49 50
	chloroform	2.91	Polg			25	H_2O, I -> 0 (KCl) (extrapolated K)	50
	chloroform	2.90	Polg			25	H_2O, 0.025 M Me_4NBr	50
	chloroform	2.91	Polg			25	H_2O, 0.025 M Bu_4NBr	50
	dimethyl carbonate	-0.10	NMR			25	C_6D_6	51
	dimethyl oxalate	-0.22	NMR			28	C_6D_6/CCl_4 (40:10 v/v)	51
	dimethyl sulfate	-0.22	NMR			28	C_6D_6	51
	eosin[e]	1.35	Spec			25	H_2O	28
	eosin[e]	2.01	Spec			25	MeOH	28
	malononitrile	2.83	NMR			9	C_6D_6	42
	malononitrile	1.25(M_2L)	NMR			9	C_6D_6 (M + ML <-> M_2L)	42
	malononitrile	2.59	NMR			17	C_6D_6	42
	malononitrile	1.08(M_2L)	NMR			17	C_6D_6 (M + ML <-> M_2L)	42
	malononitrile	2.20	NMR	-59.4	-154	25	C_6D_6	39, 41
	malononitrile	1.04(M_2L)	NMR			25	C_6D_6 (M + ML <-> M_2L)	41
	malononitrile	2.18	NMR			27	C_6D_6	42
	malononitrile	1.04(M_2L)	NMR			27	C_6D_6 (M + ML <-> M_2L)	42
	malononitrile	1.89	NMR			36	C_6D_6	42
	malononitrile	0.95(M_2L)	NMR			36	C_6D_6 (M + ML <-> M_2L)	42
	malononitrile	1.49	NMR	-22.2	-46.3	25	$CDCl_3$	39, 41
	methanol		IR	-14.6		25	CCl_4	26
	4-nitroaniline	0.86	NMR			24.5	$CDCl_3$	48
	4-nitroaniline	0.93	UV			25	$CHCl_3$	48
	nitromethane	0.48	NMR			9	C_6D_6	42
	nitromethane	0.69(M_2L)	NMR			9	C_6D_6 (M + ML <-> M_2L)	42
	nitromethane	0.26	NMR			17	C_6D_6	42
	nitromethane	0.60(M_2L)	NMR			17	C_6D_6 (M + ML <-> M_2L)	42
	nitromethane	0.08	NMR			27	C_6D_6	42
	nitromethane	0.40(M_2L)	NMR			27	C_6D_6 (M + ML <-> M_2L)	42
	nitromethane	-0.05	NMR			36	C_6D_6	42
	nitromethane	0.18(M_2L)	NMR			36	C_6D_6 (M + ML <-> M_2L)	42
	nitromethane	(ML)	NMR	-31.8	-105	9-36	C_6D_6	42
	nitromethane	0.11	Spec			25	C_6H_6	47
	nitromethane	0.15(M_2L)	Spec			25	C_6H_6 (M + ML <-> M_2L)	47
	phenol	1.90	IR	-24.7	-46.4	25	CCl_4	26
	sulfadimethoxine	1.70	Sol-UV			10	C_6H_6	52
	sulfadimethoxine	0.87	NMR			24.5	$CDCl_3$	48
	sulfadimethoxine	1.02	Sol-UV			10	$CHCl_3$	52
	sulfadimethoxine	0.80	UV			25	$CHCl_3$	48

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	sulfamerazine	nm	Sol-UV			10	C_6H_6 (poor solubility of guest)	52
	sulfamerazine	1.35	Sol-UV			10	$CHCl_3$	52
	sulfamethizole	nm	Sol-UV			10	C_6H_6 (poor solubility of guest)	52
	sulfamethizole	1.05	Sol-UV			10	$CHCl_3$	52
	sulfamethomidine	1.54	Sol-UV			10	C_6H_6	52
	sulfamethomidine	0.82	NMR			24.5	$CDCl_3$	48
	sulfamethomidine	1.31	Sol-UV			10	$CHCl_3$	52
	sulfamethomidine	0.89	UV			25	$CHCl_3$	48
	sulfamethoxazole	none	Sol-UV			10	C_6H_6	52
	sulfamethoxazole	0.89	NMR			24.5	$CDCl_3$	48
	sulfamethoxazole	1.00	Sol-UV			10	$CHCl_3$	52
	sulfamethoxazole	0.92	UV			25	$CHCl_3$	48
	sulfamethoxy-pyridazine	1.47	Sol-UV			10	C_6H_6	52
	sulfamethoxy-pyridazine	0.50	NMR			24.5	$CDCl_3$	48
	sulfamethoxy-pyridazine	1.03	Sol-UV			10	$CHCl_3$	52
	sulfamethoxy-pyridazine	0.67	UV			25	$CHCl_3$	48
	sulfamonomethoxine	2.22	Sol-UV			10	C_6H_6	52
	sulfamonomethoxine	1.15	Sol-UV			10	$CHCl_3$	52
	sulfamonomethoxine	0.83	UV			25	$CHCl_3$	48
	sulfanilamide	nm	Sol-UV			10	C_6H_6 (poor solubility of guest)	52
	sulfanilamide	1.69	Sol-UV			10	$CHCl_3$	52
	sulfaphenazole	1.62	Sol-UV			10	C_6H_6	52
	sulfaphenazole	0.74	NMR			24.5	$CDCl_3$	48
	sulfaphenazole	0.82	Sol-UV			10	$CHCl_3$	52
	sulfaphenazole	0.72	UV			25	$CHCl_3$	48
	sulfathiazole	nm	Sol-UV			10	C_6H_6 (poor solubility of guest)	52
	sulfathiazole	1.32	Sol-UV			10	$CHCl_3$	52
	sulfisomidine	nm	Sol-UV			10	C_6H_6 (poor solubility of guest)	52
	sulfisomidine	0.74	Sol-UV			10	$CHCl_3$	52
	sulfisoxazole	1.91	Sol-UV			10	C_6H_6	52
	sulfisoxazole	1.13	Sol-UV			10	$CHCl_3$	52
	sulfisoxazole	0.84	UV			25	$CHCl_3$	48
	tetrachloro-1,4-benzoquinone	0.11	Spec			25	CCl_4	18
	2,3,5,6-tetra-cyanopyrazine	~-0.82	Spec			25	CH_2Cl_2	29
	tetrafluoro-1,4-benzoquinone	0.63	Spec			25	CCl_4	18
	tetrafluoro-1,4-benzoquinone	-0.523	NMR			31.6	$CDCl_3$	30
	urea	0.2-0.7	Polg			25	MeOH, 0.1 M Et_4NI (Rb as indicator), (no reproducible value of K)	38
Cy_218C6-1 (II)	H_2O		IR	-12.6		25	CCl_4	26
	H_2O	1.31	NMR			30	$CHCl_3$	19
	HBr	~6	Spec			25	$CHCl_3$ (L + HBr <-> LH^+,Br^-)	2
	Br_2	0.80	NMR			22	CCl_4/C_2H_5Br (3:1 v/v) (Br_2 competes with $CHCl_3$)	1
	Br_2	>3	Spec	-34.3	-27.6	25	$CHCl_3$ ($LH^+,Br^- + Br_2$ <-> LH^+,Br_3^-)	2
	malononitrile	1.80	NMR	-36.0	-85.6	25	C_6D_6	39, 41
	malononitrile	1.63	NMR	-23.4	-46.3	25	$CDCl_3$	39, 41
	methanol		IR	-15.5		25	CCl_4	26
	phenol	2.29	IR	-24.3	-38.1	25	CCl_4	26
B18C6-1 (II)	malononitrile	1.48	NMR	-33.5	-82.8	25	C_6D_6	39, 41
	malononitrile	1.70	NMR	-22.6	-43.5	25	$CDCl_3$	39, 41
	tetracyanoethylene	0.41	UV			20	$CHCl_3$	53
B_218C6-1 (II)	H_2O		IR	-7.9		25	CCl_4	26
	H_2O	1.81	NMR			4	$CHCl_3$	54
	H_2O	0.89	NMR	-55.7	-167	30	$CHCl_3$	27, 54 (log$K$)
	HBr	2.32	Spec			25	$CHCl_3$ (L + HBr <-> LH^+,Br^-)	2
	Br_2	4.57	Spec			25	$CHCl_3$ ($LH^+,Br^- + Br_2$ <-> LH^+,Br_3^-)	2
	ICl	2.08	Cal	-22	-117	25	C_6H_6	16

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	ICl	1.80(M_2L)	Cal	-22		25	C_6H_6 (M + ML <-> M_2L)	16
	2,3-dichloro-5,6-dicyano-1,4-benzoquinone	1.10	Spec			0	CH_2Cl_2	31
	2,3-dichloro-5,6-dicyano-1,4-benzoquinone	0.95	Spec	-20.39	-55.2	10	CH_2Cl_2	31
	2,3-dichloro-5,6-dicyano-1,4-benzoquinone	0.69	Spec			25	CH_2Cl_2	31
	2-dicyanoethylene-1,3-indandione	0.49	Spec			3	CH_2Cl_2	32
	2-dicyanoethylene-1,3-indandione	0.35	Spec	-15.9	-46.9	12	CH_2Cl_2	32
	2-dicyanoethylene-1,3-indandione	0.33	Spec			25	CH_2Cl_2	32
	9-dicyanomethylene-2,4,7-trinitro-fluorene	0.37	Spec			5	CH_2Cl_2	33
	9-dicyanomethylene-2,4,7-trinitro-fluorene	0.16	Spec			10	CH_2Cl_2	33
	9-dicyanomethylene-2,4,7-trinitro-fluorene	-0.07	Spec	-10.04	-35	25	CH_2Cl_2	33
	malononitrile	none	NMR			25	C_6D_6 (insoluble in C_6D_6)	41
	malononitrile	2.05	NMR	-19.7	-26.7	25	$CDCl_3$	39, 41
	methanol		IR	-10.5		25	CCl_4	26
	phenol	1.35	IR	-16.7	-31.0	25	CCl_4	26
	tetracyanoethylene	0.65	UV			20	$CHCl_3$	53
	tetracyanoethylene	0.153	NMR			11	CH_2Cl_2	35
	tetracyanoethylene	0.065	NMR			24	CH_2Cl_2	35
	tetracyanoethylene	-0.007	NMR			34	CH_2Cl_2	35
	tetracyanoethylene		NMR	-10.72	-33.7	11-34	CH_2Cl_2	35
	2,3,5,6-tetra-cyanopyrazine	0.74	Spec			0.5	CH_2Cl_2	29
	2,3,5,6-tetra-cyanopyrazine	0.51	Spec			11.5	CH_2Cl_2	29
	2,3,5,6-tetra-cyanopyrazine	0.35	Spec	-20.7	-67.2	25	CH_2Cl_2	29
	tetrafluoro-1,4-benzoquinone	none	NMR			31.6	$CDCl_3$ (inadequate solubility in $CDCl_3$)	30
	2,4,5,7-tetranitro-9-fluorenone	0.60	Spec			5	CH_2Cl_2	33
	2,4,5,7-tetranitro-9-fluorenone	0.45	Spec			10	CH_2Cl_2	33
	2,4,5,7-tetranitro-9-fluorenone	0.29	Spec	-15.27	-46	25	CH_2Cl_2	33
	1,3,5-trinitro-benzene	0.038	NMR			31.5	DCE	36
	2,4,7-trinitro-9-fluorenone	0.51	Spec			5	CH_2Cl_2	33
	2,4,7-trinitro-9-fluorenone	0.26	Spec			10	CH_2Cl_2	33
	2,4,7-trinitro-9-fluorenone	-0.15	Spec	-20.57	-71.9	25	CH_2Cl_2	33
	2,4,6-trinitro-toluene	0.017	NMR	-12.5	-40.9	30	DCE	37
$B_2$18C6-2 (II)	HBr	1.30	Spec			25	$CHCl_3$ (L + HBr <-> LH^+,Br^-)	2
	Br_2	4.57	Spec			25	$CHCl_3$ (LH^+,Br^- + Br_2 <-> LH^+,Br_3^-)	2
Py18C6-1 (II)	malononitrile	1.63	NMR	-34.7	-85.6	25	C_6D_6	7, 39
	malononitrile	1.49	NMR	-10.0	-4.21	25	$CDCl_3$	7, 39
	urea	-0.40	Pot			25	H_2O, 0.1 M Et_4NCl	43
Py18C6-2 (II)	urea	<-1.0	Pot			25	H_2O, 0.1 M Et_4NCl	43
Py18C6-3 (II)	H_2O	1.59	Pot			25	H_2O	55
	H_2O	2.42	Pot			25	85.4 wt% EtOH/H_2O	55
	H_2O	2.54	Pot			25	51.2 wt% MeOH/H_2O	55
N18C6-1 (II)	malononitrile	1.53	NMR	-23.8	-50.5	25	C_6D_6	39, 41
	malononitrile	nm	NMR			25	$CDCl_3$	39, 41
$N_2$18C6-1 (II)	H_2O	2.51	NMR			30	$CHCl_3$	19

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
$N_6$18C6-1 (III)	catechol	2.20(H_2MH_3L)Polg				25	H_2O, 0.2 M $NaClO_4$, pH 7.6-8.5 (0.05-0.2 M TRIS), ($H_2M + H_3L^{3+}$ <-> $H_2MH_3L^{3+}$)	56
	cimetidine	2.74(MH_3L)	Polg			25	H_2O, 0.2 M $NaClO_4$ ($M + H_3L^{3+}$ <-> MH_3L^{3+})	57
	cimetidine	2.89(MH_3L)	Pot			25	H_2O, 0.2 M $NaClO_4$ ($M + H_3L^{3+}$ <-> MH_3L^{3+})	57
	dimaprit[e]	4.12(MH_3L)	Pot			25	H_2O, 0.2 M $NaClO_4$ ($M + H_3L^{3+}$ <-> MH_3L^{3+})	57
	dichloroiso-proterenol	2.93(MH_3L)	Polg			25	H_2O, 0.2 M $NaClO_4$, pH 7.6-8.6 (0.1 M TRIS) ($M + H_3L^{3+}$ <-> MH_3L^{3+})	56
	dopa	3.57(H_3MH_3L)	Polg			25	H_2O, 0.2 M $NaClO_4$, pH 7.8-8.6 (0.05-0.2 M TRIS), ($H_3M + H_3L^{3+}$) $H_3MH_3L^{3+}$)	56
	2-ethylamino-pyridine	none	?			25	H_2O, 0.2 M $NaClO_4$	57
	famotidine[e]	4.00(MH_3L)	Polg			25	H_2O, 0.2 M $NaClO_4$ ($M + H_3L^{3+}$ <-> MH_3L^{3+})	57
	histamine	3.05(MH_3L)	Polg			25	H_2O, 0.2 M $NaClO_4$ ($M + H_3L^{3+}$ <-> MH_3L^{3+})	57
	metiamide[e]	1.63(MH_3L)	Pot			25	H_2O, 0.2 M $NaClO_4$ ($M + H_3L^{3+}$ <-> MH_3L^{3+})	57
	nordimaprit[e]	3.78(MH_3L)	Pot			25	H_2O, 0.2 M $NaClO_4$ ($M + H_3L^{3+}$ <-> MH_3L^{3+})	57
	ranitidine[e]	3.79(MH_3L)	Pot			25	H_2O, 0.2 M $NaClO_4$ ($M + H_3L^{3+}$ <-> MH_3L^{3+})	57
	resorcinol	3.11(H_2MH_3L)	Polg			25	H_2O, 0.2 M $NaClO_4$, pH 7.6-8.8 (0.1 M TRIS) ($H_2M + H_3L^{3+}$ <-> $H_2MH_3L^{3+}$)	56
	thiourea	2.34(MH_3L)	Pot			25	H_2O, 0.2 M $NaClO_4$ ($M + H_3L^{3+}$ <-> MH_3L^{3+})	57
	urea	1.66(MH_3L)	Polg			25	H_2O, 0.2 M $NaClO_4$ ($M + H_3L^{3+}$ <-> MH_3L^{3+})	57
	veratraldehyde	2.40(MH_3L)	Polg			25	H_2O, 0.2 M $NaClO_4$, pH 8.0-8.6 (0.03-0.06 M borate), ($M + H_3L^{3+}$ <-> MH_3L^{3+})	56
$S_2$18C6-1 (III)	H_2O	0.38	NMR			30	$CHCl_3$	19
	I_2	2.41	Spec	-34	-49	25	CCl_4	20
$BS_2$18C6-1 (III)	I_2	1.97	Spec	-24.5	-26	25	CCl_4	20
(1,3-B)21C6-1 (III)	H_2O	1.15	NMR			22	$CDCl_3$	25
(1,3-B)21C6-2 (III)	malononitrile	0.70	NMR	-16.3	-40.7	25	C_6D_6	39, 41
Py21C7-1 (III)	malononitrile	0.70	NMR	-21.8	-59.0	25	C_6D_6	7, 39
	malononitrile	0.85	NMR	-14.2	-30.9	25	$CDCl_3$	7, 39
Py21C7-2 (III)	urea	-0.12	Pot			25	H_2O, 0.1 M Et_4NCl	43
Py21C7-3 (III)	H_2O	0.78	Pot			25	H_2O	55
	H_2O	1.48	Pot			25	85.4 wt% EtOH/H_2O	55
	H_2O	1.52	Pot			25	51.2 wt% MeOH/H_2O	55
$K_4N_2$21C7-1 (III)	H_2O	2.24	NMR			22	$CDCl_3$	40
$K_4N_2$21C7-2 (III)	H_2O	1.81	NMR			22	$CDCl_3$	40
(1,3-B)24C7-1 (III)	H_2O	1.30	NMR			22	$CDCl_3$	25
24C8-1 (III)	tetrafluoro-1,4-benzoquinone	-0.252	NMR			31.6	$CDCl_3$	30
$Cy_2$24C8-1 (III)	H_2O		IR	-12.1		25	CCl_4	26
	methanol		IR	-14.6		25	CCl_4	26
	phenol	2.39	IR	-23.4	-33.1	25	CCl_4	26
$B_2$24C8-1 (III)	H_2O		IR	-10.9		25	CCl_4	26
	H_2O	0.75	NMR			30	$CHCl_3$	19
	2,3-dichloro-5,6-dicyano-1,4-benzoquinone	1.15	Spec			0	CH_2Cl_2	31
	2,3-dichloro-5,6-dicyano-1,4-benzoquinone	0.98	Spec	-18.5	-56.4	9.5	CH_2Cl_2	31
	2,3-dichloro-5,6-dicyano-1,4-benzoquinone	0.88	Spec			25	CH_2Cl_2	31

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	2-dicyanoethylene-1,3-indandione	0.80	Spec			3	CH_2Cl_2	32
	2-dicyanoethylene-1,3-indandione	0.71	Spec	-20.6	-57.4	10	CH_2Cl_2	32
	2-dicyanoethylene-1,3-indandione	0.60	Spec			25	CH_2Cl_2	32
	9-dicyanomethylene-2,4,7-trinitro-fluorene	0.35	Spec			3	CH_2Cl_2	33
	9-dicyanomethylene-2,4,7-trinitro-fluorene	0.23	Spec			11	CH_2Cl_2	33
	9-dicyanomethylene-2,4,7-trinitro-fluorene	0.13	Spec	-7.23	-21.7	25	CH_2Cl_2	33
	methanol		IR	-14.2		25	CCl_4	26
	phenol	1.95	IR	-21.8	-36.9	25	CCl_4	26
	2,3,5,6-tetra-cyanopyrazine	0.85	Spec			2	CH_2Cl_2	29
	2,3,5,6-tetra-cyanopyrazine	0.72	Spec			11	CH_2Cl_2	29
	2,3,5,6-tetra-cyanopyrazine	0.53	Spec	-10.4	-25.0	25	CH_2Cl_2	29
	2,4,5,7-tetranitro-9-fluorenone	0.60	Spec			3	CH_2Cl_2	33
	2,4,5,7-tetranitro-9-fluorenone	0.48	Spec			11	CH_2Cl_2	33
	2,4,5,7-tetranitro-9-fluorenone	0.43	Spec	-9.0	-22	25	CH_2Cl_2	33
	2,4,7-trinitro-9-fluorenone	0.57	Spec			3	CH_2Cl_2	33
	2,4,7-trinitro-9-fluorenone	0.48	Spec			11	CH_2Cl_2	33
	2,4,7-trinitro-9-fluorenone	0.18	Spec	-16.6	-50.9	25	CH_2Cl_2	33
	urea	1.1	Polg			25	MeOH, 0.1 M Et_4NI (Rb as indicator)	38
Py24C8-1 (III)	malononitrile	•0.48	NMR	-18.0	-50.5	25	C_6D_6	7, 39
	malononitrile	0.30	NMR	-7.95	-19.7	25	$CDCl_3$	7, 39
Py24C8-2 (III)	urea	-0.26	Pot			25	H_2O, 0.1 M Et_4NCl	43
Py24C8-3 (III)	H_2O	0.60	Pot			25	H_2O	55
	H_2O	1.23	Pot			25	85.4 wt% EtOH/H_2O	55
	H_2O	1.32	Pot			25	51.2 wt% MeOH/H_2O	55
K_4N_224C8-1 (III)	H_2O	large	NMR			22	$CDCl_3$ (K too large to be measured)	40
K_4N_224C8-2 (III)	H_2O	3.19	NMR			22	$CDCl_3$	40
K_4N_224C8-3 (III)	H_2O	1.36	NMR			22	$CDCl_3$	40
(1,3-B)27C8-1 (III)	H_2O	1.36	NMR			22	$CDCl_3$	25
B27C9-1 (IV)	urea	1.2	Polg			25	MeOH, 0.1 M Et_4NI (Rb as indicator)	38
Py27C9-1 (IV)	malononitrile	0.48	NMR	-14.6	-39.3	25	C_6D_6	7, 39
	malononitrile	nm	NMR			25	$CDCl_3$	39
Py27C9-2 (IV)	urea	0.10	Pot			25	H_2O, 0.1 M Et_4NCl	43
Py27C9-3 (IV)	H_2O	0.30	Pot			25	H_2O	55
	H_2O	0.95	Pot			25	85.4 wt% EtOH/H_2O	55
	H_2O	1.00	Pot			25	51.2 wt% MeOH/H_2O	55
(1,3-B)30C9-1 (IV)	H_2O	1.67	NMR			22	$CDCl_3$	25
(1,3-B)30C9-2 (IV)	urea	-0.10	Pot			25	H_2O	43
B_230C10-1 (IV)	tetrafluoro-1,4-benzoquinone	none	NMR			31.6	$CDCl_3$ (inadequate solubilty in $CDCl_3$)	30
	1,3,5-trinitro-benzene	0.301	NMR	-20.43	-61.3	31.5	DCE	36
	1,3,5-trinitro-benzene	0.137	NMR			45	DCE	36
	2,4,6-trinitro-toluene	-0.070	NMR			30	DCE	37
Py30C10-1 (IV)	malononitrile	0.48	NMR	-13.4	-35.1	25	C_6D_6	7, 39
	malononitrile	nm	NMR			25	$CDCl_3$	39
	urea	0.15	Pot			25	H_2O, 0.1 M Et_4NCl	43
Py30C10-2 (IV)	urea	0.06	Pot			25	H_2O, 0.1 M Et_4NCl	43

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
(1,3-B)33C10-1 (IV)	urea	-0.17	Pot			25	H_2O	43
Py33C11-1 (IV)	malononitrile	0.60	NMR	-16.7	-44.9	25	C_6D_6	7, 39
	malononitrile	nm	NMR			25	$CDCl_3$	7, 39
($N_6$18C6)(B15C5)-1 (IV)	catechol	2.18	Polg			25	H_2O, 0.2 M $NaClO_4$, pH 7-8 (TRIS)	58, 59
			1. Coronands and Cryptands (cont.)					
			b. Hemispherands					
Spher-18C3-1 (V)	malononitrile	1.49	NMR	-33.9	-85.6	25	C_6D_6	60, 61
	malononitrile	1.45	NMR	-35.1	-89.9	25	$CDCl_3$	60, 61
Spher-Py18C3-1 (V)	malononitrile	nm	NMR			25	C_6D_6	60
	malononitrile	0.90	NMR	-19.7	-49.1	25	$CDCl_3$	60
Spher-Py18C4-1 (V)	malononitrile	1.49	NMR	-16.3	-26.7	25	C_6D_6	60, 61
	malononitrile	2.02	NMR	-16.3	-16.8	25	$CDCl_3$	60, 61
Spher-Pyrano-18C4-1 (V)	malononitrile	1.58	NMR	-23.8	-49.1	25	C_6D_6	60
	malononitrile	nm	NMR			25	$CDCl_3$	60
Spher-21C4-1 (V)	malononitrile	1.20	NMR	-25.9	-63.2	25	C_6D_6	60
	malononitrile	1.18	NMR	-7.53	-2.81	25	$CDCl_3$	60
			1. Coronands and Cryptands (cont.)					
			c. Cryptands					
[2.1.1]-1 (V)	I_2	7.48	Volt			25?	$CHCl_3$, I = ? (Bu_4NClO_4) (K = $[I^+L]/[I]_2[L]$)	62
[2.2.1]-1 (V)	I_2	6.73	Volt			25?	$CHCl_3$, I = ? (Bu_4NClO_4) (K = $[I^+L]/[I_2][L]$)	62
[2.2.2]-1 (V)	H_2O	1.17	NMR			30	$CHCl_3$	19
	I_2	6.36	Volt			25?	$CHCl_3$, I = ? (Bu_4NClO_4) (K = $[I^+L]/[I_2][L]$)	62
	ICl	(ML)	Cal	-67		25	C_6H_6	16
	ICl	(M_2L)	Cal	-65		25	C_6H_6 (M + ML <-> M_2L)	16
			2. Cyclophanes					
			a. Monocyclic with Oxygen Donor Atoms					
$Nap_2$24C4-1 (VI)	1,3,5-trinitrobenzene	2.44	NMR			?	$CDCl_3$	63
$Nap_2$28C4-1 (VI)	1,3,5-trinitrobenzene	1.88	NMR			?	$CDCl_3$	63
$(1,4\text{-B})_4$28C4-1 (VI)	1,4-diaminobenzene	<1	NMR			20	D_2O	64
	1,4-dicyanobenzene	3.18	NMR	-25.5	-20.0	20	D_2O	3, 64
	1,4-dimethoxybenzene	1.89	NMR			20	D_2O	3
	1,4-dimethoxybenzene	<1.93	NMR			20	D_2O	64
	1,4-dimethylbenzene	<1.93	NMR			20	D_2O	64
	dimethyl 1,4-benzenedicarboxylate	3.28	NMR			20	D_2O	64
	1,4-dinitrobenzene	3.13	NMR			20	D_2O	64
	ethyl anthranilate	2.30	Fluor			19.5	H_2O	3, 65
	4-nitrophenol	2.78	NMR			20	D_2O	64
	4-nitrotoluene	2.78	NMR			20	D_2O	3, 64
	p-tolunitrile	2.62	NMR			20	D_2O	64
	p-xylene	<1.93	NMR			20	D_2O	64
$(1,4\text{-B})_4$28C4-2 (IV)	1,4-diaminobenzene	1.32	NMR			20	D_2O	64
	1,4-dicyanobenzene	3.01	NMR	-30.5	-47.1	20	D_2O	65,66,67,68
	1,4-dimethoxybenzene	2.57	NMR	-23.8	-31.4	20	D_2O	64,66,67,68
	dimethyl 1,4-benzenedicarboxylate	3.32	NMR	-33.5	-49.9	20	D_2O	64,66,67,68
	hydroquinone	1.48	NMR			20	D_2O	64
	4-nitrophenol	3.34	NMR	-42.3	-79.9	20	D_2O	64, 66
	4-nitrotoluene	3.33	NMR	-35.6	-57.0	20	D_2O	64,66,67,68
	p-xylene	3.11	NMR	-26.8	-31.4	20	D_2O	64,66,67,68
	guest-1[e]	2.46	ESR	-8.4	16.7	20	H_2O (K is for host complexation with guest phenyl group)	69

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
Nap$_4$28C4-1 (VI)	guest-6[e]	none	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	70
	guest-7[e]	none	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	70
Isoquin28C4-1 (VI)	*N*-acetyl-tryptophane	weak binding	NMR			30	MeOD-d_3/0.5 aq. KD_2PO_4 (40:60 v/v)	71
	2,6-dicyano-naphthalene	considerable binding	NMR			30	MeOD-d_3/0.5 aq. KD_2PO_4 (40:60 v/v)	71
	2,6-dimethoxy-naphthalene	considerable binding	NMR			30	MeOD-d_3/0.5 aq. KD_2PO_4 (40:60 v/v)	71
	1-ethylamino-naphthalene	none	NMR			30	MeOD-d_3/0.5 aq. KD_2PO_4 (40:60 v/v)	71
	mandelic acid	weak binding	NMR			30	MeOD-d_3/0.5 aq. KD_2PO_4 (40:60 v/v)	71
	2-cyano-6-methoxy-naphthalene	2.53	NMR			30	MeOD-d_3/0.5 aq. KD_2PO_4 (44:56 v/v)	71, 72
	quinine	none	NMR			30	MeOD-d_3/0.5 aq. KD_2PO_4 (40:60 v/v)	71
	p-tolunitrile	weak binding	NMR			30	MeOD-d_3/0.5 aq. KD_2PO_4 (40:60 v/v)	71
	tryptophane	none	NMR			30	MeOD-d_3/0.5 aq. KD_2PO_4 (40:60 v/v)	71
	guest-2[e]	~1.70	NMR			30	MeOD-d_3/0.5 aq. KD_2PO_4 (40:60 v/v)	71, 72
Isoquin28C4-2 (VI)	2-cyano-6-methoxy-naphthalene	2.53	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	73
	guest-2[e]	~1.70	NMR			30	MeOD-d_3/D_2O (40:60 v/v)	73
	guest-3[e]	~2.48	NMR			30	MeOD-d_3/D_2O (40:60 v/v)	71,72,73
	guest-4[e]	~2.48	NMR			30	MeOD-d_3/D_2O (40:60 v/v)	71,72,73
Nap$_2$(1,4-B)$_2$-29C4-1 (VII)	guest-2[e]	3.40	NMR			20	MeOD-d_3/0.1 M DCl (40:60 v/v)	74
	guest-3[e]	3.49	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	74
	guest-5[e]	3.00	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	74
	guest-6[e]	3.40	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	74
	guest-8[e]	3.45	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	74
Nap$_2$(1,4-B)$_2$-29C4-2 (VII)	guest-2[e]	3.32	NMR			20	MeOD-d_3/0.1 M DCl (40:60 v/v)	74
	guest-3[e]	3.32	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	74
	guest-5[e]	2.89	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	74
	guest-6[e]	3.15	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	74
	guest-8[e]	3.25	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	74
Nap$_2$(1,4-B)$_2$-29C4-3 (VII)	2-cyano-6-methoxy-naphthalene	~4.77	NMR			20	D_2O (extrapolated K)	75
	2-cyano-6-methoxy-naphthalene	3.30	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	75, 76
	2-cyano-6-methoxy-naphthalene	2.61	NMR			20	MeOD-d_3/D_2O (60:40), 0.1 M KCl	75
	2-cyano-6-methoxy-naphthalene	1.90	NMR			20	MeOD-d_3/D_2O (80:20), 0.1 M KCl	75
	2-cyano-6-methoxy-naphthalene	1.08	NMR			20	MeOD-d_3	75
(1,4-B)$_4$30C4-1 (VII)	1,4-dicyanobenzene	2.15	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	64, 68
	1,4-dicyanobenzene	1.20	NMR			20	MeOD-d_3	64
	2,7-dihydroxy-naphthalene	3.08	Fluor			19.5	H_2O	65, 77
	1,4-dimethoxy-benzene	1.98	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	64, 68
	1,4-dimethoxy-benzene	<<1	NMR			20	MeOD-d_3	64
(1,4-B)$_4$30C4-2 (VII)	2-amino-6-nitro-naphthalene	2.01	NMR			30	MeOD-d_3	68, 78
	2-amino-6-nitro-naphthalene	2.02	NMR			30	MeOD-d_3	64
	2-amino-6-nitro-naphthalene	0.60	NMR			30	Me_2SO-d_6	64

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	2-bromo-6-methoxy-naphthalene	2.07	NMR			30	MeOD-d_3	64
	2-cyano-6-methoxy-naphthalene	2.07	NMR			30	MeOD-d_3	68, 78
	2-cyano-6-methoxy-naphthalene	2.08	NMR			30	MeOD-d_3	64
	6-cyano-2-naphthol	2.20	NMR			30	MeOD-d_3	78
	6-cyano-2-naphthol	2.22	NMR			30	MeOD-d_3	64
	6-cyano-2-naphthol	0.85	NMR			30	Me_2SO-d_6	64
	6-cyano-2-naphthol	~0.81	NMR			30	Me_2SO-d_6 (estimated K)	78
	2,6-diamino-naphthalene	1.52	NMR			30	MeOD-d_3	68, 78
	2,6-diamino-naphthalene	1.43	NMR			30	MeOD-d_3	64
	2,6-diamino-naphthalene	-0.40	NMR			30	Me_2SO-d_6	64
	1,4-dicyanobenzene	3.20	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	64, 68
	1,4-dicyanobenzene	2.11	NMR			20	MeOD-d_3	64
	2,6-dicyano-naphthalene	2.44	NMR	-31.8	-59.0	30	MeOD-d_3	68, 78
	2,6-dicyano-naphthalene	2.43	NMR			30	MeOD-d_3	64
	2,6-dicyano-naphthalene	~1.06	NMR			30	Me_2SO-d_6 (estimated K)	78
	2,6-dicyano-naphthalene	1.20	NMR			30	Me_2SO-d_6	64
	2,6-dihydroxy-naphthalene	1.38	NMR			30	MeOD-d_3	68, 78
	2,6-dihydroxy-naphthalene	1.36	NMR			30	MeOD-d_3	64
	1,4-dimethoxy-benzene	2.76	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	64, 68
	1,4-dimethoxy-benzene	1.48	NMR			20	MeOD-d_3	64
	2,6-dimethoxy-naphthalene	1.67	NMR			30	MeOD-d_3	68, 78
	2,6-dimethoxy-naphthalene	1.72	NMR			30	MeOD-d_3	64
	2,6-dimethoxy-naphthalene	~0.20	NMR			30	Me_2SO-d_6 (estimated K)	78
	2,6-dimethoxy-naphthalene dimethyl	0.30	NMR			30	Me_2SO-d_6	64
	1,4-benzene-dicarboxylate	3.62	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	64
	2,6-dimethyl-naphthalene	1.83	NMR			30	MeOD-d_3	64, 78
	2,6-dimethyl-naphthalene dimethyl	0.60	NMR			30	Me_2SO-d_6	64
	2,6-naphthalene-dicarboxylate dimethyl	2.27	NMR			30	MeOD-d_3	64,68,78
	2,6-naphthalene-dicarboxylate	1.11	NMR			30	Me_2SO-d_6	64
	dimethyl 2,6-naphthalenedione dimethyl	1.81	NMR			30	MeOD-d_8	64
	2,6-naphthalene-disulfonate	1.96	NMR			30	MeOD-d_3	64
	2,6-dimethylthio-naphthalene	2.21	NMR			30	MeOD-d_3	64
	2,6-dinitro-naphthalene	2.33	NMR			30	MeOD-d_3	64,68,78
	2,6-dinitro-naphthalene	0.95	NMR			30	Me_2SO-d_6	64
	6-methoxy-2-naphthoic acid	2.13	NMR			30	MeOD-d_3	64, 78
	6-methoxy-2-naphthoic acid	0.48	NMR			30	Me_2SO-d_6	64
	2-methoxy-6-nitro-naphthalene	2.04	NMR			30	MeOD-d_3	68, 78

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	2-methoxy-6-nitro-naphthalene	2.05	NMR			30	MeOD-d_3	64
	2-methyl-6-naphthaldehyde	1.99	NMR			30	MeOD-d_3	78
	2,6-naphthalene-diacetate	2.04	NMR			30	MeOD-d_3	64, 78
	2,6-naphthalene-dicarboxamide	1.46	NMR			30	MeOD-d_3	64
	2,6-naphthalene-dicarboxylic acid	2.32	NMR			30	MeOD-d_3	64, 78
	2,6-naphthalene-dicarboxylic acid	0.70	NMR			30	Me_2SO-d_6	64
	2,6-naphthalene-dimethanol	1.30	NMR			30	MeOD-d_3	64, 78
	2,6-naphthalene-disulfonamide	1.60	NMR			30	MeOD-d_3	64
	4-nitrophenol	3.08	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	64
	N,N,N',N'-tetraethyl 2,6-naphthalene-dicarboxamide	<1	NMR			30	MeOD-d_3	64
(1,4-B)$_4$30C4-3 (VII)	*p*-cresol	3.51	NMR	-38.1	-62.7	20	D_2O	64, 66
	p-cresol		Cal	-44.4	-84.3	20	H_2O	79
	p-cresol		Cal	-46.0		26	H_2O	79
	p-cresol		Cal	-51.9		37	H_2O	79
	2-cyano-6-methoxy-naphthalene	3.85	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	64
	2-cyano-6-methoxy-naphthalene	1.49	NMR			20	MeOD-d_3	64, 68
	1,4-diaminobenzene	2.55	NMR	-29.7	-52.8	20	D_2O	64, 66
	1,4-dicyanobenzene	3.89	NMR	-39.7	-61.3	20	D_2O	64,66,67,68
	1,4-dicyanobenzene		Cal	-43.1	-72.8	20	H_2O	79
	1,4-dicyanobenzene		Cal	-44.8		26	H_2O	79
	1,4-dicyanobenzene		Cal	-45.6		37	H_2O	79
	1,4-dicyanobenzene	2.59	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	64, 68
	1,4-dicyanobenzene	1.38	NMR	-17.6	-34.2	20	MeOD-d_3	64,66,67,68
	2,6-dicyano-naphthalene	1.89	NMR			20	MeOD-d_3	64, 68
	1,4-dimethoxy-benzene	4.01	NMR	-42.7	-68.4	20	D_2O	64,66,67,68
	1,4-dimethoxy-benzene		Cal	-41.8	-65.7	20	H_2O	79
	1,4-dimethoxy-benzene		Cal	-42.3		26	H_2O	79
	1,4-dimethoxy-benzene		Cal	-43.5		35	H_2O	79
	1,4-dimethoxy-benzene	2.53	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	64, 68
	1,4-dimethoxy-benzene	0.90	NMR	-18.4	-45.6	20	MeOD-d_3	64,66,67,68
	1,4-dimethoxy-benzene		Cal	-8.4		8	MeOH	79
	1,4-dimethoxy-benzene		Cal	-15.1		14	MeOH	79
	1,4-dimethoxy-benzene		Cal	-15.5	-35.7	20	MeOH	79
	2,6-dimethoxy-naphthalene	3.65	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	64
	2,6-dimethoxy-naphthalene dimethyl	1.08	NMR			20	MeOD-d_3	64, 68
	1,4-benzene-dicarboxylate dimethyl	5.07	NMR	-44.8	-57.0	20	D_2O	64,66,67,68,79
	1,4-benzene-dicarboxylate dimethyl-		Cal	-49.4	-71.4	20	H_2O	79
	1,4-benzene-dicarboxylate dimethyl		Cal	-49.8		26	H_2O	79
	1,4-benzene-dicarboxylate		Cal	-53.6		37	H_2O	79

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	dimethyl 1,4-benzene-dicarboxylate	3.32	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	64
	dimethyl 1,4-benzene-dicarboxylate	1.38	NMR			20	MeOD-d_3	64
	1,4-dinitrobenzene	3.89	NMR	-39.7	-61.3	20	D_2O	64, 66
	1,4-dinitrobenzene		Cal	-41.0	-65.7	20	H_2O	79
	1,4-dinitrobenzene		Cal	-41.4		26	H_2O	79
	1,4-dinitrobenzene		Cal	-43.5		35	H_2O	79
	hydroquinone	2.75	NMR			20	D_2O	64
	hydroquinone	2.71	NMR	-43.9		20	D_2O	79
	hydroquinone		Cal	-43.1	-94.2	20	H_2O	79
	hydroquinone		Cal	-46.9		26	H_2O	79
	hydroquinone		Cal	-48.1		37	H_2O	79
	4-nitrophenol	4.36	NMR	-49.0	-82.7	20	D_2O	64, 66
	4-nitrophenol		Cal	-41.8		15	H_2O	79
	4-nitrophenol		Cal	-43.9	-65.7	20	H_2O	79
	4-nitrophenol		Cal	-45.6		26	H_2O	79
	4-nitrophenol		Cal	-48.1		30	H_2O	79
	4-nitrophenol		Cal	-53.6		35	H_2O	79
	4-nitrophenol	3.00	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	64
	4-nitrophenol	1.00	NMR			20	MeOD-d_3	64
	4-nitrotoluene	4.48	NMR	-40.2	-51.3	20	D_2O	64,66,67,68
	4-nitrotoluene		Cal	-33.9	-30.0	20	H_2O	79
	4-nitrotoluene		Cal	-36.8		26	H_2O	79
	4-nitrotoluene		Cal	-37.7		37	H_2O	79
	p-tolunitrile	4.48	NMR	-41.0	-54.2	20	D_2O	64, 66
	p-tolunitrile		Cal	-33.9	-30.0	20	H_2O	79
	p-tolunitrile		Cal	-35.6		26	H_2O	79
	p-tolunitrile		Cal	-38.5		35	H_2O	79
	p-xylene	3.97	NMR	-31.0	-29.9	20	D_2O	64,66,67,68
	p-xylene		Cal	-30.1	-27.1	20	H_2O	79
	p-xylene		Cal	-31.4		26	H_2O	79
	p-xylene		Cal	-31.8		37	H_2O	79
(1,4-B)$_4$30C4-4 (VII)	benzaldehyde	2.38	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	80, 81
	2-cyano-6-methoxy-naphthalene	4.18	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	80, 81
	1,4-dicyanobenzene	3.06	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	80, 81
	2-naphthaldehyde	3.80	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	80, 81
(1,4-B)$_4$30C4-5 (VII)	benzaldehyde	2.08	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	80, 81
	2-cyano-6-methoxy-naphthalene	3.68	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	80, 81
	1,4-dicyanobenzene	2.54	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	80, 81
	2-naphthaldehyde	3.29	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	80, 81
Nap$_4$30C4-1 (VII)	guest-6[e]	2.57	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	70
	guest-7[e]	2.51	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	70
Nap$_2$(1,4-B)$_2$-31C4-1 (VII)	guest-6[e]	2.60	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	70
	guest-7[e]	2.75	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	70
IsoquinNap31C4-1 (VIII)	2-cyano-6-methoxy-naphthalene	3.33	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	73
	guest-2[e]	2.91	NMR			20	MeOD-d_3/0.01 M DCl (40:60 v/v)	73
	guest-3[e]	3.03	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	73
	guest-5[e]	2.62	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	73
	guest-6[e]	2.67	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	73
	guest-8[e]	2.95	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	73
	guest-9[e]	2.30	NMR			20	MeOD-d_3/D_2O (50:50 v/v)	73
IsoquinNap31C4-2 (VIII)	2-cyano-6-methoxy-naphthalene	3.33	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	73
	guest-2[e]	2.97	NMR			20	MeOD-d_3/0.01 M DCl (40:60 v/v)	73
	guest-3[e]	3.05	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	73
	guest-5[e]	2.65	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	73
	guest-6[e]	2.86	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	73
	guest-8[e]	3.08	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	73
	guest-9[e]	2.36	NMR			20	MeOD-d_3/D_2O (50:50 v/v)	73
(1,4-B)$_4$32C4-1 (VIII)	fluoranthene	<0.30	NMR			30	$CDCl_3$	82
	fluoranthene	2.04	NMR			30	MeOD-d_3	82

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	naphthalene	~1.15	NMR			30	MeOD-d_3	82
	perylene	2.92	Tit-EAS			30	MeOH	3,82
	pyrene	~2.08	NMR			30	MeOD-d_3	82
	pyrene	~1.20	NMR			30	Me_2SO-d_6	82
(1,4-B)$_4$32C4-2 (VIII)	1-adamantanol	2.20	Fluor			19.5	H_2O	3, 83
	azulene	4.32	Solv Extr-EAS		20-22	H_2O	3,83,84	
	biphenyl	4.34	Solv Extr-EAS		20-22	H_2O	3,83,84	
	1,5-bis(dimethylamino)naphthalene	3.99	Sol-UV			20-22	H_2O, 0.015 M K_2CO_3 pH ~11	3, 85
	trans-1,4-cyclohexanedimethanol	2.70	Fluor			19.5	H_2O	3, 85
	1,3-dihydroxynaphthalene	3.99	Fluor			19.5	H_2O	3, 83
	2,6-dihydroxynaphthalene	4.0	NMR			30	D_2O	86
	2,7-dihydroxynaphthalene	4.28	Fluor			19.5	H_2O	3, 83
	1-(dimethylamino)naphthalene	3.97	Solv Extr-EAS		20-22	H_2O	3, 83	
	1-(dimethylamino)naphthalene	3.97	Fluor			19.5	H_2O	83
	1,5-dimethylnaphthalene	4.52	Sol-EAS			20-22	H_2O	3, 83
	2,6-dimethylnaphthalene	4.42	Sol-EAS			20-22	H_2O	3, 83
	durene	3.30	Sol-EAS			20-22	H_2O	83
	durene	3.28	Solv Extr-EAS		20-22	H_2O	3,83,84	
	fluoranthene	6.08	Sol-EAS			20-22	H_2O	83
	fluoranthene	6.26	Solv Extr-EAS		20-22	H_2O	3,83,84	
	naphthalene	4.20	Fluor			19.5	H_2O	83
	naphthalene	4.18	Sol-EAS			20-22	H_2O	83
	naphthalene	4.08	Solv Extr-EAS		20-22	H_2O	3,83,84	
	perylene	7.20	Sol-EAS			20-22	H_2O	3,83,84
	pyrene	6.04	Sol-EAS			20-22	H_2O	83
	pyrene	6.26	Solv Extr-EAS		20-22	H_2O	3,83,84	
	pyrene	1.85	NMR			30	MeOD-d_3	3, 86
	pyrene	nm or none	NMR			30	Me_2SO-d_6	86
	N,N,N',N'-tetramethylbenzidine	4.23	Sol-UV			20-22	H_2O, 0.015 M K_2CO_3 pH ~11	3, 85
Nap$_4$32C4-1 (VIII)	guest-6[e]	2.66	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	70
	guest-7[e]	2.64	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	70
(1,4-B)$_2$32C4-1 (VIII)	isoquinoline	0.15	NMR			22	$CDCl_3$	87
	quinoline	none	NMR			22	$CDCl_3$	87
(1,4-B)$_2$32C4-2 (VIII)	indole	3.15	NMR			22	D_2O, pD ~9 (borate-*d*)	88
	isoquinoline	4.67	NMR			22	D_2O, pD ~9 (borate-*d*)	87, 88
	isoquinoline	4.70	NMR	-41.0	-46	25	D_2O, pD ~9 (borate-*d*)	89
	lepidine	4.58	NMR			22	D_2O, pD ~9 (borate-*d*)	88
	lepidine	5.21	NMR	-41.0	-38	25	D_2O, pD ~9 (borate-*d*)	89
	1-methylindole	3.32	NMR			22	D_2O, pD ~9 (borate-*d*)	88
	1-methylindole	2.93	NMR	-6.7	34	25	D_2O, pD ~9 (borate-*d*)	89
	1-methylisoquinoline	4.74	NMR			22	D_2O, pD ~9 (borate-*d*)	88
	quinaldine	4.04	NMR			22	D_2O, pD ~9 (borate-*d*)	88
	quinoline	4.00	NMR			22	D_2O, pD ~9 (borate-*d*)	87, 88
	quinoline	4.40	NMR	-46	-71	25	D_2O, pD ~9 (borate-*d*)	89
(1,4-Cy)$_2$32C4-1 (VIII)	indole	3.20	NMR			22	D_2O, pD ~9 (borate-*d*)	88
	isoquinoline	4.66	NMR			22	D_2O, pD ~9 (borate-*d*)	88
	isoquinoline	4.62	NMR	-12.1	46	25	D_2O, pD ~9 (borate-*d*)	89
	lepidine	4.48	NMR			22	D_2O, pD ~9 (borate-*d*)	88
	lepidine	4.62	NMR	4.2	100	25	D_2O, pD ~9 (borate-*d*)	89
	1-methylindole	3.58	NMR			22	D_2O, pD ~9 (borate-*d*)	88
	1-methylindole	3.67	NMR	1.3	75	25	D_2O, pD ~9 (borate-*d*)	89
	1-methylisoquinoline	5.00	NMR			22	D_2O, pD ~9 (borate-*d*)	88
	quinaldine	4.30	NMR			22	D_2O, pD ~9 (borate-*d*)	88
	quinoline	4.34	NMR			22	D_2O, pD ~9 (borate-*d*)	88
	quinoline	4.70	NMR	-31.4	-16	25	D_2O, pD ~9 (borate-*d*)	89

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
$Nap_2(1,4\text{-}B)_2$-34C4-1 (VIII)	camphor	2.16	NMR			20	MeOD-d_3/D_2O (50:50 v/v)	90
	chenodeoxycholic acid	2.91	NMR			20	MeOD-d_3/D_2O (50:50 v/v) 0.01 M Na_2CO_3	90
	cholic acid	2.16	NMR			20	MeOD-d_3/D_2O (50:50 v/v) 0.01 M Na_2CO_3	90
	cortisone	3.18	NMR			20	MeOD-d_3/D_2O (50:50 v/v)	90
	deoxycholic acid	2.40	NMR			20	MeOD-d_3/D_2O (50:50 v/v) 0.01 M Na_2CO_3	68, 90
	hydrocortisone	3.04	NMR			20	MeOD-d_3/D_2O (50:50 v/v)	90
	lithocholic acid	3.85	NMR			20	MeOD-d_3/D_2O (50:50 v/v) 0.01 M Na_2CO_3	68, 90
	testosterone	3.55	NMR			20	MeOD-d_3/D_2O (50:50 v/v)	90
	ursodeoxycholic acid	3.24	NMR			20	MeOD-d_3/D_2O (50:50 v/v) 0.01 M Na_2CO_3	90
	guest-10[e]	2.92	NMR			20	MeOD-d_3/D_2O (50:50 v/v) 0.01 M Na_2CO_3	90
	guest-11[e]	2.66	NMR			20	MeOD-d_3/D_2O (50:50 v/v)	90
	guest-12[e]	2.72	NMR			20	MeOD-d_3/D_2O (50:50 v/v) 0.01 M Na_2CO_3	90
	guest-13[e]	2.30	NMR			20	MeOD-d_3/D_2O (50:50 v/v) 0.01 M Na_2CO_3	90
	guest-14[e]	2.57	NMR			20	MeOD-d_3/D_2O (50:50 v/v) 0.01 M Na_2CO_3	90
	guest-15[e]	2.64	NMR			20	MeOD-d_3/D_2O (50:50 v/v) 0.01 M Na_2CO_3	90
	guest-16[e]	2.63	NMR			20	MeOD-d_3/D_2O (50:50 v/v) 0.01 M Na_2CO_3	90
			2. Cyclophanes (cont.)					
			b. Monocyclic with Nitrogen Donor Atoms					
$(1,4\text{-}B)_3N_321C3$-1 (IX)	1-(2-pyridylazo)-2-naphthol	5.87	Spec			30	H_2O, 0.1 M KCl, pH 8 (0.01 M HEPES)	91, 92
$(1,4\text{-}B)_3N_321C3$-2 (IX)	1-(2-pyridylazo)-2-naphthol	7.58	Spec			30	H_2O, 0.1 M KCl pH 8 (0.01 M HEPES)	93
$K_4Py_2(1,4\text{-}B)_2N_4$-26C4-1 (IX)	*N*-benzyl-1,4-dihydronicotinamide	3.15	Fluor			30	Me_2SO/H_2O (5:95 v/v), 0.1 M KCl, pH 10 (0.01 M CAPS)	94, 95
	indole	3.83	Fluor			30	Me_2SO/H_2O (5:95 v/v), pH 10 (0.01 M CAPS)	95
	indole	3.63	Fluor			30	Me_2SO/H_2O (5:95 v/v), 0.1 M KCl, pH 10 (0.01 M CAPS)	94
	N-phenyl-1-aminonaphthalene	2.86	Fluor			30	Me_2SO/H_2O (5:95 v/v), 0.1 M KCl, pH 10 (0.01 M CAPS)	94, 95
$K_4Py_2(1,4\text{-}B)_2N_4$-26C4-2 (IX)	*N*-benzyl-1,4-dihydronicotinamide	3.76	Fluor			30	Me_2SO/H_2O (5:95 v/v), 0.1 M KCl, pH 10 (0.01 M CAPS)	94, 95
	indole	4.11	Fluor			30	Me_2SO/H_2O (5:95 v/v), pH 10 (0.01 M CAPS)	95
	indole	3.66	Fluor			30	Me_2SO/H_2O (5:95 v/v), 0.1 M KCl, pH 10 (0.01 M CAPS)	94
	N-phenyl-1-aminonaphthalene	none	Fluor			30	Me_2SO/H_2O (5:95 v/v), 0.1 M KCl, pH 10 (0.01 M CAPS)	94, 95
$(1,4\text{-}B)_4N_428C4$-1 (IX)	*N*-phenyl-1-aminonaphthalene	2.79	Fluor			30	H_2O, 0.1 M KCl, pH 10 (0.01 M CAPS)	96

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
(1,4-B)$_4$N$_4$28C4-2 (IX)	*N*-phenyl-1-amino-naphthalene	5.00	Fluor			30	H_2O, 0.1 M KCl, pH 8 (0.01 M HEPES)	97, 98
	N-phenyl-2-amino-naphthalene	5.36	Fluor			30	H_2O, 0.1 M KCl, pH 8 (0.01 M HEPES)	97, 98
(1,4-B)$_4$N$_4$28C4-3 (IX)	*N*-phenyl-1-amino-naphthalene	5.32	Fluor			30	H_2O, 0.1 M KCl, pH 8 (0.01 M HEPES)	98
	N-phenyl-2-amino-naphthalene	5.15	Fluor			30	H_2O, 0.1 M KCl, pH 8 (0.01 M HEPES)	98
(1,4-B)$_4$N$_4$28C4-4 (IX)	*N*-phenyl-1-amino-naphthalene	3.32	Fluor			30	H_2O, 0.1 M KCl, pH 4 (acetate buffer)	99
K$_4$(1,4-B)$_4$N$_4$-28C4-1 (IX)	*N*-benzyl-1,4-di-hydronicotinamide	none	Fluor			30	Me_2SO/H_2O (5:95 v/v), 0.1 M KCl, pH 10 (0.01 M CAPS)	94, 95
	indole	3.40	Fluor			30	Me_2SO/H_2O (5:95 v/v), pH 10 (0.01 M CAPS)	95
	indole	3.18	Fluor			30	Me_2SO/H_2O (5:95 v/v), 0.1 M KCl, pH 10 (0.01 M CAPS)	94, 96
	N-phenyl-1-amino-naphthalene	none	Fluor			30	Me_2SO/H_2O (5:95 v/v), 0.1 M KCl, pH 10 (0.01 M CAPS)	94, 95
K$_4$(1,4-B)$_4$N$_4$-28C4-2 (IX)	*N*-benzyl-1,4-di-hydronicotinamide	3.30	Fluor			30	Me_2SO/H_2O (5:95 v/v), 0.1 M KCl, pH 10 (0.01 M CAPS)	94,95,96
	indole	3.40	Fluor			30	Me_2SO/H_2O (5:95 v/v), pH 10 (0.01 M CAPS)	95
	indole	3.18	Fluor			30	Me_2SO/H_2O (5:95 v/v), 0.1 M KCl, pH 10 (0.01 M CAPS)	94, 96
	N-phenyl-1-amino-naphthalene	3.20	Fluor			30	Me_2SO/H_2O (5:95 v/v), 0.1 M KCl, pH 10 (0.01 M CAPS)	94,95,96
	1-(2-pyridylazo)-2-naphthol	3.17	Spec			39.4	Me_2SO/EtOH/H_2O (10:1:89 v/v) 0.15 M KCl, pH 10.29	100
K$_4$(1,4-B)$_4$N$_4$-28C4-3 (IX)	1-(2-pyridylazo)-2-naphthol	2.55	Spec	2.55		30	EtOH/MeOH/H_2O (5:2:95 v/v), 0.1 M KCl, pH 8.7	101
K$_4$(1,4-B)$_4$N$_4$-28C4-4 (IX)	*N*-phenyl-1-amino-naphthalene	3.66	Fluor			30	EtOH/H_2O (5:95 v/v), 0.1 M KCl, pH 6 (0.01 M MES)	95,96,102
	1-(2-pyridylazo)-2-naphthol	2.51	Spec			30	H_2O, 0.1 M KCl, pH 6 (0.01 M MES)	96
K$_4$(1,4-B)$_4$N$_4$-28C4-5 (IX)	*N*-phenyl-1-amino-naphthalene	6.11	Fluor			30	EtOH/H_2O (5:95 v/v), 0.1 M KCl, pH 6 (0.01 M MES)	95,96,102
	1-(2-pyridylazo)-2-naphthol	5.57	Spec			30	EtOH/H_2O (5:95 v/v), 0.1 M KCl, pH 6 (0.01 MES)	96,103

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
$K_4(1,4\text{-B})_4N_4$-28C4-6 (IX)	*N*-phenyl-1-amino-naphthalene	5.41	Fluor			30	EtOH/H_2O (5:95 v/v), 0.1 M KCl, pH 8 (0.01 M HEPES)	96, 103
	pyrene	6.08	Fluor			30	EtOH/H_2O (0.1:99.9 v/v) 0.1 M KCl, pH 8 (0.01 M HEPES)	92,96,103
	pyrene	6.38(M_2L)	Fluor			30	EtOH/H_2O (0.1:99.9 v/v) 0.1 M KCl, pH 8 (0.01 M HEPES) (M + ML <-> M_2L)	92,96,103
$Py_4(1,4\text{-B})_2$-28C4-1 (IX)	1,2-dimethoxy-benzene	0.90	Spec			?	MeCN	104
	1,3-dimethoxy-benzene	0.90	Spec			?	MeCN	104
	1,4-dimethoxy-benzene	1.23	Spec			?	MeCN	104, 105
$(1,4\text{-B})_4N_430C4$-1 (X)	2,7-dihydroxy-naphthalene	3.45	Fluor			25	H_2O, pH 1.95 (KCl/HCl buffer)	106, 107
$(1,4\text{-B})_4N_430C4$-2 (X)	benzene	3.00	NMR			27	D_2O	108
	biphenyl	3.92	NMR			27	D_2O	108
	2,7-dihydroxy-naphthalene	2.90	NMR			?	MeOD-d_3/0.33 M DCl-D_2O (10:40)	109
	naphthalene	3.65	NMR			27	D_2O	108
	tetralin	3.23	NMR			27	D_2O	108
	toluene	3.01	NMR			27	D_2O	108
$(1,4\text{-B})_4N_430C4$-3 (X)	2,7-dihydroxy-naphthalene	3.18	NMR			28	D_2O	109, 110
$(1,4\text{-B})_4N_630C6$-1 (X)	4-acetylphenol	0.81	NMR			?	D_2O/DCl, pH < 3	111
	4-chlorophenol	1.23	NMR			?	D_2O/DCl, pH < 3	111
	p-cresol	1.76	NMR			?	D_2O/DCl, pH < 3	111
	4-methoxyphenol	1.18	NMR			?	D_2O/DCl, pH < 3	111
	4-nitrophenol	0.46	NMR			?	D_2O/DCl, pH < 3	111
$(1,4\text{-B})_4(1,3\text{-B})_2$-$N_432C4$-1 (X)	1,4-benzoquinone	2.00	NMR			room	$CDCl_3$/MeOD-d_3 (90:10)	112
	1,4-benzoquinone	3.08	NMR			room	$CDCl_3$	112
$Py_2(1,4\text{-B})_4N_4$-32C6-1 (X)	4-nitrophenol	1.30	NMR			25	D_2O	113
$(1,4\text{-B})_4N_433C4$-1 (X)	2,7-dihydroxy-naphthalene	2.41	Fluor			25	H_2O, pH 1.95 (KCl/HCl buffer)	106, 107
$(1,4\text{-B})_4N_434C4$-1 (X)	1-aminonaphthalene	3.33	NMR			25	D_2O	114
	1-aminonaphthalene	2.77	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	115
	benzene	1.77	NMR			25	D_2O	116
	benzene	1.75	NMR			25	MeOD-d_3/D_2O (5:95 v/v)	117
	benzyl bromide	1.40	NMR			30	Diox-H_2O (50:50)	118
	2-bromomethyl-naphthalene	0.54	NMR			30	Diox-H_2O (50:50)	118
	p-cresol	1.76	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	119
	dansylamide	3.70	Fluor			25	H_2O	120
	dansylamide	3.68	Fluor			25	H_2O, pH ~7	121
	dansylamide	3.68	Fluor			25	H_2O, [L] = <0.001 M	121
	dansylamide	3.69	Fluor			25	H_2O, 0.1 M NaCl	121
	dansylamide	3.45	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	122
	dansylamide	2.97	Fluor			25	MeOH/H_2O (20:80 v/v), pH ~7	121
	dansylamide	2.11	NMR			25	MeOD-d_3/D_2O (50:50 v/v), pH ~7	121
	dansylamide	3.20	NMR			25	MeOD-d_3/D_2O (50:50 v/v)	120
	dansylamide	3.45	Fluor			25	MeOH/H_2O (10:90 v/v), pH ~7	121
	decalin	1.17	Sol			25	H_2O	119, 123
	4,4-diaminodi-phenylmethane	2.54	NMR			25	MeOD-d_3/D_2O (5:95 v/v)	117

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	dichloromethane	<0.18	NMR			25	MeOD-d_3/D_2O (10:90 v/v)	117
	2,7-dihydroxy-naphthalene	2.95	NMR			28	D_2O	110
	diiodomethane	1.32	NMR			25	MeOD-d_3/D_2O (10:90 v/v)	117
	3,5-dimethyl-cyclohexanol	0.37-0.81	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	119
	3,5-dimethylphenol	1.98	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	119
	diphenylamine	2.54	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	117
	trans-4-methyl-cyclohexanol	0.59	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	119
	1-methyl-naphthalene	3.15	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	122
	2-methyl-naphthalene	3.01	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	122
	naphthalene	3.09	NMR			25	D_2O	116
	naphthalene	3.33	NMR			25	D_2O	114
	naphthalene	2.93	Sol			25	H_2O	119, 123
	naphthalene	3.03	NMR			25	MeOD-d_3/D_2O (10:90 v/v)	117
	naphthalene	2.93	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	119,122,123
	naphthalene	2.96	NMR			25	MeOD-d_3/D_2O (20:80 v/v) pH ~7	115, 121
	naphthalene	2.86	Fluor			25	MeOH/H_2O (20:80 v/v) 0.01 M NaCl	122
	naphthalene	1.88	NMR			25	MeOD-d_3/D_2O (50:50 v/v) pH ~7	121
	naphthalene	0.90	NMR			25	MeOD-d_3/D_2O (80:20 v/v) pH ~7	121
	naphthoic acid	3.16	NMR			25	D_2O	114
	1-naphthol	3.68	NMR			25	D_2O	114
	1-naphthol	3.15	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	122, 123
	2-naphthol	3.33	NMR			25	D_2O	114
	2-naphthol	2.86	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	119,122,123
	nitrophenyl acetate	2.05	NMR			25	MeOD-d_3/D_2O (10:90 v/v) pH ~7	121
	nitrophenyl acetate	1.81	NMR			25	MeOD-d_3/D_2O (20:80 v/v) pH ~7	121
	nitrophenyl acetate	1.58	NMR			25	MeOD-d_3/D_2O (30:70 v/v) pH ~7	121
	5,6,7,8,-tetra-hydro-2-naphthol	1.98	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	119
	tetralin	2.44	NMR			25	D_2O	116
	tetralin	1.98	Sol			25	H_2O	119, 123
	tetralin	2.27	NMR			25	MeOD-d_3/D_2O (20:08 v/v)	119
	toluene	2.10	NMR			25	D_2O	116
	guest-17[e]	7.34	Fluor			25?	H_2O (ethidium bromide as indicator)	124
	guest-18[e]	4.77	Fluor			25?	H_2O (ethidium bromide as indicator)	124
	guest-19[e]	4.40	Fluor			25?	H_2O (ethidium bromide as indicator)	124
	guest-20[e]	5.14	Fluor			25?	H_2O (ethidium bromide as indicator)	124
(1,4-B)$_4$N$_4$34C4-2 (X)	1-aminonaphthalene	2.58	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	115
	p-cresol	1.32	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	119
	3,5-dimethyl-cyclohexanol	0.66-1.10	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	119
	3,5-dimethylphenol	1.17	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	119
	trans-4-methyl-cyclohexanol	0.73-1.25	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	119
	naphthalene	2.27	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	115, 119
(1,4-B)$_4$N$_4$34C4-3 (X)	1-aminonaphthalene	2.02	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	115
	naphthalene	2.35	NMR			25	MeOD-d_3/D_2O (20:80 v/v)	115
(1,4-B)$_4$N$_4$34C4-4 (X)	β-estradiol	1.32	NMR			25?	MeOD-d_3/D_2O (50:50 v/v)	125
	5,6,7,8-tetrahydro-2-naphthol	2.00	NMR			25?	MeOD-d_3/D_2O (20:80 v/v)	125
Cy_2(1,4-B)$_4$N$_4$-34C4-1 (XI)	2,7-dihydroxy-naphthalene	3.63	Fluor			25	H_2O, pH 1.95 (KCl/HCl buffer)	107

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
$Cy_2(1,4\text{-}B)_4N_4$-34C4-2 (XI)	2,7-dihydroxy-naphthalene	3.63	Fluor			25	H_2O, pH 1.95 (KCl/HCl buffer)	106
$Nap_2(1,4\text{-}B)_2N_4$-34C4-1 (XI)	2,7-dihydroxy-naphthalene	2.30	NMR			?	MeOD-d_3/0.33 M DCl-D_2O (10:40)	109
$Nap_2(1,4\text{-}B)_2N_4$-34C4-2 (XI)	2,7-dihydroxy-naphthalene	2.48	NMR			?	D_2O	109
	2,7-dihydroxy-naphthalene	2.52	NMR			28	D_2O	110
$Nap_2(1,4\text{-}B)_2N_4$-36C4-1 (XI)	2,7-dihydroxy-naphthalene	2.40	NMR			28	D_2O	110
$Nap_2(1,4\text{-}B)_2N_4$-38C4-1 (XI)	2,7-dihydroxy-naphthalene	2.49	NMR			28	D_2O	110
$(1,4\text{-}B)_4N_4$38C4-1 (XI)	naphthalene	2.63	NMR			25	D_2O	116
	tetralin	2.10	NMR			25	D_2O	116
Cholaphane-1 (XI)	guest-21[e]	3.24	NMR			25?	$CDCl_3$	126
Cholaphane-2 (XI)	guest-21[e]	none	NMR			25?	$CDCl_3$ (no significant spectra changes)	126
Cholaphane-3 (XI)	guest-21[e]	none	NMR			25?	$CDCl_3$ (no significant spectra changes)	126
Cholaphane-4 (XI)	guest-21[e]	none	NMR			25?	$CDCl_3$ (no significant spectra changes)	126
Cholaphane-5 (XI)	guest-21[e]	2.85	NMR			25?	$CDCl_3$	126
			2. Cyclophanes (cont.)					
			c. Monocyclic with Various Donor Atoms					
$NapPyN_220C5$-1 (XII)	*N*-butylthymine[e]	2.46	NMR			25	$CDCl_3$	127,128,129
	guest-22[e]	3.65	Fluor			25	$CDCl_3$	130
	guest-23[e]	none	Fluor			25	$CDCl_3$	130
	guest-24[e]	3.54	Fluor			25	$CDCl_3$	130
	guest-25[e]	none	Fluor			25	$CDCl_3$	130
$NapPyN_220C5$-2 (XII)	*N*-butylthymine[e]	2.76	NMR			25	$CDCl_3$	129, 131
$NapPyN_220C5$-3 (XII)	*N*-butylthymine[e]	2.14	NMR			25	$CDCl_3$	129, 131
$NapPyN_220C5$-4 (XII)	guest-27[e]	3.20	NMR			25	$CDCl_3$	132
$NapPyN_222C5$-1 (XII)	*N*-butyltymine[e]	2.40	NMR			25	$CDCl_3$	127
$NapPy_2N_223C6$-1 (XII)	9-butyladenine[e]	1.86	Spec			25	$CDCl_3$	133
$NapPy_2N_225C6$-1 (XII)	9-butyladenine[e]	3.51	Spec			25	$CDCl_3$	133
NapNaphthyrN-23C7-1 (XII)	2',3',5'-tri-*O*-pentanoylguanosine[e]	2.85	NMR			25	$CDCl_3$	134
NapNaphthyrN-25C7-1 (XII)	2',3',5'-tri-*O*-pentanoylguanosine[e]	2.73	NMR			25	$CDCl_3$	127, 134
$(1,4\text{-}B)_4N_428C6$-1 (XII)	*p*-cresol	1.05	NMR			25	D_2O	135
	4-cyanophenol	1.70	NMR			25	D_2O	135
	4-toluenosulfonic acid	1.74	NMR			25	D_2O	135
	2,4,6-trimethyl-phenol	1.10	NMR			25	D_2O	135
$(1,4\text{-}B)_4N_430C6$-1 (XII)	*p*-cresol	1.22	NMR			25	D_2O	135
	4-cyanophenol	1.48	NMR			25	D_2O	135
	4-toluenosulfonic acid	1.82	NMR			25	D_2O	135

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	2,4,6-trimethylphenol	1.15	NMR			25	D_2O	135
(1,4-B)$_4$N$_4$30C6-2 (XII)	*p*-cresol	1.72	NMR			25?	D_2O, pD 1.9 (0.1 M KCl/DCl buffer)	136
	4-cyanophenol	2.22	NMR			25?	D_2O, pD 1.9 (0.1 M KCl/DCl buffer)	136
	1,3-dihydroxynaphthalene	2.52	NMR			25?	D_2O, pD 2.3 (0.1 M KCl/DCl buffer)	136
	4-methoxyphenol	1.77	NMR			25?	D_2O, pD 1.9 (0.1 M KCl/DCl buffer)	136
	4-nitrophenylacetate	2.15	NMR			25?	MeOD-d_3/D_2O (1:9)	136
	4-toluenesulfonic acid	2.52	NMR			25?	D_2O, pD 1.9 (0.1 M KCl/DCl buffer)	136
	2,4,6-trimethylphenol	2.00	NMR			25?	D_2O, pD 1.9 (0.1 M KCl/DCl buffer)	136
(1,4-B)$_4$N$_4$30C6-3 (XII)	*p*-cresol	1.64	NMR			25?	D_2O, pD 1.9 (0.1 M KCl/DCl buffer)	136
	4-cyanophenol	1.82	NMR			25?	D_2O, pD 1.9 (0.1 M KCl/DCl buffer)	136
	1,3-dihydroxynaphthalene	2.30	NMR			25?	D_2O, pD 2.3 (0.1 M KCl/DCl buffer)	136
	4-toluenesulfonic acid	2.40	NMR			25?	D_2O, pD 1.9 (0.1 M KCl/DCl buffer)	136
	2,4,6-trimethylphenol	1.85	NMR			25?	D_2O, pD 1.9 (0.1 M KCl/DCl buffer)	136
(1,4-B)$_4$N$_4$30C6-4 (XII)	*p*-cresol	1.64	NMR			25	D_2O	135
	p-cresol	1.63	NMR			25	D_2O, pD 1.8 (KCl/DCl buffer)	137
	4-cyanophenol	1.82	NMR			25	D_2O	135
	4-cyanophenol	1.89	NMR			25	D_2O, pD 1.8 (KCl/DCl buffer)	137
	4-toluenesulfonic acid	2.40	NMR			25	D_2O, pD 1.8 (KCl/DCl buffer)	137
	2,4,6-trimethylphenol	1.82	NMR			25	D_2O	135
	2,4,6-trimethylphenol	1.88	NMR			25	D_2O, pD 1.8 (KCl/DCl buffer)	137
N$_4$S$_2$30C6-1 (XII)	(-) menthol	3.40	NMR			20	D_2O, pD 9 ($ND_4^+Cl^-$/ND_3 buffer)	138
	(+) menthol	3.30	NMR			20	D_2O, pD 9 ($ND_4^+Cl^-$/ND_3 buffer)	138
	(+) isomenthol	3.00	NMR			20	D_2O, pD 9 ($ND_4^+Cl^-$/ND_3 buffer)	138
Nap(1,3-B)Py$_2$N$_2$-32C8-1 (XIII)	diethylmalonic acid	3.04	NMR			25	$CDCl_3$	139
	ethylmalonic acid	3.86	NMR			25	$CDCl_3$	139
Nap(1,3-B)Py$_2$N$_2$-32C8-2 (XIII)	barbital	2.49	NMR			25	$CDCl_3$	140
Nap(1,3-B)Py$_2$N$_4$-32C8-1 (XIII)	barbital	5.13	NMR			25	$CDCl_3$	127
	barbital	5.40	Spec			25	CH_2Cl_2	140
	cyclic urea[e]	2.60	NMR			25	$CDCl_3$	140
	DL-glutethimide	2.94	NMR			25	$CDCl_3$	140
	mephobarbital	2.69	NMR			25	$CDCl_3$	140
	phenobarbital	5.45	NMR			25	$CDCl_3$	127
	thiobarbital	2.87	NMR			25	$CDCl_3$	140
NapPy$_3$N$_4$32C8-1 (XIII)	barbital	4.61	Spec			25	CH_2Cl_2	140
(1,3-B)(1,4-B)-Py$_2$N$_4$34C8-1 (XIII)	barbital	6.14	NMR			25	$CDCl_3$	127, 141
	barbital	5.78	Spec			25	CH_2Cl_2	140

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	mephobarbital	2.83	NMR			25	$CDCl_3$	127, 140, 141
	phenobarbital	5.29	NMR			25	$CDCl_3$	27, 141
$Py_6Pd_4$36C4-1 (XIII)	1,4-benzenedimethanol	<1	NMR			25	D_2O	142
	1,4-bis(methoxymethyl)benzene	1.00	NMR			25	D_2O	142
	1,2-dimethoxybenzene	1.48	NMR			25	D_2O	142
	1,3-dimethoxybenzene	2.76	NMR			25	D_2O	142
	1,4-dimethoxybenzene	2.52	NMR			25	D_2O	142
	1,4-dimethoxycyclohexane	none	NMR			25	D_2O	142
	4-methoxybenzyl methyl sulfoxide	2.23	NMR			25	D_2O	142
	2,4-dimethyl-2-pentanol	1.48	NMR			25	D_2O	142
	1,3,5-trimethoxybenzene	2.88	NMR			25	D_2O	142, 143
$Py_6Pt_4$36C4-1 (XIII)	1,2-dimethoxybenzene	1.30	NMR			25	D_2O	142
	1,3-dimethoxybenzene	2.74	NMR			25	D_2O	142
	1,4-dimethoxybenzene	2.41	NMR			25	D_2O	142
$(NapPyN_220C5)_2$-1 (XIV)	guest-28[e]	4.31	NMR			25	$CDCl_3$	132
Flavinophane-1 (XIV)	6-cyano-2-naphthol	2.21	NMR			20	D_2O, pD 10.4 (borate-*d*) (apparent K)	81,144,145
	6-methoxy-2-naphthoic acid	2.97	NMR			22	D_2O, pD 10.4 (borate-*d*) (apparent K)	81, 145
	6-methoxy-2-naphthol	2.45	NMR			22	D_2O, pD 10.4 (borate-*d*) (apparent K)	145
	2-naphthol	2.16	NMR			22	D_2O, pD 10.4 (borate-*d*) (apparent K)	145
Flavinophane-2 (XIV)	6-cyano-2-naphthol	2.39	NMR			20	D_2O, pD 10.4 (borate-*d*) (true K)	144
	6-cyano-2-naphthol	2.36	NMR			22	D_2O, pD 10.4 (borate-*d*) (true K)	81, 145
	6-methoxy-2-naphthoic acid	2.46	NMR			22	D_2O, pD 10.4 (borate-*d*) (true K)	81, 145
	6-methoxy-2-naphthol	2.51	NMR			22	D_2O, pD 10.4 (borate-*d*) (true K)	145
	2-naphthol	2.30	NMR			22	D_2O, pD 10.4 (borate-*d*) (true K)	145
			2. Cyclophanes (cont.)					
			d. Mono- and Bi-cyclic without Heteroatoms					
(1,3-B)(1,4-B)-11C-1 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	2.08	Spec			20	CH_2Cl_2	146
	tetracyanoethylene	1.89	Spec			20	CH_2Cl_2	146
(1,3-B)(1,4-B)-11C-2 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	1.97	Spec			20	CH_2Cl_2	146
	tetracyanoethylene	1.81	Spec			20	CH_2Cl_2	146
(1,3-B)(1,4-B)-11C-3 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	1.86	Spec			20	CH_2Cl_2	146
	tetracyanoethylene	1.72	Spec			20	CH_2Cl_2	146
$(1,4\text{-B})_2$12C-1 (XV)	I_2	0.37	Spec			25	CH_2Cl_2	147
	2,3-dichloro-5,6-dicyanobenzoquinone	0.83	Spec			25	CH_2Cl_2	148
	tetracyanoethylene	3.63	Spec			25	CH_2Cl_2 (apparent K)	149

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
(1,4-B)$_2$12C-2 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	2.14	Spec			20	CH_2Cl_2	146
	tetracyanoethylene	1.94	Spec			20	CH_2Cl_2	146
(1,4-B)$_2$12C-3 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	2.11	Spec			20	CH_2Cl_2	146
	tetracyanoethylene	1.91	Spec			20	CH_2Cl_2	146
(1,4-B)$_2$12C-4 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	1.98	Spec			20	CH_2Cl_2	146
	tetracyanoethylene	1.85	Spec			20	CH_2Cl_2	146
(1,4-B)$_2$12C-5 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	1.96	Spec			20	CH_2Cl_2	146
	tetracyanoethylene	1.83	Spec			20	CH_2Cl_2	146
(1,4-B)$_2$12C-6 (XV)	I_2	0.54	Spec			25	CH_2Cl_2	147
	2,3-dichloro-5,6-dicyanobenzoquinone	0.85	Spec			25	CH_2Cl_2	148
	tetracyanoethylene	3.95	Spec			25	CH_2Cl_2 (apparent K)	149
(1,4-B)$_2$12C-7 (XV)	I_2	0.97	Spec			25	CH_2Cl_2	147
	2,3-dichloro-5,6-dicyanobenzoquinone	1.01	Spec			25	CH_2Cl_2	148
	2,3-dichloro-5,6-dicyanobenzoquinone	4.93	Spec			25	CH_2Cl_2 (apparent K)	149
	tetrachloro-1,4-benzoquinone	3.28	Spec			25	CH_2Cl_2 (apparent K)	149
	tetrachloro-1,4-benzoquinone	0.90	Spec			25	CH_2Cl_2	148
	tetracyanoethylene	4.42	Spec			25	C_6H_6 (apparent K)	149
	tetracyanoethylene	1.99	Spec			22	CH_2Cl_2	150
	tetracyanoethylene	4.65	Spec			25	CH_2Cl_2 (apparent K)	149
	tetracyanoethylene	4.21	Spec			25	$(C_2H_5)_2O$ (apparent K)	149
(1,4-B)$_2$12C-8 (XV)	I_2	0.81	Spec			25	CH_2Cl_2	147
(1,4-B)$_2$12C-9 (XV)	I_2	0.12	Spec			25	CH_2Cl_2	147
(1,4-B)$_2$12C-10 (XV)	I_2	0.11	Spec			25	CH_2Cl_2	147
(1,4-B)$_2$12C-11 (XV)	tetracyanoethylene	2.04	Spec			22	CH_2Cl_2	150
(1,4-B)$_2$12C-12 (XV)	2-dicyanoethylene-1,3-indandione	1.87	Spec			22	CH_2Cl_2	150
	tetracyanoethylene	2.18	Spec			22	CH_2Cl_2	150
(1,4-B)$_2$12C-13 (XV)	2-dicyanoethylene-1,3-indandione	1.26	Spec			22	CH_2Cl_2	150
	tetracyanoethylene	2.05	Spec			22	CH_2Cl_2	150
(1,4-B)$_2$12C-14 (XV)	2-dicyanoethylene-1,3-indandione	2.02	Spec			22	CH_2Cl_2	150
	tetracyanoethylene	2.52	Spec			22	CH_2Cl_2	150
(1,4-B)$_2$12C-15 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	0.87	Spec			25	CH_2Cl_2	148
(1,4-B)$_2$12C-16 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	3.83	Spec			25	CH_2Cl_2	151
	tetracyanoethylene	3.97	Spec			25	CH_2Cl_2	151
(1,4-B)$_2$12C-17 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	3.79	Spec			25	CH_2Cl_2	151
(1,4-B)$_2$12C-18 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	3.98	Spec			25	CH_2Cl_2	151
	tetracyanoethylene	3.99	Spec			25	CH_2Cl_2	151
(1,4-B)$_2$12C-19 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	4.52	Spec			25	CH_2Cl_2	151
(1,4-B)$_2$12C-20 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	1.11	Spec			22	CH_2Cl_2	152
(1,4-B)$_2$12C-21 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	0.99	Spec			22	CH_2Cl_2	152
(1,4-B)$_2$12C-22 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	1.12	Spec			22	CH_2Cl_2	152
(1,4-B)$_2$12C-23 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	1.14	Spec			22	CH_2Cl_2	152
(1,4-B)$_2$12C-24 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	0.98	Spec			22	CH_2Cl_2	152
(1,4-B$_2$12C-25 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	0.97	Spec			22	CH_2Cl_2	152
(1,4-B)$_2$12C-26 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	1.05	Spec			22	CH_2Cl_2	152
(1,4-B)$_2$12C-27 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	1.10	Spec			22	CH_2Cl_2	152
(1,4-B)$_2$12C-28 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	1.00	Spec			22	CH_2Cl_2	152
(1,4-B)$_2$12C-29 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	0.96	Spec			22	CH_2Cl_2	152

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
(1,4-B)$_2$12C-30 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	1.04	Spec			22	CH_2Cl_2	152
(1,4-B)$_2$12C-31 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	1.08	Spec			22	CH_2Cl_2	152
(1,4-B)$_2$12C-32 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	1.90	Spec			20	CH_2Cl_2	153
	tetracyanoethylene	1.71	Spec			20	CH_2Cl_2	153
(1,4-B)$_2$12C-33 (XV)	2-dicyanoethylene-1,3-indandione	1.37	Spec			20	CH_2Cl_2	153
	2,3-dichloro-5,6-dicyanobenzoquinone	1.96	Spec			20	CH_2Cl_2	153
	tetrachloro-1,4-benzoquinone	1.47	Spec			20	CH_2Cl_2	153
	tetracyanoethylene	1.77	Spec			20	CH_2Cl_2	153
	7,7,8,8-tetracyanoquinodimethane	1.08	Spec			20	CH_2Cl_2	153
(1,4-B)$_2$12C-34 (XV)	2-dicyanoethylene-1,3-indandione	1.38	Spec			20	CH_2Cl_2	153
	2,3-dichloro-5,6-dicyanobenzoquinone	1.99	Spec			20	CH_2Cl_2	153
	tetrachloro-1,4-benzoquinone	1.52	Spec			20	CH_2Cl_2	153
	tetracyanoethylene	1.81	Spec			20	CH_2Cl_2	153
	7,7,8,8-tetracyanoquinodimethane	1.17	Spec			20	CH_2Cl_2	153
(1,4-B)$_2$12C-35 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	3.85	Spec			25	CH_2Cl_2	154
	tetrabromo-1,4 benzoquinone	3.32	Spec			25	CH_2Cl_2	154
	tetrachloro-1,4-benzoquinone	3.28	Spec			25	CH_2Cl_2	154
	tetracyanoethylene	3.40	Spec			25	CH_2Cl_2	154
(1,4-B)$_2$12C-36 (XV)	2,3-dichloro-5,6-dicyanobenzoquinone	5.53	Spec			25	CH_2Cl_2	154
	tetrabromo-1,4-benzoquinone	3.91	Spec			25	CH_2Cl_2	154
	tetrachloro-1,4-benzoquinone	3.88	Spec			25	CH_2Cl_2	154
	tetracyanoethylene	3.93	Spec			25	CH_2Cl_2	154
			2. Cyclophanes (cont.)					
			e. Polycyclic with Various Donor Atoms					
(20C6)(29C4)-1 (XVI)	2-cyano-6-methoxynaphthalene	~5	NMR			20	H_2O (extrapolated K)	75
	2-cyano-6-methoxynaphthalene	3.65	NMR			20	MeOD-d_3/D_2O (40:60 v/v)	67,75,76
	2-cyano-6-methoxynaphthalene	2.64	NMR			20	MeOD-d_3/D_2O (40:60 v/v) 0.1 M KCl	67,75,76
	2-cyano-6-methoxynaphthalene	2.15	NMR			20	MeOD-d_3/D_2O (40:60 v/v) 0.05 M KCl	67,75,76
	2-cyano-6-methoxynaphthalene	1.38	NMR			20	MeOD-d_3	67,75,76
Cyclophane-1 (XVI)	4-nitro-1-naphthol	3.18	NMR			25	MeOD-d_3/D_2O (30:70 v/v)	155
Cyclophane-2 (XVI)	4-nitro-1-naphthol	3.54	NMR			25	MeOD-d_3/D_2O (30:70 v/v)	155
Cyclophane-3 (XVI)	durene	1.43	Fluor			30	MeOH	3, 82
	fluoranthene	3.04	NMR			30	Me_2CO-d_6	82
	fluoranthene	4.86	Fluor			30	MeOH	3, 82
	fluoranthene	2.08	NMR			30	THF-d_8	82
	naphthalene	<1	NMR			30	Me_2CO-d_6	82
	naphthalene	2.08	Fluor			30	MeOH	3, 82
	naphthalene	<1	NMR			30	Me_2SO-d_6	82
	naphthalene	<0.48	NMR			30	THF-d_6	82
	perylene	1.43	NMR			30	C_6D_6	82
	perylene	1.62	NMR			30	$CDCl_3$	82
	perylene	2.56	NMR			30	DMF-d_7	82
	perylene	5.28	Fluor			10	EtOH	82
	perylene	5.03	Fluor			20	EtOH	82
	perylene	4.80	Fluor	-44.8	-56.1	30	EtOH	3, 82
	perylene	4.53	Fluor			40	EtOH	82
	perylene	4.28	Fluor			50	EtOH	82
	perylene	3.34	Fluor			30	Me_2CO	82
	perylene	3.18	NMR			30	Me_2CO-d_6	82
	perylene	5.04	Fluor			30	MeOH	3,68,82

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	perylene	2.90	NMR			30	Me_2SO-d_6	82
	perylene	2.18	NMR			30	THF-d_8	82
	pyrene	~4	Sol-EAS			20-22	H_2O, 0.5 M KH_2PO_4	3
	pyrene	1.08	NMR			30	C_6D_6	68,82,156
	pyrene		Cal	-3.35	9.67	30	C_6H_6	79
	pyrene	1.63	NMR			30	$CDCl_3$	68,82,156
	pyrene		Cal	-13.0	-11.0	30	$CHCl_3$	79
	pyrene	2.08	NMR			30	CD_2Cl_2	68, 156
	pyrene	0.95	NMR			30	CS_2	68,82,156
	pyrene	3.04	NMR			30	DMAC/Me_2SO-d_6 (90:10 v/v)	68, 156
	pyrene	3.17	Cal	-8.37	33.1	30	DMAC	79
	pyrene	2.20	NMR			30	DMF-d_7/Me_2SO-d_6 (90:10 v/v)	68, 156
	pyrene		Cal	-15.5	-11.0	30	DMF	79
	pyrene	2.20	NMR			30	DMF-d_7	68,82,156
	pyrene	4.42	NMR			30	EtOD-d_5	82
	pyrene		Cal	-46.0	-67.7	30	EtOH	79
	pyrene	4.40	Fluor			30	EtOH	68,82,156
	pyrene	4.38	Tit-EAS			30	EtOH	82
	pyrene	5.26	Fluor			30	ethylene glycol/Me_2SO (90:10 v/v)	68, 156
	pyrene	4.48	Fluor			30	Form/Me_2SO (90:10 v/v)	68, 156
	pyrene	3.17	Cal	-27.6	-31.8	30	Me_2CO	79
	pyrene	3.08	Fluor			30	Me_2CO	68,82,156
	pyrene	2.92	Tit-EAS			30	Me_2CO	82
	pyrene	2.95	NMR			30	Me_2CO-d_6	82
	pyrene	4.52	NMR			30	MeOD-d_3	82
	pyrene	4.62	Cal	-50.2	-77.3	30	MeOH	79
	pyrene	4.64	Fluor			30	MeOH	3,68,82,156
	pyrene	4.53	Tit-EAS			30	MeOH	82
	pyrene	6.78	Fluor			30	Me_2SO/H_2O (1:99 v/v) 0.001 M Na_2CO_3	68, 156
	pyrene	2.81	Cal	-26.8	-34.5	30	Me_2SO	79
	pyrene	2.84	NMR			30	Me_2SO-d_6	68,82,156
	pyrene	4.18	Fluor			30	*N*-methylacetamide/ Me_2SO (90:10 v/v)	68, 156
	pyrene		Cal	-37.7	-44.2	30	*N*-methylacetamide	79
	pyrene	3.68	Fluor			30	NMF/Me_2SO (90:10 v/v)	68, 156
	pyrene		Cal	-23.4	-6.90	30	NMF	79
	pyrene		Cal	-12.6	-4.14	30	THF	79
	pyrene	1.92	NMR			30	THF-d_8	68,82,156
	pyrene	5.62	Fluor			30	2,2,2-trifluoroethanol/ Me_2SO/ (99:1 v/v)	68, 156
	pyrene		Cal	-83.7	-168	30	2,2,2-trifluoroethanol	79
Cyclophane-4 (XVI)	naphthalene	4.08	Sol-EAS			20-22	H_2O, 0.5 M KH_2PO_4	82, 157
	naphthalene	4.20	Solv Extr-EAS			20-22	H_2O, 0.5 M KH_2PO_4	3, 82
	naphthalene	1.40	NMR			30	MeOD-d_3	82
	perylene	<0.48	NMR			30	$CDCl_3$	82
	perylene	1.04	NMR			30	DMF-d_7	82
	perylene	2.75	Tit-EAS			30	MeOH	68, 82
	perylene	1.58	NMR			30	Me_2SO-d_6	82
	pyrene	6.61	Sol-EAS			20-22	H_2O, 0.5 M KH_2PO_4	82, 157
	pyrene	6.49	Solv Extr-EAS			20-22	H_2O, 0.5 M KH_2PO_4	3, 82
	pyrene	<1	NMR			30	DMF-d_7	82
	pyrene	1.74	NMR			30	MeOD-d_3	82
	pyrene	1.81	Tit-EAS			30	MeOH	3, 82
	pyrene	1.43	NMR			30	Me_2SO-d_6	82
	pyrene	<30	NMR			30	THF-d_8	82
Cyclophane-5 (XVI)	*N*-acetylmethyl-L-histidine	1.32	NMR			25?	$CDCl_3$	158
	N-acetylmethyl-L-phenylalanine	none	NMR			25?	$CDCl_3$	158
	4-aminopyridine	2.20	NMR			25?	$CDCl_3$	158
	aniline	none	NMR			25?	$CDCl_3$	158
	benzimidazole	3.37	NMR			25?	$CDCl_3$	158
	benzotriazole	3.08	NMR			25?	$CDCl_3$	158
	imidazole	3.30	NMR			25?	$CDCl_3$	158
	2-methyl-benzimidazole	1.94	NMR			25?	$CDCl_3$	158
	1-methylimidazole	none	NMR			25?	$CDCl_3$	158
	2-methylimidazole	2.53	NMR			25?	$CDCl_3$	158
	4-methylimidazole	3.12	NMR			25?	$CDCl_3$	158
	pyrazole	none	NMR			25?	$CDCl_3$	158
	pyridine	none	NMR			25?	$CDCl_3$	158

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	2-pyridinol	2.71	NMR			25?	$CDCl_3$	158
	3-pyridinol	2.86	NMR			25?	$CDCl_3$	158
	4-pyridinol	3.56	NMR			25?	$CDCl_3$	158
	pyrrole	none	NMR			25?	$CDCl_3$	158
Cyclophane-6 (XVI)	imidazole	1.82	UV			25	*t*-BuOH	159
	imidazole	2.75	UV			25	*t*-butyl methyl ester	159
	imidazole	3.91	UV			25	CH_3CCl_3	159
	imidazole	2.69	UV			25	$CHCl_3$	159
	imidazole	2.38	UV			25	CH_2Cl_2	159
	imidazole	5.11	UV			25	$(CHCl_2)_2$	159
	imidazole	1.94	UV			25	Diox	159
	imidazole	none	UV			25	MeCN	159
	imidazole	1.89	UV			25	2-Me-THF	159
	imidazole	2.19	UV			25	2,2-Me_2-THF	159
	imidazole	2.27	UV			25	2,5-Me_2-THF	159
	imidazole	3.03	UV			25	2,2,5,5-Me_4-THF	159
	imidazole	1.11	UV			25	*i*-PrOH	159
	imidazole	2.02	UV			25	tetrahydropyran	159
	imidazole	1.46	UV			25	THF	159
Cyclophane-7 (XVII)	BnNHCOH	2.36	NMR			27	C_6D_6	160
	BnNHCOMe	2.07	NMR			27	C_6D_6	160
	$BnNHCOCF_3$	none	NMR			27	C_6D_6	160
	BnNHCOEt	1.70	NMR			27	C_6D_6	160
	BnOAlaNHCOMe(R)	1.32	NMR			27	C_6D_6	160
	BnOAlaNHCOMe(S)	1.67	NMR			27	C_6D_6	160
	MeNHCOMe	2.31	NMR			27	C_6D_6	160
	MeNHCOBn	1.59	NMR			27	C_6D_6	160
	MeOPGlyNHCOMe(R)	1.50	NMR			27	C_6D_6	160
	MeOPGlyNHCOMe(S)	1.39	NMR			27	C_6D_6	160
	1-NapCHMeNHCOMe(R)	1.68	NMR			27	C_6D_6	160
	1-NapCHMeNHCOMe(S)	1.87	NMR			27	C_6D_6	160
	PhCHMeNHCOMe(R)	1.91	NMR			27	C_6D_6	160
	PhCHMeNHCOMe(S)	2.22	NMR			27	C_6D_6	160
	PhCHMeNHCOH(R)	2.08	NMR			27	C_6D_6	160
	PhCHMeNHCOH(S)	2.32	NMR			27	C_6D_6	160
	PhCHMeNHCOEt(R)	1.13	NMR			27	C_6D_6	160
	PhCHMeNHCOEt(S)	1.31	NMR			27	C_6D_6	160
Cyclophane-8 (XVII)	Ac-D-Ala-NHBn	1.00	NMR			25	$CDCl_3$	161
	Ac-L-Ala-NHBn	1.73	NMR			25	$CDCl_3$	161
	Ac-D-Ala-OBn	0.63	NMR			25	$CDCl_3$	161
	Ac-L-Ala-OBn	0.93	NMR			25	$CDCl_3$	161
	Ac-D-Ala-OBn	2.15	NMR			25	C_6D_6	161
	Ac-L-Ala-OBn	2.54	NMR			25	C_6D_6	161
	Ac-D-Ala-D-Ala-OBn	1.09	NMR			25	$CDCl_3$	161
	Ac-D-Ala-L-Ala-OBn	1.23	NMR			25	$CDCl_3$	161
	Ac-L-Ala-D-Ala-OBn	1.64	NMR			25	$CDCl_3$	161
	Ac-L-Ala-L-Ala-OBn	1.89	NMR			25	$CDCl_3$	161
	Ac-D-Ala-NH-*t*-Bu	0.76	NMR			25	$CDCl_3$	161
	Ac-L-Ala-NH-*t*-Bu	1.72	NMR			25	$CDCl_3$	161
	Ac-D-Ala-NH-*t*-Bu	2.43	NMR			25	C_6D_6	161
	Ac-L-Ala-NH-*t*-Bu	3.21	NMR			25	C_6D_6	161
	N-*t*-butylacetamide	1.09	NMR			25	$CDCl_3$	161
	N-methylacetamide	2.44	NMR			25	$CDCl_3$	161
	PhAc-D-Ala-NHMe	1.40	NMR			25	$CDCl_3$	161
	PhAc-L-Ala-NHMe	1.48	NMR			25	$CDCl_3$	161
Cyclophane-9 (XVII)	*N*-Boc-D-Ala-NHMe	1.54	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
	N-Boc-L-Ala-NHMe	2.79	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
	N-Boc-D-Leu-NHMe	1.17	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
	N-Boc-L-Leu-NHMe	2.79	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
	N-Boc-D-Ser-NHME	3.23	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
	N-Boc-L-Ser-NHMe	>4.55	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
	N-Boc-D-Thr-NHMe	2.64	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	N-Boc-L-Thr-NHMe	large	NMR			25	$CDCl_3$ (K too large to be measured) (Boc = butoxycarbonyl)	162
	N-Boc-D-Val-NHMe	1.10	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
	N-Boc-L-Val-NHMe	2.93	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
Cyclophane-10 (XVII)	*N*-Ac-D-Ala-NHMe	1.98	NMR			25	$CDCl_3$	162
	N-Ac-L-Ala-NHMe	2.86	NMR			25	$CDCl_3$	162
	N-Ac-D-Ala-NH-*t*-Bu	1.47	NMR			25	$CDCl_3$	162
	N-Ac-L-Ala-NH-*t*-Bu	2.20	NMR			25	$CDCl_3$	162
	N-Boc-D-Ala-NHMe	1.25	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
	N-Boc-L-Ala-NHMe	2.86	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
	N-Boc-L-Ala-NHBn	1.03	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
	N-Boc-L-Ala-NH-*t*-Bu	none	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
	N-Boc-D-Leu-NHMe	1.10	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
	N-Boc-L-Leu-NHMe	3.01	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
	N-Boc-D-Ser-NHMe	2.79	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
	N-Boc-L-Ser-NHMe	>4.48	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
	N-Boc-L-Ser(OBn)-NHMe	2.27	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
	N-Boc-D-Thr-NHMe	2.35	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
	N-Boc-L-Thr-NHMe	>4.55	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
	N-Boc-D-Val-NHMe	1.10	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
	N-Boc-L-Val-NHMe	3.23	NMR			25	$CDCl_3$ (Boc = butoxycarbonyl)	162
Cyclophane-11 (XVII)	4-cyanophenol	2.91	NMR			?	$CDCl_3$	163
	6-nitro-2-naphthol	2.32	NMR			?	$CDCl_3$	163
	3-nitrophenol	2.06	NMR			?	$CDCl_3$	163
	4-nitrophenol	3.37	NMR			?	$CDCl_3$	163
	4-propoxybenzoic acid	0.90	NMR			?	$CDCl_3$	163
Cyclophane-12 (XVII)	4-cyanophenol	2.51	NMR			?	$CDCl_3$	163
	3-nitrophenol	1.72	NMR			?	$CDCl_3$	163
	4-nitrophenol	2.85	NMR			?	$CDCl_3$	163
	4-propoxybenzoic acid	0.85	NMR			?	$CDCl_3$	163
Cyclophane-13 (XVII)	4-cyanophenol	3.99	NMR			?	$CDCl_3$	164
	4-(2',4'-dinitrophenylazo)phenol	4.10	NMR			?	$CDCl_3$	164
	4-nitrophenol	4.20	NMR			?	$CDCl_3$	163
	4-nitrophenol	4.14	NMR			?	$CDCl_3$	164
	4-nitrophenol	4.15	NMR			?	$CDCl_3$	165
	4-nitrophenol	4.36	NMR			?	$CDCl_3$ (competitive NMR)	165
	4-(4'-nitrophenylazo)phenol	3.53	NMR			?	$CDCl_3$	164
	4-propoxybenzoic acid	3.76	NMR			?	$CDCl_3$	164
Cyclophane-14 (XVII)	4-nitrophenol	4.04	NMR			?	$CDCl_3$	163
Cyclophane-15 (XVII)	4-cyanophenol	2.39	NMR			?	$CDCl_3$	163
	3-nitrophenol	2.15	NMR			?	$CDCl_3$	163
	4-nitrophenol	3.06	NMR			?	$CDCl_3$	163
Cyclophane-16 (XVII)	4-cyanophenol	1.97	NMR			?	$CDCl_3$	163
	3-nitrophenol	1.28	NMR			?	$CDCl_3$	163
	4-nitrophenol	2.32	NMR			?	$CDCl_3$	163
	4-propoxybenzoic acid	0.90	NMR			?	$CDCl_3$	163
Cyclophane-17 (XVII)	4-carboethoxyphenol	~1.70	NMR			?	$CDCl_3$	166
	4-cyanophenol	3.04	NMR			?	$CDCl_3$	166
	4-cyanophenol	3.06	NMR			?	$CDCl_3$	164
	4-(2',4'-dinitrophenylazo)phenol	3.34	NMR			?	$CDCl_3$	164
	4-nitrophenol	3.78	NMR			?	$CDCl_3$	163,165

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	4-nitrophenol	3.48	NMR			?	$CDCl_3$	164, 166
	4-(4'-nitrophenyl-azo)phenol	2.70	NMR			?	$CDCl_3$	166
	4-(4'-nitrophenyl-azo)phenol	2.72	NMR			?	$CDCl_3$	164
	phenol	~1.30	NMR			?	$CDCl_3$	166
	4-propoxybenzoic acid	<2	NMR			?	$CDCl_3$	164
Cyclophane-18 (XVII)	4-nitrophenol	3.99	NMR			?	$CDCl_3$	165
	4-nitrophenol	4.67	NMR			?	$CDCl_3$ (competitive NMR)	165
Cyclophane-19 (XVII)	6-nitro-2-naphthol	3.85	NMR			?	CD_2Cl_2	165
	4-nitrophenol	4.38	NMR			?	CD_2Cl_2	165
	4-nitrophenol	4.98	NMR			?	CD_2Cl_2 (competitive NMR)	165
Cyclophane-20 (XVIII)	adenosine	4.00	Spec			20	H_2O, I = constant (0.01 M $(CH_3)_2As(O)Na$, pH 7.8, 0.01 M Na_2SO_4)	167
Cyclophane-21 (XVIII)	adenosine	3.87	Spec			20	H_2O, I = constant (0.01 M $(CH_3)_2As(O)Na$, pH 7.8, 0.01 M Na_2SO_4)	167
	cytidine	3.94	Spec			20	H_2O, I = constant (0.01 M $(CH_3)_2As(O)Na$, pH 7.8, 0.01 M Na_2SO_4)	167
	2'-deoxyuridine	4.06	Spec			20	H_2O, I = constant (0.01 M $(CH_3)_2As(O)Na$, pH 7.8, 0.01 M Na_2SO_4)	167
	guanosine	4.30	Spec			20	H_2O, I = constant (0.01 M $(CH_3)_2As(O)Na$, pH 7.8, 0.01 M Na_2SO_4)	167
	thymidine	3.86	Spec			20	H_2O, I = constant (0.01 M $(CH_3)_2As(O)Na$, pH 7.8, 0.01 M Na_2SO_4)	167
	uridine	4.05	Spec			20	H_2O, I = constant (0.01 M $(CH_3)_2As(O)Na$, pH 7.8, 0.01 M Na_2SO_4)	167
Cyclophane-22 (XVIII)	adenosine	3.86	Spec			20	H_2O, I = constant (0.01 M $(CH_3)_2As(O)Na$, pH 7.8, 0.01 M Na_2SO_4)	167
Cyclophane-23 (XVIII)	adenosine	3.99	Spec			20	H_2O, I = constant (0.01 M $(CH_3)_2As(O)Na$, pH 7.8, 0.01 M Na_2SO_4)	167
Cyclophane-24 (XVIII)	4-cyanophenol	2.08	^{31}P NMR			25	$CDCl_3$	168
	4-nitrophenol	2.20	^{31}P NMR			25	$CDCl_3$	168
	pentafluorophenol	1.80	^{31}P NMR			25	$CDCl_3$	168
Cyclophane-25 (XVIII)	4-cyanophenol	1.98	^{31}P NMR			25	$CDCl_3$	168
	4-nitrophenol	2.01	^{31}P NMR			25	$CDCl_3$	168
	pentafluorophenol	1.87	^{31}P NMR			25	$CDCl_3$	168
Cyclophane-26 (XVIII)	acetic acid	2.58	^{31}P NMR			25	$CDCl_3$ (endo complex)	168
	acetic acid	0.30(M_2L)	^{31}P NMR			25	$CDCl_3$ (exo complex) (M + ML <-> M_2L)	168
	benzoic acid	nm	^1H NMR			25	$CDCl_3$ (no substantial spectra changes)	168
	4-cyanophenol	2.06	^1H NMR			25	$CDCl_3$ (endo complex)	168
	4-cyanophenol	2.69(M_2L)	^1H NMR			25	$CDCl_3$ (exo complex) (M + ML <-> M_2L)	168
	4-cyanophenol	2.65	^{31}P NMR			25	$CDCl_3$ (endo complex)	168
	4-cyanophenol	2.06(M_2L)	^{31}P NMR			25	$CDCl_3$ (exo complex) (M + ML <-> M_2L)	168
	3,4-difluorophenol	2.44	^1H NMR			25	$CDCl_3$ (endo complex)	168
	3,4-difluorophenol	1.85(M_2L)	^1H NMR			25	$CDCl_3$ (exo complex) (M + ML <-> M_2L)	168
	2,6-dimethyl-4-nitrophenol	2.40	^{31}P NMR			25	$CDCl_3$ (endo complex)	168
	2,6-dimethyl-4-nitrophenol	0.78(M_2L)	^{31}P NMR			25	$CDCl_3$ (exo complex) (M + ML <-> M_2L)	168

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K-mol	T, °C	conditions[d]	ref
	2,4-dinitrophenol	nm	^{1}H NMR			25	$CDCl_3$ (no substantial spectra changes)	168
	4-fluorophenol	1.77	^{1}H NMR			25	$CDCl_3$ (endo complex)	168
	4-fluorophenol	1.18(M_2L)	^{1}H NMR			25	$CDCl_3$ (exo complex) (M + ML <-> M_2L)	168
	6-nitro-2-naphthol	2.21	^{1}H NMR			25	$CDCl_3$ (endo complex)	168
	6-nitro-2-naphthol	2.50(M_2L)	^{1}H NMR			25	$CDCl_3$ (exo complex) (M + ML <-> M_2L)	168
	4-nitrophenol	2.55	^{1}H NMR			25	$CDCl_3$ (endo complex)	168
	4-nitrophenol	2.51(M_2L)	^{1}H NMR			25	$CDCl_3$ (exo complex) (M + ML <-> M_2L)	169 168, 169
	4-nitrophenol	2.56	^{31}P NMR			25	$CDCl_3$ (endo complex)	168
	4-nitrophenol	2.57(M_2L)	^{31}P NMR			25	$CDCl_3$ (exo complex) (M + ML <-> M_2L)	168
	4-[(*p*-nitrophenyl)-azo]phenol	2.34	^{1}H NMR			25	$CDCl_3$ (endo complex)	168
	4-[(*p*-nitrophenyl)-azo]phenol	2.31(M_2L)	^{1}H NMR			25	$CDCl_3$ (exo complex) (M + ML <-> M_2L)	168
	4-nitrothiophenol	nm	^{1}H NMR			25	$CDCl_3$ (no substantial spectra changes)	168
	pentafluorophenol	1.97	^{1}H NMR			25	$CDCl_3$ (endo complex)	168
	pentafluorophenol	1.81(M_2L)	^{1}H NMR			25	$CDCl_3$ (exo complex) (M + ML <-> M_2L)	168
	pentafluorophenol	2.22	^{31}P NMR			25	$CDCl_3$ (endo complex)	168
	pentafluorophenol	1.62(M_2L)	^{31}P NMR			25	$CDCl_3$ (exo complex) (M + ML <-> M_2L)	168
	phenol	1.26	^{1}H NMR			25	$CDCl_3$ (endo complex)	168
	phenol	0(M_2L)	^{1}H NMR			25	$CDCl_3$ (exo complex) (M + ML <-> M_2L)	168 168
	4-(trifluoro-methyl)phenol	2.54	^{1}H NMR			25	$CDCl_3$ (endo complex)	168
	4-(trifluoro-methyl)phenol	2.52(M_2L)	^{1}H NMR			25	$CDCl_3$ (exo complex) (M + ML <-> M_2L)	168 168
	4-(trifluoro-methyl)phenol	2.30	^{31}P NMR			25	$CDCl_3$ (endo complex)	168
	4-(trifluoro-methyl)phenol	1.71(M_2L)	^{31}P NMR			25	$CDCl_3$ (exo complex) (M + ML <-> M_2L)	168 168
Cyclophane-27 (XVIII)	benzoic acid	nm	^{1}H NMR			25	$CDCl_3$ (no substantial spectra changes)	168
	4-cyanophenol	2.85	^{1}H NMR			25	$CDCl_3$ (exo complex)	168
	4-cyanophenol	1.93(M_2L)	^{1}H NMR			25	$CDCl_3$ (endo complex) (M + ML <-> M_2L)	168
	4-cyanophenol	2.69	^{31}P NMR			25	$CDCl_3$ (exo complex)	168
	4-cyanophenol	2.10(M_2L)	^{31}P NMR			25	$CDCl_3$ (endo complex) (M + ML <-> M_2L)	168
	3,4-difluorophenol	2.26	^{1}H NMR			25	$CDCl_3$ (exo complex)	168
	3,4-difluorophenol	1.67(M_2L)	^{1}H NMR			25	$CDCl_3$ (endo complex) (M + ML <-> M_2L)	168
	2,6-dimethyl-4-nitrophenol	2.69	^{31}P NMR			25	$CDCl_3$ (exo complex)	168
	2,6-dimethyl-4-nitrophenol	0.70(M_2L)	^{31}P NMR			25	$CDCl_3$ (endo complex) (M + ML <-> M_2L)	168
	2,4-dinitrophenol	nm	^{1}H NMR			25	$CDCl_3$ (no substantial spectra changes)	168
	4-fluorophenol	1.40	^{1}H NMR			25	$CDCl_3$ (exo complex)	168
	4-fluorophenol	1.38(M_2L)	^{1}H NMR			25	$CDCl_3$ (endo complex) (M + ML <-> M_2L)	168
	6-nitro-2-naphthol	2.65	^{1}H NMR			25	$CDCl_3$ (exo complex)	168
	6-nitro-2-naphthol	2.05(M_2L)	^{1}H NMR			25	$CDCl_3$ (endo complex) (M + ML <-> M_2L)	168
	4-nitrophenol	2.94	^{1}H NMR			25	$CDCl_3$ (exo complex)	168,169
	4-nitrophenol	2.36(M_2L)	^{1}H NMR			25	$CDCl_3$ (endo complex) (M + ML <-> M_2L)	169 168
	4-nitrophenol	2.99	^{31}P NMR			25	$CDCl_3$ (exo complex)	168
	4-nitrophenol	2.42(M_2L)	^{31}P NMR			25	$CDCl_3$ (endo complex) (M + ML <-> M_2L)	168
	4-[(*p*-nitrophenyl)-azo]phenol	2.48	^{1}H NMR			25	$CDCl_3$ (exo complex)	168
	4-[(*p*-nitrophenyl)-azo]phenol	1.89(M_2L)	^{1}H NMR			25	$CDCl_3$ (endo complex) (M + ML <-> M_2L)	168

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	4-nitrothiophenol	nm	^{1}H NMR			25	$CDCl_3$ (no substantial spectra changes)	168
	pentafluorophenol	2.43	^{1}H NMR			25	$CDCl_3$ (exo complex)	168
	pentafluorophenol	1.84(M_2L)	^{1}H NMR			25	$CDCl_3$ (endo complex) (M + ML <-> M_2L)	168
	pentafluorophenol	2.55	^{31}P NMR			25	$CDCl_3$ (exo complex)	168
	pentafluorophenol	1.96(M_2L)	^{31}P NMR			25	$CDCl_3$ (endo complex) (M + ML <-> M_2L)	168
	4-(trifluro-methyl)phenol	2.35	^{1}H NMR			25	$CDCl_3$ (exo complex)	168
	4-(trifluoro-methyl)phenol	1.81(M_2L)	^{1}H NMR			25	$CDCl_3$ (endo complex) (M + ML <-> M_2L)	168
	4-(trifluoro-methyl)phenol	2.33	^{31}P NMR			25	$CDCl_3$ (exo complex)	168
	4-(trifluoro-methyl)phenol	1.74(M_2L)	^{31}P NMR			25	$CDCl_3$ (endo complex) (M + ML <-> M_2L)	168
Cyclophane-28 (XVIII)	adenine	4.28	Sol-UV			25?	CH_2Cl_2	170
	cytosine	4.57	Sol-UV			25?	CH_2Cl_2	170
	2,6-diaminopurine	4.64	Sol-UV			25?	CH_2Cl_2	170
	guanine	4.38	Sol-UV			25?	CH_2Cl_2	170
	2,4-dihydroxy-pteridine	<3	Sol-UV			25?	CH_2Cl_2	170
	melamine	4.00	Sol-UV			25?	CH_2Cl_2	170
	pterine	4.70	Sol-UV			25?	CH_2Cl_2	170
	uracil	<3	Sol-UV			25?	CH_2Cl_2	170
Cyclophane-29 (XIX)	phloroglucinol	4.04	Sol			25	CH_2Cl_2	171
Cyclophane-30 (XIX)	*N*-phenyl-1-amino-naphthalene	4.71	Fluor			30	EtOH/H_2O (10:90 v/v), 0.1 M KCl, pH 8 (0.01 M HEPES)	172 96
Cyclophane-31 (XIX)	1,3-dihydroxy-naphthalene	none	Fluor			30	H_2O, I = 0.1 (KCl), pH 4 (0.01 M acetate) 0.1 M KCl, pH 8 (0.01 M HEPES)	172 96,99
	1-(dimethyl-amino)naphthalene	4.43	Fluor			30	H_2O, I = 0.1 (KCl), pH 4 (0.01 M acetate)	99
	naphthalene	3.48	Fluor			30	H_2O, I = 0.1 (KCl), pH 4 (0.01 M acetate)	97,99,173
	perylene	2.85	Fluor			30	H_2O, I = 0.1 (KCl), pH 4 (0.01 M acetate)	97,99,173
	N-phenyl-1-amino-naphthalene	2.95	Fluor			30	H_2O, I = 0.1 (KCl), pH 3 (0.01 M acetate)	97,99
	N-phenyl-1-amino-naphthalene	4.94	Fluor			30	H_2O, I = 0.1 (KCl), pH 4 (0.01 M acetate)	97,99,173
	N-phenyl-2-amino-naphthalene	4.84	Fluor			30	H_2O, I = 0.1 (KCl), pH 4 (0.01 M acetate)	97,99,173
	pyrene	3.75	Fluor			30	H_2O, I = 0.1 (KCl), pH 4 (0.01 M acetate)	97,173,174
Cyclophane-32 (XIX)	D-phenylalanine	nm	Fluor			30	H_2O, I = 0.1 (KCl), pH 4.1 (0.01 M acetate)	175
	L-phenylalanine	2.90	Fluor			30	H_2O, I = 0.1 (KCl), pH 4.1 (0.01 M acetate)	175
	D-tryptophan	2.85	Fluor			30	H_2O, I = 0.1 (KCl), pH 4.1 (0.01 M acetate)	175
	L-tryptophan	nm	Fluor			30	H_2O, I = 0.1 (KCl), pH 4.1 (0.01 M acetate)	175
Cyclophane-33 (XIX)	methyl yellow	5.81	Spec			30	H_2O, I = 0.1 (KCl), pH 7 (0.01 M HEPES)	176
	1-(2-pyridylazo)-2-naphthol	6.00	Spec			30	H_2O, I = 0.1 (KCl), pH 7 (0.01 M HEPES)	176

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
			3. Calixarenes					
Calix4-16C-1 (XX)	1-butylimidazole	none	NMR			25	$CDCl_3$	177
	imidazole	1.15	NMR			25	$CDCl_3$	177
	1-methylimidazole	0.70	NMR			25	$CDCl_3$	177
	4-methylimidazole	0.95	NMR			25	$CDCl_3$	177
Calix4-16C-2 (XX)	pyrene	5.79	Fluor			30	H_2O	178
Calix4-16C-3 (XX)	imidazole	1.08	NMR			25	$CDCl_3$	177
Calix4-16C-4 (XX)	imidazole	decomp	NMR			25	$CDCl_3$	177
Calix4-16C-5 (XX)	imidazole	0.85	NMR			25	$CDCl_3$	177
	1-methylimidazole	0.60	NMR			25	$CDCl_3$	177
Calix4-16C-6 (XX)	acetic acid	2.48	Fluor			25	CH_2Cl_2	179
	benzoic acid	2.48	Fluor			25	CH_2Cl_2	179
	chloroacetic acid	2.74	Fluor			25	CH_2Cl_2	179
	dichloroacetic acid	2.91	Fluor			25	CH_2Cl_2	179
	trichloroacetic acid	3.08	Fluor			25	CH_2Cl_2	179
	trifluoroacetic acid	3.28	Fluor			25	CH_2Cl_2	179
Calix4-16C-7 (XX)	acetic acid	2.48	Fluor			25	CH_2Cl_2	179
	benzoic acid	2.48	Fluor			25	CH_2Cl_2	179
	chloroacetic acid	3.36	Fluor			25	CH_2Cl_2	179
	dichloroacetic acid	3.73	Fluor			25	CH_2Cl_2	179
	2,6-dihydroxybenzoic acid	3.34	Fluor			25	CH_2Cl_2	179
	4-nitrobenzoic acid	2.72	Fluor			25	CH_2Cl_2	179
	trichloroacetic acid	4.04	Fluor			25	CH_2Cl_2	179
	trifluoroacetic acid	4.15	Fluor			25	CH_2Cl_2	179
Calix4-16C-8 (XX)	ferrocenecarboxylic acid	none	CD			20	$CHCl_3$	180
Calix4-16C-9 (XX)	t-butylamine	4.68	Spec			25?	MeCN	181, 182
	neopentylamine	4.78	Spec			25?	MeCN	181, 182
Calix4-16C-10 (XX)	acetone	none	NMR			coalescent	$CDCl_3$	183
	acetonitrile	none	NMR			coalescent	$CDCl_3$	183
	anisole	none	NMR			coalescent	$CDCl_3$	183
	t-amylamine	4.70	Spec			25?	MeCN	181, 182
	benzonitrile	none	NMR			coalescent	$CDCl_3$	183
	bromobenzene	none	NMR			coalescent	$CDCl_3$	183
	n-butylamine	4.98	Spec			25?	MeCN	181, 182
	t-butylamine	4.67	Spec			25?	MeCN	181, 182
	t-butylcyclohexanol	none	NMR			coalescent	$CDCl_3$	183
	4-t-butylphenol	none	NMR			coalescent	$CDCl_3$	183
	neopentylamine	4.48	Spec			25?	MeCN	181, 182
	nitrobenzene	none	NMR			coalescent	$CDCl_3$	183
	phenylacetylene	none	NMR			coalescent	$CDCl_3$	183
	(trichloromethyl)benzene	none	NMR			coalescent	$CDCl_3$	183
	(trifluoromethyl)benzene	none	NMR			coalescent	$CDCl_3$	183

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	(trimethylaceto)-nitrile	none	NMR			coalescent	$CDCl_3$	183
	p-xylene	none	NMR			coalescent	$CDCl_3$	183
Calix4-16C-11 (XX)	acetone	none	NMR			coalescent	$CDCl_3$	183
	acetonitrile	none	NMR			coalescent	$CDCl_3$	183
	anisole	none	NMR			coalescent	$CDCl_3$	183
	benzonitrile	none	NMR			coalescent	$CDCl_3$	183
	bromobenzene	none	NMR			coalescent	$CDCl_3$	183
	t-butylcyclo-hexanol	none	NMR			coalescent	$CDCl_3$	183
	4-*t*-butylphenol	none	NMR			coalescent	$CDCl_3$	183
	nitrobenzene	none	NMR			coalescent	$CDCl_3$	183
	phenylacetylene	none	NMR			coalescent	$CDCl_3$	183
	(trichloromethyl)-benzene	none	NMR			coalescent	$CDCl_3$	183
	(trifluoromethyl)-benzene	none	NMR			coalescent	$CDCl_3$	183
	(trimethylaceto)-nitrile	none	NMR			coalescent	$CDCl_3$	183
	p-xylene	none	NMR			coalescent	$CDCl_3$	183
Calix4-16C-12 (XX)	benzonitrile	none	NMR			coalescent	$MeCN/H_2O$ (3:1)	183
	benzonitrile	none	NMR			coalescent	Me_2SO/H_2O (3:1)	183
	chloroform	none	NMR			coalescent	$MeCN/H_2O$ (3:1)	183
	chloroform	none	NMR			coalescent	Me_2SO/H_2O (3:1)	183
	4-nitrophenol	none	NMR			coalescent	$MeCN/H_2O$ (3:1)	183
	4-nitrophenol	none	NMR			coalescent	Me_2SO/H_2O (3:1)	183
	toluene	none	NMR			coalescent	$MeCN/H_2O$ (3:1)	183
	toluene	none	NMR			coalescent	Me_2SO/H_2O (3:1)	183
	(trichloromethyl)-benzene	none	NMR			coalescent	$MeCN/H_2O$ (3:1)	183
	(trichloromethyl)-benzene	none	NMR			coalescent	Me_2SO/H_2O (3:1)	183
Calix4-16C-13 (XX)	benzonitrile	none	NMR			coalescent	$MeCN/H_2O$ (3:1)	183
	benzonitrile	none	NMR			coalescent	Me_2SO/H_2O (3:1)	183
	chloroform	none	NMR			coalescent	$MeCN/H_2O$ (3:1)	183
	chloroform	none	NMR			coalescent	Me_2SO/H_2O (3:1)	183
	4-nitrophenol	none	NMR			coalescent	$MeCN/H_2O$ (3:1)	183
	4-nitrophenol	none	NMR			coalescent	Me_2SO/H_2O (3:1)	183
	toluene	none	NMR			coalescent	$MeCN/H_2O$ (3:1)	183

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	toluene	none	NMR			coalescent	Me_2SO/H_2O (3:1)	183
	(trichloromethyl)-benzene	none	NMR			coalescent	$MeCN/H_2O$ (3:1)	183
	(trichloromethyl)-benzene	none	NMR			coalescent	Me_2SO/H_2O (3:1)	183
Calix4-16C-14 (XX)	anthracene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	coronene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	decacyclene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	durene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	fluoranthene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	naphthalene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	perylene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	phenanthrene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	pyrene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
Calix4-16C-15 (XX)	anthracene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
	coronene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
	decacyclene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
	durene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
	fluoranthene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
	naphthalene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
	perylene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
	phenanthrene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
	pyrene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
Calix4-16C-16 (XX)	*t*-butylamine	2.60	Spec			25?	MeCN	181
Calix4-16C-17 (XX)	imidazole	1.00	NMR			25	$CDCl_3$	177
Calix4-16C-18 (XX)	imidazole	1.00	NMR			25	$CDCl_3$	177
	1-methylimidazole	0.70	NMR			25	$CDCl_3$	177
	4-methylimidazole	0.78	NMR			25	$CDCl_3$	177
Calix4-16C-19 (XX)	anthrol blue[e]	3.26	PhotoTit			30	H_2O, pH 5.5 ($MH^+ + L <-> MH^+L$)	185,186,187
	phenol blue	4.67	PhotoTit			30	H_2O, pH 6.4 ($MH^+ + L <-> MH^+L$)	185,186,187
	pyrene	6.55	Fluor			30	H_2O	178,187,188
Calix4-16C-20 (XX)	imidazole	none	NMR			25	$CDCl_3$	177
Calix4-16C-21 (XX)	2-methyl-2-propanol	0.81	NMR			25	D_2O, 0.5 M NaOD	123,189,190
Calix4-16C-22 (XX)	*cis*-4-*t*-butyl-cyclohexanol	0.89	NMR			25	$CDCl_3$	191
	trans-4-*t*-butyl-cyclohexanol	0.92	NMR			25	$CDCl_3$	191
	cyclohexanol	1.04	NMR			25	$CDCl_3$	191
	cis-1,2-cyclo-hexanediol	2.42	NMR			25	$CDCl_3$	191
	trans-1,2-cyclo-hexanediol	2.03	NMR			25	$CDCl_3$	191
	cis-1,3-cyclo-hexanediol	2.09	NMR			25	$CDCl_3$	191
	trans-1,3-cyclo-hexanediol	2.26	NMR			25	$CDCl_3$	191
	cis-1,4-cyclo-hexanediol	3.02	NMR			25	$CDCl_3$	191
	trans-1,4-cyclo-hexanediol	2.11	NMR			25	$CDCl_3$	191
	glutaric acid	5.08	NMR			25	$CDCl_3$	192
	glutaric acid monomethyl ester	1.49	NMR			25	$CDCl_3$	192
	2,5-hexanediol	1.56	NMR			25	$CDCl_3$	191
	2,4-pentanediol	1.63	NMR			25	$CDCl_3$	191
	pimelic acid	3.04	NMR			25	$CDCl_3$	192
	valeric acid	1.85	NMR			25	$CDCl_3$	192
	vitamin B_{12}	2.36	Solv Extr-Spec			25?	C_6H_6	193

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	guest-26[e]	2.32	Solv Extr-Spec			25?	C_6H_6	193
Calix4-16C-23 (XX)	adamantane	4.30	Spec			30	H_2O, pH 5.4	194
	coronene	4.66	Spec			30	H_2O, pH 5.4	194
	pyrene	4.57	Spec			30	H_2O, pH 5.4	194
Calix4-18C1-1 (XX)	*t*-butylamine	4.23	Spec			25?	MeCN	181
	neopentylamine	4.15	Spec			25?	MeCN	181
Calix5-20C-1 (XXI)	anthracene	3.96	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184, 195
	coronene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	decacyclene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	durene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	fluoranthene	3.60	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184, 195
	naphthalene	3.57	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184, 195
	perylene	<2	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184, 195
	phenanthrene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	pyrene	<2	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184, 195
Calix5-20C-2 (XXI)	anthracene	3.95	Sol-UV			25?	H_2O, 0.01 M HCl	184, 195
	coronene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
	decacyclene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
	durene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
	fluoranthene	3.30	Sol-UV			25?	H_2O, 0.01 M HCl	184, 195
	naphthalene	3.52	Sol-UV			25?	H_2O, 0.01 M HCl	184, 195
	perylene	<2	Sol-UV			25?	H_2O, 0.01 M HCl	184, 195
	phenanthrene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
	pyrene	<2	Sol-UV			25?	H_2O, 0.01 M HCl	184, 195
Calix6-24C-1 (XXI)	anthracene	4.11	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184,195,196
	coronene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	decacyclene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	durene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	fluoranthene	3.53	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184, 196
	naphthalene	3.57	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184,195,196
	perylene	<2	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184,195,196
	phenanthrene	3.48	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184, 196
	pyrene	<2	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184,195,196
Calix6-24C-2 (XXI)	anthracene	3.20	Sol-UV			25?	H_2O, 0.01 M HCl	184
	coronene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
	decacyclene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
	durene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
	fluoranthene	3.60	Sol-UV			25?	H_2O, 0.01 M HCl	184, 195
	naphthalene	3.65	Sol-UV			25?	H_2O, 0.01 M HCl	184, 195
	perylene	<2	Sol-UV			25?	H_2O, 0.01 M HCl	184, 195
	phenanthrene	3.28	Sol-UV			25?	H_2O, 0.01 M HCl	184
	pyrene	<2	Sol-UV			25?	H_2O, 0.01 M HCl	184, 195
Calix6-24C-3 (XXI)	*N*-benzyl-1,4-dihydronicotinamide	2.75	Kin			30	H_2O, pH 6.3 (0.01 M phosphate)	197, 198
Calix6-24C-4 (XXI)	phenol blue	2.75	Spec			30	H_2O	188, 199
Calix6-24C-5 (XXI)	*t*-butylamine	5.90	Spec			25?	MeCN	181
	neopentylamine	5.90	Spec			25?	MeCN	181
Calix6-24C-6 (XXI)	*N*-benzyl-1,4-dihydronicotinamide	3.13	Kin			30	H_2O, pH 6.3 (0.01 M phosphate)	197, 198
	N-benzyl-1,4-dihydronicotinamide	3.01	Kin			30	H_2O, pH 4 (0.01 M acetate)	197, 198
Calix6-24C-7 (XXI)	*N*-benzyl-1,4-dihydronicotinamide	2.46	Kin			30	H_2O, pH 4 (0.01 M acetate)	197, 198
	pyrene	4.08	Fluor			30	H_2O	178
Calix6-24C-8 (XXI)	anthrol blue[e]	3.97	PhotoTit			30	H_2O, pH 5.5 ($MH^+ + L <-> MH^+L$)	185,186,187
	phenol blue	4.75	PhotoTit			30	H_2O, pH 6.4 ($MH^+ + L <-> MH^+L$)	185,186,187

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	pyrene	6.59	Fluor			30	H_2O	178,187,188
Calix6-24C-9 (XXI)	pyrene	6.36	Fluor			30	H_2O	178
Calix6-24C-10 (XXI)	*N*-benzyl-1,4-dihydronicotinamide	3.46	Fluor			30	H_2O, pH 10.11	197, 198
	N-benzyl-1,4-dihydronicotinamide	3.33	Kin			30	H_2O, pH 6.3 (0.01 M phosphate)	197, 198
Calix6-24C-11 (XXI)	1-butanol	nm	CD			20	H_2O/DMF (98.6:1.4 v/v) pH 6.9 (0.067 M phosphate	200
	cyclohexanol	1.90	CD			20	H_2O/DMF (98.6:1.4 v/v) pH 6.9 (0.067 M phosphate)	187, 201
	1-decanol	3.71	CD			20	H2O/DMF (98.6:1.4 v/v) pH 6.9 (0.067 M phosphate)	187, 200
	2,2-dimethyl-3-hexanol	2.40	CD			20	H2O/DMF (98.6:1.4 v/v) pH 6.9 (0.067 M phosphate)	187
	1-dodecanol	4.15	CD			20	H2O/DMF (98.6:1.4 v/v) pH 6.9 (0.067 M phosphate)	187, 200
	ethanol	nm	CD			20	H_2O/DMF (98.6:1.4 v/v) pH 6.9 (0.067 M phosphate	200
	1-heptanol	3.08	CD			20	H_2O/DMF (98.6:1.4 v/v) pH 6.9 (0.067 M phosphate)	185,187,201
	1-hexanol	2.15	CD			20	H_2O/DMF (98.6:1.4 v/v) pH 6.9 (0.067 M phosphate)	185,187,200,201
	1-octanol	3.89	CD			20	H_2O/DMF (98.6:1.4 v/v) pH 6.9 (0.067 M phosphate)	185,187,200,201
Calix6-24C-12 (XXI)	2-anilinonaphthalene	5.92	Fluor			30	H_2O	188, 199
	orange OT	7.36	Sol			30	H_2O	188, 199
Calix6-24C-13 (XXI)	2-anilinonaphthalene	5.53	Fluor			30	H_2O	188, 199
	orange OT	5.72	Sol			30	H_2O	188, 199
	phenol blue	5.30	Spec			30	H_2O	188, 199
Calix6-24C-14 (XXI)	pyrene	5.80	Fluor			30	H_2O	178
Calix6-24C-15 (XXI)	pyrene	6.61	Fluor			30	H_2O	178
Calix6-24C-16 (XXI)	anthracene	3.30	Sol-UV			25?	H_2O (K_2CO_3)	196
	fluoranthene	3.83	Sol-UV			25?	H_2O (K_2CO_3)	196
	naphthalene	3.30	Sol-UV			25?	H_2O (K_2CO_3)	196
	perylene	3.52	Sol-UV			25?	H_2O (K_2CO_3)	196
	phenanthrene	3.67	Sol-UV			25?	H_2O (K_2CO_3)	196
	pyrene	4.15	Sol-UV			25?	H_2O (K_2CO_3)	196
Calix6-24C-17 (XXI)	anthracene	none	Sol-UV			25?	H_2O (K_2CO_3)	196
	fluoranthene	none	Sol-UV			25?	H_2O (K_2CO_3)	196
	naphthalene	none	Sol-UV			25?	H_2O (K_2CO_3)	196
	perylene	none	Sol-UV			25?	H_2O (K_2CO_3)	196
	phenanthrene	none	Sol-UV			25?	H_2O (K_2CO_3)	196
	pyrene	none	Sol-UV			25?	H_2O (K_2CO_3)	196
Calix6-24C-18 (XXI)	ferrocenecarboxylic acid	2.83	CD			20	$CHCl_3$	180
	ferrocenecarboxylic acid	none	CD			20	Me_2SO	180
	ferrocene	none	CD			20	$CHCl_3$	180
	methyl ferrocenecarboxylate	none	CD			20	$CHCl_3$	180

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
Calix6-24C-19 (XXI)	anthracene	3.98	Sol-UV			25?	H_2O (1.5×10^{-3} M K_2CO_3)	196
	anthracene	3.54	Sol-UV			25?	H_2O (6×10^{-3} M K_2CO_3)	196
	fluoranthene	<2	Sol-UV			25?	H_2O (K_2CO_3)	196
	naphthalene	3.38	Sol-UV			25?	H_2O (K_2CO_3)	196
	perylene	<2	Sol-UV			25?	H_2O (K_2CO_3)	196
	pyrene	<2	Sol-UV			25?	H_2O (K_2CO_3)	196
Calix6-24C-20 (XXI)	anthracene	none	Sol-UV			25?	H_2O (K_2CO_3)	196
	fluoranthene	none	Sol-UV			25?	H_2O (K_2CO_3)	196
	naphthalene	none	Sol-UV			25?	H_2O (K_2CO_3)	196
	perylene	none	Sol-UV			25?	H_2O (K_2CO_3)	196
	phenanthrene	none	Sol-UV			25?	H_2O (K_2CO_3)	196
	pyrene	none	Sol-UV			25?	H_2O (K_2CO_3)	196
Calix6-24C-21 (XXI)	anthracene	none	Sol-UV			25?	H_2O (K_2CO_3)	196
	fluoranthene	none	Sol-UV			25?	H_2O (K_2CO_3)	196
	naphthalene	none	Sol-UV			25?	H_2O (K_2CO_3)	196
	perylene	none	Sol-UV			25?	H_2O (K_2CO_3)	196
	phenanthrene	none	Sol-UV			25?	H_2O (K_2CO_3)	196
	pyrene	none	Sol-UV			25?	H_2O (K_2CO_3)	196
Calix7-28C-1 (XXII)	anthracene	4.04	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184, 195
	coronene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO3	184
	decacyclene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	durene	3.59	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	fluoranthene	3.56	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184, 195
	naphthalene	3.59	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184, 195
	perylene	3.95	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184, 195
	phenanthrene	3.95	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	pyrene	4.04	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184, 195
Calix7-28C-2 (XXII)	anthracene	3.92	Sol-UV			25?	H_2O, 0.01 M HCl	184, 195
	coronene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
	decacyclene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
	durene	3.59	Sol-UV			25?	H_2O, 0.01 M HCl	184
	fluoranthene	3.48	Sol-UV			25?	H_2O, 0.01 M HCl	184, 195
	naphthalene	3.48	Sol-UV			25?	H_2O, 0.01 M HCl	184, 195
	perylene	4.00	Sol-UV			25?	H_2O, 0.01 M HCl	184, 195
	phenanthrene	3.95	Sol-UV			25?	H_2O, 0.01 M HCl	184
	pyrene	3.95	Sol-UV			25?	H_2O, 0.01 M HCl	184, 195
Calix8-32C-1 (XXII)	anthracene	4.15	Sol-UV			25?	H_2O (K_2CO_3)	196
	anthracene	3.97	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	coronene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	decacyclene	none	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	durene	3.45	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184
	fluoranthene	4.15	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184,195,196
	naphthalene	2.79	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184,195,196
	perylene	3.92	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184,195,196
	phenanthrene	3.61	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184, 196
	pyrene	4.64	Sol-UV			25?	H_2O, 0.01 M K_2CO_3	184,195,196
Calix8-32C-2 (XXII)	anthracene	3.88	Sol-UV			25?	H_2O, 0.01 M HCl	184
	coronene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
	decacyclene	none	Sol-UV			25?	H_2O, 0.01 M HCl	184
	durene	3.45	Sol-UV			25?	H_2O, 0.01 M HCl	184
	fluoranthene	4.18	Sol-UV			25?	H_2O, 0.01 M HCl	184, 195
	naphthalene	3.04	Sol-UV			25?	H_2O, 0.01 M HCl	184, 195
	perylene	4.00	Sol-UV			25?	H_2O, 0.01 M HCl	184, 195
	phenanthrene	3.61	Sol-UV			25?	H_2O, 0.01 M HCl	184
	pyrene	4.56	Sol-UV			25?	H_2O, 0.01 M HCl	184, 195
Calix8-32C-3 (XXII)	anthracene	4.46	Sol-UV			25?	H_2O (K_2CO_3)	196
	fluoranthene	4.20	Sol-UV			25?	H_2O (K_2CO_3)	196
	naphthalene	3.48	Sol-UV			25?	H_2O (K_2CO_3)	196
	perylene	4.60	Sol-UV			25?	H_2O (K_2CO_3)	196
	phenanthrene	4.30	Sol-UV			25?	H_2O (K_2CO_3)	196
	pyrene	4.86	Sol-UV			25?	H_2O (K_2CO_3)	196
Calix8-32C-4 (XXII)	anthrol blue[e]	4.18	PhotoTit			30	H_2O, pH 5.5 ($MH^+ + L <-> MH^+L$)	185,186,187

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	phenol blue	4.13	PhotoTit			30	H_2O, pH 6.4 ($MH^+ + L <-> MH^+L$)	185,186,187
	pyrene	6.75	Fluor			30	H_2O	178,187,188
Calix8-32C-5 (XXII)	pyrene	5.57	Fluor			30	H_2O	178
Calix8-32C-6 (XXII)	1-butanol	nm	CD			20	H_2O/DMF (98.6:1.4 v/v) pH 6.9 (0.067 M phosphate	200
	cyclohexanol	nm	CD			20	H_2O/DMF (98.6:1.4 v/v) pH 6.9 (0.067 M phosphate)	187
	1-decanol	3.04	CD			20	H2O/DMF (98.6:1.4 v/v) pH 6.9 (0.067 M phosphate)	187, 200
	2,2-dimethyl-3-hexanol	1.90	CD			20	H_2O/DMF (98.6:1.4 v/v) pH 6.9 (0.067 M phosphate)	187
	1-dodecanol	4.00	CD			20	H_2O/DMF (98.6:1.4 v/v) pH 6.9 (0.067 M phosphate)	187, 200
	ethanol	nm	CD			20	H_2O/DMF (98.6:1.4 v/v) pH 6.9 (0.067 M phosphate	200
	1-heptanol	nm	CD			20	H2O/$_D$MF (98.6:1.4 v/v) pH 6.9 (0.067 M phosphate)	187, 200
	1-hexanol	nm	CD			20	H2O/DMF (98.6:1.4 v/v) pH 6.9 (0.067 M phosphate)	187, 200
	1-octanol	1.85	CD			20	H2O/DMF (98.6:1.4 v/v) pH 6.9 (0.067 M phosphate)	187, 200
Double Calix-1 (XXII)	2-aminopropanol	none	NMR			25	$CDCl_3$	177
	2-bromophenol	none	NMR			25	$CDCl_3$	177
	4-bromophenol	1.00	NMR			25	$CDCl_3$	177
	2-bromopropionic acid	1.00	NMR			25	$CDCl_3$	177
	n-butylamine	none	NMR			25	$CDCl_3$	177
	4-*n*-butylbenzoic acid	1.08	NMR			25	$CDCl_3$	177
	butyric acid	none	NMR			25	$CDCl_3$	177
	dibromoacetic acid	1.18	NMR			25	$CDCl_3$	177
	2,4-dinitrophenol	none	NMR			25	$CDCl_3$	177
	4-methoxybenzyl-amine	none	NMR			25	$CDCl_3$	177
	4-methoxyphenyl-ethylamine	none	NMR			25	$CDCl_3$	177
	imidazole	1.23	NMR			25	$CDCl_3$	177
	neopentylamine	none	NMR			25	$CDCl_3$	177
	4-nitro-3,5-di-methylphenol	none	NMR			25	$CDCl_3$	177
	2-nitrophenol	none	NMR			25	$CDCl_3$	177
	3-nitrophenol	1.57	NMR			25	$CDCl_3$	177
	4-nitrophenol	1.60	NMR			25	$CDCl_3$	177
	phenol	none	NMR			25	$CDCl_3$	177
	pyridine	none	NMR			25	$CDCl_3$	177
Double Calix-2 (XXII)	2-aminopropanol	1.30	NMR			25	$CDCl_3$	4, 177
	3-aminopropanol	1.18	NMR			25	$CDCl_3$	4, 177
	aniline	none	NMR			25	$CDCl_3$	177
	bromoacetic acid	0.70	NMR			25	$CDCl_3$	4, 177
	2-bromophenol	none	NMR			25	$CDCl_3$	4, 177
	4-bromophenol	1.32	NMR			25	$CDCl_3$	4, 177
	2-bromopropionic acid	1.18	NMR			25	$CDCl_3$	177
	n-butylamine	1.08	NMR			25	$CDCl_3$	4, 177
	sec-butylamine	none	NMR			25	$CDCl_3$	4, 177
	t-butylamine	none	NMR			25	$CDCl_3$	177
	4-*n*-butylbenzoic acid	1.11	NMR			25	$CDCl_3$	177

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K-mol	T, °C	conditions[d]	ref
	4-*t*-butylbenzoic acid	none	NMR			25	$CDCl_3$	177
	butyric acid	1.26	NMR			25	$CDCl_3$	177
	3-chloropropionic acid	0.70	NMR			25	$CDCl_3$	4, 177
	2,4,6-collidine	none	NMR			25	$CDCl_3$	177
	4-cyanophenol	1.49	NMR			25	$CDCl_3$	4, 177
	4-cyanopyridine	none	NMR			25	$CDCl_3$	4, 177
	dibromoacetic acid	0.70	NMR			25	$CDCl_3$	4, 177
	dichloroacetic acid	0.78	NMR			25	$CDCl_3$	4, 177
	diethylamine	none	NMR			25	$CDCl_3$	4, 177
	2,4-dinitrophenol	none	NMR			25	$CDCl_3$	4, 177
	2-hydroxypropyl-amine	1.04	NMR			25	$CDCl_3$	4, 177
	imidazole	1.20	NMR			25	$CDCl_3$	4, 177
	iodoacetic acid	0.95	NMR			25	$CDCl_3$	4, 177
	isobutylamine	1.11	NMR			25	$CDCl_3$	4, 177
	isobutyric acid	o.85	NMR			25	$CDCl_3$	177
	isopropylamine	1.11	NMR			25	$CDCl_3$	4, 177
	2,6-lutidine	none	NMR			25	$CDCl_3$	4, 177
	4-methoxybenzyl-amine	1.28	NMR			25	$CDCl_3$	4, 177
	4-methoxyphenyl-ethylamine	1.20	NMR			25	$CDCl_3$	4, 177
	4-methoxyphenyl-propylamine	1.28	NMR			25	$CDCl_3$	4, 177
	neopentylamine	none	NMR			25	$CDCl_3$	4, 177
	4-nitro-3,5-di-methylphenol	none	NMR			25	$CDCl_3$	4, 177
	2-nitrophenol	none	NMR			25	$CDCl_3$	4, 177
	3-nitrophenol	1.60	NMR			25	$CDCl_3$	4, 177
	4-nitrophenol	1.74	NMR			25	$CDCl_3$	4, 177
	phenol	0.85	NMR			25	$CDCl_3$	177
	4-picoline	0.78	NMR			25	$CDCl_3$	4, 177
	pyridine	1.52	NMR			25	$CDCl_3$	4, 177
	4-trifluoro-methylphenol	1.32	NMR			25	$CDCl_3$	4, 177
	trimethylacetic acid	none	NMR			25	$CDCl_3$	177
Double Calix-3 (XXII)	2-aminopropanol	none	NMR			25	$CDCl_3$	177
	4-bromophenol	1.20	NMR			25	$CDCl_3$	177
	2-bromopropionic acid	1.11	NMR			25	$CDCl_3$	177
	n-butylamine	none	NMR			25	$CDCl_3$	177
	butyric acid	none	NMR			25	$CDCl_3$	177
	dibromoacetic acid	1.28	NMR			25	$CDCl_3$	177
	imidazole	1.23	NMR			25	$CDCl_3$	177
	4-methoxybenzyl-amine	none	NMR			25	$CDCl_3$	177
	4-nitrophenol	1.68	NMR			25	$CDCl_3$	177
	phenol	0.70	NMR			25	$CDCl_3$	177
	pyridine	none	NMR			25	$CDCl_3$	177
			4. Cryptophanes					
Cryptophane-1 (XXIII)	(+)bromochloro-fluoromethane	-0.52	NMR			59	$CDCl_3$ (apparent K)	202, 203
	(-)bromochloro-fluoromethane	-0.66	NMR			59	$CDCl_3$ (apparent K)	202, 203
	bromochloro-fluoromethane	1.58	NMR			27	$(CDCl_2)_2$	203, 204
	bromochloromethane	-0.05	NMR			-50	$CDCl_3$ (apparent K)	205
	bromochloromethane	2.35	NMR			27	$(CDCl_2)_2$	203, 204
	chloroform	1.03	NMR	-26.8	-66.9	27	$(CDCl_2)_2$	203, 204
	chloroform	~-1	NMR			37-57	?	202
	dibromomethane	-0.82	NMR			-50	$CDCl_3$ (apparent K)	205
	dibromomethane	1.76	NMR			27	$(CDCl_2)_2$	203, 204
	dibromomethane	-0.15	NMR			37-57	$CDCl_3$ (apparent K)	202
	dichloromethane	0.26	NMR			-50	$CDCl_3$ (apparent K)	205, 206
	dichloromethane	~2.51	NMR			27	$CDCl_3$ (estimated K)	203, 204
	dichloromethane	0.41	NMR			37-57	$CDCl_3$ (apparent K)	202
	dichloromethane	2.57	NMR	-16.3	-4.2	27	$(CDCl_2)_2$	203, 204
	iodomethane	1.76	NMR			27	$(CDCl_2)_2$	203, 204

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
Cryptophane-2 (XXIII)	chloroform	2.41	NMR	-34.3	-66.9	27	$(CDCl_2)_2$	203,204,207
	dibromomethane	2.55	NMR	-5.4	-29.3	27	$(CDCl_2)_2$	203, 204
	dichloromethane	2.70	NMR	-13.8	4.2	27	$(CDCl_2)_2$	203,204,207
Cryptophane-3 (XXIII)	dichloromethane	~-0.72	NMR			below -53	$CDCl_3$ (apparent K)	208
	dichloromethane	~-0.55	NMR			above 27	$CDCl_3$ (apparent K)	208
	dichloromethane	0.26	NMR			-50	$CDCl_3$ (apparent K)	206
Cryptophane-4 (XXIII)	acetone	0.95	NMR			27	$(CDCl_2)_2$	204, 209
	bromochloro-fluoromethane	2.11	NMR			27	$(CDCl_2)_2$	210
	bromochloro-fluoromethane	2.20	NMR			27	$(CDCl_2)_2$	204
	bromodichloro-methane	2.48	NMR	-21.8	-25	27	$(CDCl_2)_2$	204, 209
	bromoform	1.68	NMR	-5.9	17	27	$(CDCl_2)_2$	204, 209
	bromoform	1.60	NMR			27	$(CDCl_2)_2$	210, 211
	i-butane	2.04	NMR	-15.9	-13	27	$(CDCl_2)_2$	204, 209
	i-butane	2.06	NMR	-15.9	-13	27	$(CDCl_2)_2$	210
	carbon tetrachloride	0.87	NMR			27	$(CDCl_2)_2$	204, 209
	carbon tetrachloride	0.85	NMR			27	$(CDCl_2)_2$	210
	chlorodibromo-methane	2.11	NMR	-6.3	17	27	$(CDCl_2)_2$	204, 209
	chlorodibromo-methane	2.08	NMR			27	$(CDCl_2)_2$	210
	chloroform	2.70	NMR	-25.1	-29	27	$(CDCl_2)_2$	204, 209
	chloroform	2.67	NMR	-28.9	-46	27	$(CDCl_2)_2$	210, 211
	2-chloro-2-methyl-propane	-0.58	NMR			27	$(CDCl_2)_2$	204, 209
	dibromomethane	2.19	NMR			27	$(CDCl_2)_2$	209
	dichloromethane	2.04	NMR	4.2	25	27	$(CDCl_2)_2$	204, 209
	dichloromethane	2.08	NMR			27	$(CDCl_2)_2$	210, 211
	2,2-dichloropropane	-0.07	NMR			27	$(CDCl_2)_2$	204, 209
	iodomethane	1.75	NMR			27	$(CDCl_2)_2$	209
	1,1,1-trichloro-ethane	0.15	NMR			27	$(CDCl_2)_2$	204, 209
Cryptophane-5 (XXIII)	chloroform	3.89	NMR			27	D_2O	203,204,207
	dichloromethane	3.70	NMR			27	D_2O	203,204,207
Cryptophane-6 (XXIII)	*n*-butane	3.78	NMR			27	D_2O	203, 204
	i-butane	4.78	NMR			27	D_2O	203, 204
	i-butene	3.08	NMR			27	D_2O	203, 204
Cryptophane-7 (XXIV)	benzene	~3	NMR			21	$(CCl_3)CO$	212
	chloroform	4.89	NMR			-20	$(CCl_3)CO$ (direct study)	212
	cubane	3.60	NMR			-20	$(CCl_3)CO$ (direct study)	212
	dichloromethane	4.11	NMR			-20	$(CCl_3)CO$ (competition study)	212
	2-methyl-2-propanol	4.20	NMR			-20	$(CCl_3)CO$ (direct study)	212
	propylene oxide	3.78	NMR			-20	$(CCl_3)CO$ (competition study)	212
	1,1,2,2-tetra-chloroethane	~1-2	NMR			21	$(CCl_3)CO$	212
Cryptophane-8 (XXIV)	cubane	none	NMR			-20 to 40	$(CCl_3)_2CO$	212
	dichloromethane	none	NMR			-20 to 40	$(CCl_3)_2CO$	212
Cryptophane-9 (XXIV)	acetonitrile	0-1	NMR			22	$CDCl_3$	213
	ethanol	<0.70	NMR			22	$CDCl_3$	213
	methanol	1.71	NMR	-35.6	-88	22	$CDCl_3$	213
Cryptophane-10 (XXVI)	N_2	~2	NMR			-40	$CDCl_3$	213
	O_2	~2	NMR			-40	$CDCl_3$	213
	acetonitrile	nm	NMR			22	$CDCl_3$	213
	methanol	1.04	NMR	-27.6	-75	22	$CDCl_3$	213
				5. Miscellaneous				
				a. Cavitands and Carcerands				
Cavitand-1 (XXV)	carbon disulfide	0.41	NMR	-14.6	-61.2	-61	$CDCl_3$	214

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	carbon disulfide	-0.09	NMR			-23	$CDCl_3$	214
	carbon disulfide	-0.66	NMR			27	$CDCl_3$	214
	carbon disulfide	-0.74	NMR			27	C_6D_6	214
Cavitand-2 (XXV)	carbon disulfide	0.91	NMR			-23	$CDCl_3$	214
Cavitand-3 (XXV)	carbon disulfide	1.12	NMR			-23	$CDCl_3$	214
Cavitand-4 (XXV)	acetonitrile-d_3	2.20	NMR			0	CCl_4 + 0.3% v/v Me_4Si	215
	acetonitrile-d_3	1.65	NMR	-26.8	-56.9	27	CCl_4 + 0.3% v/v Me_4Si	215
	acetonitrile-d_3	1.34	NMR			55	CCl_4 + 0.3% v/v Me_4Si	215
Cavitand-5 (XXV)	acetonitrile-d_3	2.50	NMR			0	CCl_4 + 0.3% v/v Me_4Si	215
	acetonitrile-d_3	1.95	NMR	-25.9	-47.7	27	CCl_4 + 0.3% v/v Me_4Si	215
	acetonitrile-d_3	1.65	NMR			55	CCl_4 + 0.3% v/v Me_4Si	215
Cavitand-6 (XXV)	benzene	1.82	NMR			25	Me_2CO-d_6	216
	fluorobenzene	3.36	NMR			25	Me_2CO-d_6	216
	toluene	1.93	NMR			25	Me_2CO-d_6	216
Cavitand-7 (XXV)	Cavitand-7[f]	~10.01	NMR			-18?	H_2O (extrapolated K)	217
	Cavitand-7[f]	5.81	NMR			-18	$CDCl_3$	217
	Cavitand-7[f]	4.94	NMR			12	$CDCl_3$	217
	Cavitand-7[f]	~9.43	NMR			-18?	MeOH (extrapolated K)	217
	Cavitand-9[f]	5.42	NMR			-18	$CDCl_3$	217
Cavitand-8 (XXV)	Cavitand-7[f]	none	NMR			-18?	$CDCl_3$	217
	Cavitand-9[f]	none	NMR			-18?	$CDCl_3$	217
Cavitand-9 (XXV)	Cavitand-9[f]	4.37	NMR			-18	$CDCl_3/Me_2CO$-d_6 (75:25 v/v)	217
	Cavitand-9[f]		NMR	-16.7	8.4	?	$CDCl_3/Me_2CO$-d_6 (90:10 v/v)	217
	Cavitand-9[f]	>4.8	NMR			-18	$CDCl_3$/MeOD-d_3 75:25 v/v)	217
	Cavitand-9[f]		NMR	-15.5	12.6	?	$CDCl_3$/MeOD-d_3 (90:10 v/v)	217
	Cavitand-9[f]	4.55	NMR			-18	$CDCl_3/MeNO_2$-d_3 (75:25 v/v)	217
	Cavitand-9[f]	3.85	NMR			-46	$CDCl_3$	217
	Cavitand-9[f]	3.72	NMR			-36	$CDCl_3$	217
	Cavitand-9[f]	3.66	NMR			-32	$CDCl_3$	217
	Cavitand-9[f]	3.49	NMR			-20	$CDCl_3$	217
	Cavitand-9[f]	3.49	NMR			-18	$CDCl_3$	217
	Cavitand-9[f]	3.36	NMR			-10	$CDCl_3$	217
	Cavitand-9[f]		NMR	-15.9	4.6	-46 to -10	$CDCl_3$	217
	Cavitand-9[f]	3.12	Kin			12	$CDCl_3$	217
	Cavitand-9[f]	4.14	NMR			-46	CD_2Cl_2	217
	Cavitand-9[f]	3.37	NMR			-46	toluene-d_6	217
Cavitand-10 (XXVI)	ethyl acetate	0.09	NMR			21	CD_2Cl_2	218
	nitrobenzene-d_5	-0.23	NMR			21	CD_2Cl_2	218
	toluene-d_8	0.26	NMR			21	CD_2Cl_2	218
	p-xylene-d_{10}	0.20	NMR			21	CD_2Cl_2	218
Carcerand-1 (XXVI)	N_2	~2.26	NMR			22	$CDCl_3$	219
	O_2	~1.64	NMR			22	$CDCl_3$	219
	Xe	~2.30	NMR			22	$CDCl_3$	219
			5. Miscellaneous (cont.)					
			b. Porphyrins and Porphyrin Derivatives					
Porphyrin-1 (XXVIII)	1,4-benzoquinone	-0.22	Spec			15	CH_2Cl_2	220
	4,6-dinitrobenzofuroxan	1.75	Spec	-16.8	-22.9	25	CH_2Cl_2	221
	2,4,5,7-tetranitrofluorenone	2.06	Spec	-12.7	-31.8	25	CH_2Cl_2	222
	2,4,7-trinitrofluorenone	2.00	Spec	-3.3	26.9	25	CH_2Cl_2	223
Porphyrin-2 (XXVIII)	1,4-benzoquinone	0.51	Spec			15	MeCN	220
Porphyrin-3 (XXVIII)	1,4-benzoquinone	0.38	Spec			15	MeCN	220
Porphyrin-4 (XXVIII)	1,4-benzoquinone	0.48	Fluor			25	Me_2CO (apparent K)	224
	1,4-benzoquinone	-0.52	Spec			25	Me_2CO (apparent K)	224
	1,4-benzoquinone	-0.30	Spec			25	Me_2CO (ground state complex)	224
Porphyrin-5 (XXVIII)	1,4-benzoquinone	-1.70	Spec			15	MeCN	220
Porphyrin-6 (XXVIII)	1,4-benzoquinone	0.89	Spec			7	CH_2Cl_2	220

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	1,4-benzoquinone	0.61	Spec			15	MeCN	220
Porphyrin-7 (XXVIII)	1,4-naphthoquinone	1.11	Spec			20	MeOH	220
	1,4-benzoquinone	2.17	Fluor			20	H_2O	220
	1,4-benzoquinone	2.18	Spec			20	H_2O	220
	1,4-benzoquinone	1.93	Fluor	-34	-73	25	H_2O	220
	1,4-benzoquinone	1.92	Fluor			30	H_2O	220
	1,4-benzoquinone	1.90	Fluor			35	H_2O	220
	1,4-benzoquinone	0.43	Spec			20	MeOH	220
Porphyrin-8 (XXVIII)	1,4-benzoquinone	1.90	Spec			20	H_2O	220
	1,4-benzoquinone	1.86	Fluor			20	H_2O	220
	1,4-benzoquinone	1.85	Fluor	-28	-56	25	H_2O	220
	1,4-benzoquinone	1.83	Fluor			30	H_2O	220
	1,4-benzoquinone	1.80	Fluor			35	H_2O	220
	1,4-benzoquinone	0.60	Spec			20	MeOH	220
	1,4-naphthoquinone	0.88	Spec			20	MeOH	220
	4-nitrophenol	3.11	Fluor	-46.1	-99.9	10	H_2O	225
	4-nitrophenol	3.05	Fluor			15	H_2O	225
	4-nitrophenol	2.89	Fluor			20	H_2O	225
	4-nitrophenol	2.74	Fluor			25	H_2O	225
	4-nitrophenol	2.58	Fluor			30	H_2O	225
Porphyrin-9 (XXVIII)	3-acetylpyridine	3.26	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	226
	3-acetylpyridine	-0.22(M_2L)	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4 ($M + ML = M_2L$)	226
	4-acetylpyridine	3.38	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	226
	4-acetylpyridine	-0.22(M_2L)	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4 ($M + ML = M_2L$)	226
	2-aminopyridine	3.05	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	226
	2-aminopyridine	-0.16(M_2L)	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4 ($M + ML = M_2L$)	226
	3-bromopyridine	2.63	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	226
	3-bromopyridine	-0.36(M_2L)	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4 ($M + ML = M_2L$)	226
	3-chloropyridine	2.49	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	226
	3-chloropyridine	-0.10(M_2L)	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4 ($M + ML = M_2L$)	226
	3-cyanopyridine	2.20	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	226
	3-cyanopyridine	0.16(M_2L)	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4 ($M + ML = M_2L$)	226
	4-cyanopyridine	2.33	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	226
	4-cyanopyridine	-0.02(M_2L)	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4 ($M + ML = M_2L$)	226
	3,5-dichloropyridine	1.88	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	226
	3,5-dichloropyridine	-0.14(M_2L)	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4 ($M + ML = M_2L$)	226
	4-(*N*,*N*-dimethylamino)pyridine	4.49	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	226
	4-(*N*,*N*-dimethylamino)pyridine	0.29(M_2L)	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4 ($M + ML = M_2L$)	226
	imidazole	4.98	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	226
	imidazole	0.21(M_2L)	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4 ($M + ML = M_2L$)	226
	3,4-lutidine	4.23	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	226
	3,4-lutidine	-0.89(M_2L)	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4 ($M + ML = M_2L$)	226
	1-methylimidazole	5.40	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	226
	1-methylimidazole	-0.96(M_2L)	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4 ($M + ML = M_2L$)	226
	2-methylimidazole	5.76	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	226
	2-methylimidazole	4.15(M_2L)	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4 ($M + ML = M_2L$)	226
	2-picoline	2.47	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	226
	2-picoline	-0.20(M_2L)	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4 ($M + ML = M_2L$)	226
	3-picoline	4.19	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	226
	3-picoline	-0.85(M_2L)	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4 ($M + ML = M_2L$)	226
	4-picoline	4.21	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	226
	4-picoline	-0.80(M_2L)	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4 ($M + ML = M_2L$)	226

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	piperidine	4.33	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	226
	piperidine	-0.52(M_2L)	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4 ($M + ML = M_2L$)	226
	propylene oxide	~-0.3	Spec			20	C_6H_6	227
	propylene sulfide	<<-1	Spec			20	C_6H_6	227
	pyridine	3.30	Spec			29.9	C_6H_6 (estimated K)	228
	pyridine	-0.24(M_2L)	Spec	-10.9	-41	29.9	C_6H_6 ($M + ML <-> M_2L$)	228
	pyridine	3.63	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	226
	pyridine	-0.73(M_2L)	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4 ($M + ML = M_2L$)	226
	pyridine	-0.78(M_2L)	Spec	-9.92	-47.7	30	2,6-lutidine ($M + ML <-> M_2L$)	229
Porphyrin-10 (XXVIII)	*N,N'*-dimidazolylmethane	3.48	Spec			-20	DMF	230
	4,6-dinitrobenzofuroxan	2.02	Spec	-8.7	9.2	25	CH_2Cl_2	221
	1-methylimidazole	3.4	Spec			-20	DMF	230
	4-picoline	3.11	Spec			-20	DMF	230
	2,4,5,7-tetranitrofluorenone	2.76	Spec	-2.8	43.2	25	CH_2Cl_2	222
	1,3,5-trinitrobenzene	1.93	Spec	-14.0	-10.0	25	$CHCl_3$	231
	2,4,7-trinitrofluorenone	2.70	Spec	-3.2	40.8	25	CH_2Cl_2	223
Porphyrin-11 (XXVIII)	4-aminopyridine	2.57	Spec	-31.8	-59	25	$CHCl_3$	232
	4-cyanopyridine	2.86	Spec	-18.0	-4	25	C_6H_6	232
	4-cyanopyridine	2.57	Spec	29.3	146	25	$CHCl_3$	232
	4,6-dinitrobenzofuroxan	1.74	Spec	-13.8	-13.2	25	CH_2Cl_2	221
	methyl 4-pyridineacetate	3.15	Spec	6.3	25	25	$CHCl_3$	232
	4-picoline	3.08	Spec	-27.6	-33	25	C_6H_6	232
	pyridine	3.15	Spec	-26.4	-29	25	C_6H_6	232
	pyridine	3.01	Spec	-17.6	0	25	$CHCl_3$	232
	4-pyridinecarboxaldehyde	2.27	Spec	25.1	130	25	$CHCl_3$	232
	2,4,5,7-tetranitrofluorenone	2.25	Spec	-5.5	24.7	25	CH_2Cl_2	222
	1,3,5-trinitrobenzene	1.23	Spec	-30.0	-80.0	25	$CHCl_3$	231
	2,4,7-trinitrofluorenone	2.15	Spec	-8.5	12.7	25	CH_2Cl_2	223
Porphyrin-12 (XXVIII)	4,6-dinitrobenzofuroxan	1.89	Spec	-18.9	-27.15	25	CH_2Cl_2	221
	pyridine	-1.3	Spec			29.9	C_6H_6	228
	2,4,5,7-tetranitrofluorenone	2.65	Spec	-5.3	33.0	25	CH_2Cl_2	222
	1,3,5-trinitrobenzene	1.65	Spec	-20.0	-34.5	25	$CHCl_3$	231
	2,4,7-trinitrofluorenone	2.64	Spec	-1.0	46.9	25	CH_2Cl_2	223
	2,4,7-trinitrofluorenone	2.75	Spec	-2.7	43.5	25	$CHCl_3$	223
	2,4,7-trinitrofluorenone	2.74	Spec	-2.6	43.6	25	Diox	223
	2,4,7-trinitrofluorenone	2.03	Spec	-8.2	16.8	25	toluene	223
	2,4,7-trinitrofluorenone	2.70	Spec	-4.0	38.1	25	ethyl acetate	223
Porphyrin-13 (XXVIII)	3-acetylpyridine	3.31	Spec			25	CH_2Cl_2	233
	3-acetylpyridine	3.19	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	4-acetylpyridine	3.51	Spec			25	CH_2Cl_2	233
	4-acetylpyridine	3.27	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	2-aminopyridine	2.87	Spec			25	CH_2Cl_2	233
	2-aminopyridine	2.76	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	4-aminopyridine	4.62	Spec	-58.2	-109	25	C_6H_6	232
	4-aminopyridine	4.65	Spec			25	C_6H_6	234
	4-aminopyridine	3.52	Spec	-21.3	-4	25	$CHCl_3$	232
	4-aminopyridine	4.67	Spec			25	CH_2Cl_2	233
	4-aminopyridine	4.49	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	anisole	none	Spec			24	C_6H_6	235

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	benzaldehyde	0	Spec			24	C_6H_6	235
	benzhydrol	0.39	Spec			24	C_6H_6	235
	benzyl alcohol	1.21	Spec			24	C_6H_6	235
	3-bromopyridine	3.14	Spec			25	CH_2Cl_2	233
	3-bromopyridine	3.06	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	1-butanol	1.06	Spec			24	C_6H_6	235
	2-butanol	1.03	Spec			24	C_6H_6	235
	butyl acetate	0.05	Spec			24	C_6H_6	235
	4-butyrolactone	0.30	Spec			24	C_6H_6	235
	3-chloropyridine	3.11	Spec			25	CH_2Cl_2	233
	3-chloropyridine	3.00	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	2,4,6-collidine	1.82	Spec			25	C_6H_6	234
	o-cresol	none	Spec			24	C_6H_6	235
	m-cresol	-0.40	Spec			24	C_6H_6	235
	p-cresol	-0.41	Spec			24	C_6H_6	235
	3-cyanopyridine	2.80	Spec			25	C_6H_6	234
	3-cyanopyridine	2.82	Spec			25	CH_2Cl_2	233
	3-cyanopyridine	2.70	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	4-cyanopyridine	2.20	Spec	-18.0	-4	25	C_6H_6	232
	4-cyanopyridine	2.90	Spec			25	C_6H_6	234
	4-cyanopyridine	2.05	Spec	-20.1	-4	25	$CHCl_3$	232
	4-cyanopyridine	3.00	Spec			25	CH_2Cl_2	233
	4-cyanopyridine	2.84	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	cyclohexanol	0.97	Spec			24	C_6H_6	235
	cyclohexanone	0.38	Spec			24	C_6H_6	235
	3,5-dichloro-pyridine	2.45	Spec			25	CH_2Cl_2	233
	3,5-dichloro-pyridine	2.50	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	diethyl ether	0.16	Spec			24	C_6H_6	235
	N,N'-diimidazolyl-methane	4.67	Spec			24	C_6H_6	230
	4-(*N,N*-dimethyl-amino)pyridine	4.84	Spec			25	CH_2Cl_2	233
	4-(*N,N*-dimethyl-amino)pyridine	4.61	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	dimethylformamide	1.77	Spec			24	C_6H_6	235
	1,2-dimethyl-imidazole	5.57	Spec			25	CH_2Cl_2	233
	1,2-dimethyl-imidazole	5.47	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	dimethylsulfoxide	2.85	Spec			24	C_6H_6	235
	dimethylsulfoxide	3.58	Spec	-36.4	53.6	25	cyclohexane	236
	4,6-dinitro-benzofuroxan	1.15	Spec	-14.0	-25.1	25	CH_2Cl_2	221
	4,4'-dipyridyl-methane	4.17	Spec			24	C_6H_6	230
	ethanol	1.00	Spec			24	C_6H_6	235
	ethyl acetate	0.04	Spec			24	C_6H_6	235
	imidazole	5.11	Spec			25	CH_2Cl_2	233
	imidazole	5.28	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	imidazole	4.69	Spec	-50.6	-80	25	C_6H_5Cl	237
	imidazole	4.92	Spec	-40.6	-42	25	1-chlorobutane	237
	3,4-lutidine	4.15	Spec			25	CH_2Cl_2	233
	3,4-lutidine	3.98	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	methanol	0.98	Spec			24	C_6H_6	235
	methyl ethyl ketone	-0.04	Spec			24	C_6H_6	235
	1-methylimidazole	4.66	Spec			24	C_6H_6	230
	1-methylimidazole	5.38	Spec			25	CH_2Cl_2	233
	1-methylimidazole	5.16	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	2-methylimidazole	5.45	Spec			25	CH_2Cl_2	233
	2-methylimidazole	5.32	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	2-methyl-1-propanol	0.94	Spec			24	C_6H_6	235
	2-methyl-2-propanol	0.60	Spec			24	C_6H_6	235
	methyl 4-pyridine-acetate	3.23	Spec	-19.7	-4	25	$CHCl_3$	232
	7-oxabicyclo-[2.2.1]heptane	2.68	Spec	-29.7	49.0	25	cyclohexane	236
	1-pentanol	1.06	Spec			24	C_6H_6	235
	perfluoro-1,1-dihydroethanol	-0.72	Spec			24	C_6H_6	235
	phenol	-0.08	Spec			24	C_6H_6	235
	2-picoline	2.30	Spec			25	C_6H_6	234

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	2-picoline	2.36	Spec			25	CH_2Cl_2	233
	2-picoline	2.25	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	2-picoline	2.45	Spec	-33.5	-67	25	C_6H_5Cl	237
	2-picoline	2.75	Spec	-32.2	-56	25	1-chlorobutane	237
	3-picoline	3.81	Spec			25	C_6H_6	234
	3-picoline	3.92	Spec			25	CH_2Cl_2	233
	3-picoline	3.76	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	4-picoline	4.08	Spec			24	C_6H_6	230
	4-picoline	4.02	Spec			25	C_6H_6	234
	4-picoline	3.96	Spec			25	CH_2Cl_2	233
	4-picoline	3.82	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	piperidine	5.05	Spec			25	C_6H_6	234
	piperidine	5.09	Spec			25	CH_2Cl_2	233
	piperidine	4.90	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	propylene oxide	0.78	Spec			20	C_6H_6	227
	propylene sulfide	0.48	Spec			20	C_6H_6	227
	pyridine	3.60	Spec	-36.8	-54	25	C_6H_6	232
	pyridine	3.78	Spec			25	C_6H_6	234
	pyridine	3.72	Spec			25	C_6H_6	238
	pyridine	3.57	Spec	-38.5	-59	29.9	C_6H_6	228
	pyridine	2.79	Spec	-16.7	0	25	$CHCl_3$	232
	pyridine	3.82	Spec			25	CH_2Cl_2	233
	pyridine	3.84	Spec			25	CH_2Cl_2	239
	pyridine	3.62	Spec			25	CH_2Cl_2, 0.1 M Bu_4NClO_4	233
	pyridine	3.68	Spec			25	CH_2Cl_2, 1.24×10^{-2} M Bu_4NClO_4	239
	pyridine	3.75	Spec	-43.5	-71	25	C_6H_5Cl	237
	pyridine	4.23	Spec	-39.3	-50	25	1-chlorobutane	237
	pyridine	4.40	Spec	-41.8	56.5	25	cyclohexane	236
	pyridine	3.68	Spec	-38.9	-59	25	toluene	237
	4-pyridine-carboxaldehyde	3.24	Spec			25	C_6H_6	234
	tetrahydrofuran	1.66	Spec			24	C_6H_6	235
	tetrahydrothiophene	1.98	Spec	-28.0	56.1	25	cyclohexane	236
	tetramethylene sulfoxide	2.74	Spec			24	C_6H_6	235
	1,1,3,3-tetra-methylthiourea	1.08	Spec	-23.4	-57.7	25	C_6H_6	240
	1,1,3,3-tetra-methylurea	1.86	Spec	-27.2	-55.6	25	C_6H_6	240
	2,4,5,7-tetra-nitrofluorenone	1.89	Spec	-9.4	4.5	25	CH_2Cl_2	222
	1,3,5-trinitro-benzene	-0.30	Spec	-120	-406	25	$CHCl_3$	231
	1,3,5-trinitro-benzene	2.01	Spec			25	ether	231
	2,4,7-trinitro-fluorenone	1.97	Spec	-6.6	15.7	25	$CHCl_3$	223
	2,4,7-trinitro-fluorenone	1.60	Spec	-6.3	9.4	25	CH_2Cl_2	223
	2,4,7-trinitro-fluorenone	1.79	Spec	-11.2	-3.74	25	ethyl acetate	223
	2,4,7-trinitro-fluorenone	1.79	Spec	-11.7	-4.9	25	Diox	223
	2,4,7-trinitro-fluorenone	1.76	Spec	-12.3	-7.8	25	toluene	223
	triphenylcarbinol	none	Spec			24	C_6H_6	235
	triphenylphosphine	1.42	Spec	-32.2	-81.2	25	C_6H_6	240
Porphyrin-14 (XXVIII)	4-aminopyridine	4.73	Spec			25	C_6H_6	241
	t-butylthiirane	1.60	Spec			20	C_6H_6	227
	4-cyanopyridine	2.27	Spec			25	C_6H_6	241
	epichlorohydrin	<<-1	Spec			20	C_6H_6	227
	4-picoline	3.83	Spec			25	C_6H_6	241
	propylene oxide	~-0.3	Spec			20	C_6H_6	227
	propylene sulfide	1.30	Spec			20	C_6H_6	227
	pyridine	3.51	Spec			25	C_6H_6	241
	pyridine	3.43	Spec	-36.4	-54	29.9	C_6H_6	228
	2,4,5,7-tetra-nitrofluorenone	2.82	Spec	-3.9	40.7	25	CH_2Cl_2	222
	1,3,5-trinitro-benzene	2.10	Spec	-13.0	-33	25	ether	231
	2,4,7-trinitro-fluorenone	2.77	Spec	-2.1	45.7	25	CH_2Cl_2	223

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
Porphyrin-15 (XXVIII)	4-aminopyridine	2.92	Spec			25	C_6H_6	241
	4-cyanopyridine	0.22	Spec			25	C_6H_6	241
	3-picoline	1.41	Spec			25	C_6H_6	241
	4-picoline	1.62	Spec			25	C_6H_6	241
	pyridine	1.21	Spec			25	C_6H_6	241
	pyridine	1.08	Spec	-20.5	-46	29.9	C_6H_6	228
Porphyrin-16 (XXVIII)	pyridine	3.80	Spec			25	C_6H_6	238
Porphyrin-17 (XXVIII)	pyridine	3.72	Spec			25	C_6H_6	238
	1,4-benzoquinone	0.48	Fluor			25	Me_2CO (apparent K)	224
	1,4-benzoquinone	-0.30	Spec			25	Me_2CO (apparent K)	224
	1,4-benzoquinone	-0.15	Spec			25	Me_2CO (ground state complex)	224
Porphyrin-18 (XXVIII)	pyridine	3.84	Spec			25	C_6H_6	238
Porphyrin-19 (XXVIII)	pyridine	3.69	Spec			25	C_6H_6	238
Porphyrin-20 (XXVIII)	4-ethylpyridine	4.38	NMR/UV			20	$CDCl_3/CHCl_3$	242
	imidazole	4.51	NMR/UV			20	$CDCl_3/CHCl_3$	242
	3,5-lutidine	4.15	NMR/UV			20	$CDCl_3/CHCl_3$	242
	purine	3.61	NMR/UV			20	$CDCl_3/CHCl_3$	242
	pyrazine N-oxide	2.86	NMR/UV			20	$CDCl_3/CHCl_3$	242
	pyridine	4.04	NMR/UV			20	$CDCl_3/CHCl_3$	242
	3-pyridinol	4.08	NMR/UV			20	$CDCl_3/CHCl_3$	242
	4-pyridinol	3.11	NMR/UV			20	$CDCl_3/CHCl_3$	242
	tropine	1.70	NMR/UV			20	$CDCl_3/CHCl_3$	242
Porphyrin-21 (XXVIII)	pyridine	4.09	Spec			25	C_6H_6	238
Porphyrin-22 (XXVIII)	pyridine	3.91	Spec			25	C_6H_6	238
Porphyrin-23 (XXVIII)	pyridine	4.14	Spec			25	C_6H_6	238
Porphyrin-24 (XXVIII)	pyridine	4.04	Spec			25	C_6H_6	238
Porphyrin-25 (XXVIII)	pyridine	4.19	Spec			25	C_6H_6	238
Porphyrin-26 (XXVIII)	pyridine	-0.92	Spec			25	$CDCl_3$	243
Porphyrin-27 (XXVIII)	pyridine	0.40	Spec			25	$CDCl_3$	243
Porphyrin-28 (XXVIII)	pyridine	0.7	Spec			25	$CDCl_3$	243
Porphyrin-29 (XXVIII)	pyridine	2.7	Spec			25	$CDCl_3$	243
Porphyrin-30 (XXVIII)	pyridine	-1.1	Spec			25	$CDCl_3$	243
Porphyrin-31 (XXVIII)	pyridine	3.76	Spec			25	$CDCl_3$	243
Porphyrin-32 (XXIX)	4,4'-bipyridine	3.38	Spec			25?	CH_2Cl_2 (microscopic K)	244
	1,2-bis(4-pyridyl)-ethane	3.63	Spec			25?	CH_2Cl_2 (microscopic K)	244
	pyridine	3.45	Spec			25?	CH_2Cl_2 (microscopic K)	244
	2,4,6-tri(4-pyridyl)-1,3,5-triazine	3.11	Spec			25?	CH_2Cl_2 (microscopic K)	244
Porphyrin-33 (XXIX)	4,4'-bipyridine	3.9	Spec			25?	CH_2Cl_2	245
	1,2-bis(4-pyridyl)-ethane	4.1	Spec			25?	CH_2Cl_2	245
	1,3-bis(4-pyridyl)-propane	4.2	Spec			25?	CH_2Cl_2	245
	pyridine	3.7	Spec			25?	CH_2Cl_2	245
	2,4,6-tri(4-pyridyl)-1,3,5-triazine	3.9	Spec			25?	CH_2Cl_2	245
Porphyrin-34 (XXIX)	9,10-anthraquinone	3.95	NMR			-30	$CDCl_3$	246
	9,10-anthraquinone	3.30	NMR			-15	$CDCl_3$	246
	9,10-anthraquinone	2.93	NMR			0	$CDCl_3$	246
	9,10-anthraquinone	2.36	NMR	-33.1	-66	25	$CDCl_3$	246
	9,10-anthraquinone	2.30	UV			25	$CHCl_3$	246
	anthrone	1.20	NMR			-15	$CDCl_3$	246
	anthrone	1.08	NMR			0	$CDCl_3$	246

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	anthrone	0.62	NMR	-21.8	-60	25	$CDCl_3$	246
	anthrone	0.67	UV			25	$CHCl_3$	246
	1,4-benzoquinone	2.68	NMR			-30	$CDCl_3$	246
	1,4-benzoquinone	2.38	NMR			-15	$CDCl_3$	246
	1,4-benzoquinone	2.11	NMR			0	$CDCl_3$	246
	1,4-benzoquinone	1.74	NMR	-23.4	-46	25	$CDCl_3$	246
	1,4-benzoquinone	1.65	UV			25	$CHCl_3$	246
	2-chloro-1,4-benzoquinone	3.15	NMR			-30	$CDCl_3$	246
	2-chloro-1,4-benzoquinone	2.76	NMR			-15	$CDCl_3$	246
	2-chloro-1,4-benzoquinone	2.49	NMR			0	$CDCl_3$	246
	2-chloro-1,4-benzoquinone	2.08	NMR	-27.2	-52	25	$CDCl_3$	246
	1,4-cyclohexane-dione	1.34	NMR			-15	$CDCl_3$	246
	1,4-cyclohexane-dione	1.23	NMR			0	$CDCl_3$	246
	1,4-cyclohexane-dione	1.00	NMR	-12.1	-21	25	$CDCl_3$	246
	cyclohexanone	-0.42	NMR			-15	$CDCl_3$	246
	cyclohexanone	-0.49	NMR			0	$CDCl_3$	246
	cyclohexanone	-0.62	NMR	-7.53	-37	25	$CDCl_3$	246
	2,5-dichloro-1,4 benzoquinone	3.75	NMR			-30	$CDCl_3$	246
	2,5-dichloro-1,4 benzoquinone	3.18	NMR			-15	$CDCl_3$	246
	2,5-dichloro-1,4-benzoquinone	2.81	NMR			0	$CDCl_3$	246
	2,5-dichloro-1,4-benzoquinone	2.34	NMR	-35.1	-74	25	$CDCl_3$	246
	2,3-dimethoxy-5-methyl-1,4-benzoquinone	1.54	NMR	-25.1	-56	25	$CDCl_3$	246
	2,3-dimethoxy-5-methyl-1,4-benzoquinone	1.32	NMR			40	$CDCl_3$	246
	2,3-dimethoxy-5-methyl-1,4-benzoquinone	1.11	NMR			55	$CDCl_3$	246
	2,5-dimethyl-1,4-benzoquinone	3.15	NMR			-30	$CDCl_3$	246
	2,5-dimethyl-1,4-benzoquinone	2.78	NMR			-15	$CDCl_3$	246
	2,5-dimethyl-1,4-benzoquinone	2.52	NMR			0	$CDCl_3$	246
	2,5-dimethyl-1,4 benzoquinone	2.04	NMR	-28.5	-56	25	$CDCl_3$	246
	2-methyl-1,4-benzoquinone	2.98	NMR			-30	$CDCl_3$	246
	2-methyl-1,4-benzoquinone	2.65	NMR			-15	$CDCl_3$	246
	2-methyl-1,4-benzoquinone	2.38	NMR			0	$CDCl_3$	246
	2-methyl-1,4-benzoquinone	1.94	NMR	-26.4	-51	25	$CDCl_3$	246
	1,2-naphthoquinone	1.23	NMR			-15	$CDCl_3$	246
	1,2-naphthoquinone	1.11	NMR			0	$CDCl_3$	246
	1,2-naphthoquinone	0.94	NMR	-10.9	-18	25	$CDCl_3$	246
	1,4-naphthoquinone	3.59	NMR			-30	$CDCl_3$	246
	1,4-naphthoquinone	2.71	NMR			-15	$CDCl_3$	246
	1,4-naphthoquinone	2.23	NMR	-34.7	-74	25	$CDCl_3$	246
	tetrachloro-1,4-benzoquinone	2.60	NMR	-36.0	-72	25	$CDCl_3$	246
	tetrachloro-1,4-benzoquinone	2.26	NMR			40	$CDCl_3$	246
	tetrachloro-1,4-benzoquinone	2.00	NMR			55	$CDCl_3$	246
	tetrafluoro-1,4-benzoquinone	2.57	NMR	-33.5	-63	25	$CDCl_3$	246
	tetrafluoro-1,4-benzoquinone	2.30	NMR			40	$CDCl_3$	246
	tetrafluoro-1,4-benzoquinone	2.04	NMR			55	$CDCl_3$	246

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	tetramethoxy-1,4-benzoquinone	1.60	NMR			-30	$CDCl_3$	246
	tetramethoxy-1,4-benzoquinone	1.43	NMR			-15	$CDCl_3$	246
	tetramethoxy-1,4-benzoquinone	1.23	NMR			0	$CDCl_3$	246
	tetramethoxy-1,4-benzoquinone	0.89	NMR	-18.0	-44	25	$CDCl_3$	246
	tetramethoxy-1,4-benzoquinone	0.90	UV			25	$CHCl_3$	246
	tetramethyl-1,4-benzoquinone	2.62	NMR	-37.7	-77	25	$CDCl_3$	246
	tetramethyl-1,4-benzoquinone	2.23	NMR			40	$CDCl_3$	246
	tetramethyl-1,4-benzoquinone	1.95	NMR			55	$CDCl_3$	246
Porphyrin-35 (XXIX)	2-aminobenzoic acid	3.15	Spec			0	$CHCl_3$	247
	2-aminobenzoic acid	2.89	Spec	-25.9	-35.1	15	$CHCl_3$	247
	2-aminobenzoic acid	2.64	Spec			30	$CHCl_3$	247
	2-aminobenzoic acid	2.47	Spec			45	$CHCl_3$	247
	4-aminobenzoic acid	3.59	Spec			0	$CHCl_3$	247
	4-aminobenzoic acid	3.33	Spec			15	$CHCl_3$	247
	4-aminobenzoic acid	3.11	Spec	-25.1	-22.6	30	$CHCl_3$	247
	4-aminobenzoic acid	2.91	Spec			45	$CHCl_3$	247
	2-aminobenzoic acid methyl ester	3.47	Spec			0	$CHCl_3$	247
	2-aminobenzoic acid methyl ester	3.20	Spec	-25.9	-28.9	15	$CHCl_3$	247
	2-aminobenzoic acid methyl ester	2.94	Spec			30	$CHCl_3$	247
	4-aminobenzoic acid methyl ester	3.65	Spec			0	$CHCl_3$	247
	4-aminobenzoic acid methyl ester	3.39	Spec	-23.0	-15.1	15	$CHCl_3$	247
	4-aminobenzoic acid methyl ester	3.17	Spec			30	$CHCl_3$	247
	4-aminoheptane	5.59	Spec			15	$CHCl_3$	248
	L-leucine methyl ester	5.20	Spec			15	$CHCl_3$	248
Porphyrin-36 (XXIX)	9,10-anthraquinone	1.49	NMR			-30	$CDCl_3$	246
	9,10-anthraquinone	1.32	NMR			-15	$CDCl_3$	246
	9,10-anthraquinone	1.11	NMR			0	$CDCl_3$	246
	9,10-anthraquinone	0.77	NMR	-15.9	-36	25	$CDCl_3$	246
	anthrone	1.36	NMR			-30	$CDCl_3$	246
	anthrone	1.08	NMR			-15	$CDCl_3$	246
	anthrone	0.90	NMR			0	$CDCl_3$	246
	anthrone	0.65	NMR	-17.2	-45	25	$CDCl_3$	246
	1,4-benzoquinone	1.11	NMR			-30	$CDCl_3$	246
	1,4-benzoquinone	0.91	NMR			-15	$CDCl_3$	246
	1,4-benzoquinone	0.73	NMR			0	$CDCl_3$	246
	1,4-benzoquinone	0.51	NMR	-15.1	-41	25	$CDCl_3$	246
	tetramethyl-1,4-benzoquinone	1.15	NMR			-30	$CDCl_3$	246
	tetramethyl-1,4 benzoquinone	0.94	NMR			-15	$CDCl_3$	246
	tetramethyl-1,4-benzoquinone	0.76	NMR			0	$CDCl_3$	246
	tetramethyl-1,4-benzoquinone	0.48	NMR	-17.2	-48	25	$CDCl_3$	246
Porphyrin-37 (XXIX)	2-aminobenzoic acid	5.47	Spec			0	$CHCl_3$	247
	2-aminobenzoic acid	5.08	Spec	-39.3	-38.9	15	$CHCl_3$	247
	2-aminobenzoic acid	4.71	Spec			30	$CHCl_3$	247
	2-aminobenzoic acid	4.40	Spec			45	$CHCl_3$	247
	4-aminobenzoic acid	3.73	Spec			0	$CHCl_3$	247
	4-aminobenzoic acid	3.50	Spec	-23.4	-14.6	15	$CHCl_3$	247
	4-aminobenzoic acid	3.27	Spec			30	$CHCl_3$	247
	4-aminobenzoic acid	3.08	Spec			45	$CHCl_3$	247
	2-aminobenzoic acid methyl ester	4.61	Spec			0	$CHCl_3$	247
	2-aminobenzoic acid methyl ester	4.25	Spec	-38.1	-52.3	15	$CHCl_3$	247

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	2-aminobenzoic acid methyl ester	3.88	Spec			30	$CHCl_3$	247
	4-aminobenzoic acid methyl ester	3.67	Spec			0	$CHCl_3$	247
	4-aminobenzoic acid methyl ester	3.47	Spec	-23.8	-16.7	15	$CHCl_3$	247
	4-aminobenzoic acid methyl ester	3.24	Spec			30	$CHCl_3$	247
	4-aminoheptane	5.46	Spec			15	$CHCl_3$	248
	L-leucine ethyl ester	6.70	Spec			15	$CHCl_3$	248
Porphyrin-38 (XXIX)	4-ethylpyridine	-0.82(M_2L)	Spec			30	2,6-lutidine (M + ML <-> M_2L)	229
	4-methoxypyridine	-0.46(M_2L)	Spec			30	2,6-lutidine (M + ML <-> M_2L)	229
	4-picoline	-0.80(M_2L)	Spec			30	2,6-lutidine (M + ML <-> M_2L)	229
	pyridine	-0.61(M_2L)	Spec	-16.3	-62.3	30	2,6-lutidine (M + ML <-> M_2L)	229
	4-vinylpyridine	-1.05(M_2L)	Spec			30	2,6-lutidine (M + ML <-> M_2L)	229
Porphyrin-39 (XXIX)	4-carboxy-*n*-butyl-pyridine	3.52(M_2L)	Spec	-28.0	-29	25	C_6H_6 (2M + L <-> M_2L)	249
	4-cyanopyridine	3.08(M_2L)	Spec	-72.8	-184	25	CCl_4 (2M + L <-> M_2L)	250
	4-cyanopyridine	3.52(M_2L)	Spec	-28.9	-29	25	C_6H_6 (2M + L <-> M_2L)	249, 250
	4-cyanopyridine	1.54(M_2L)	Spec	-50.2	-138	25	$CHCl_3$ (2M + L <-> M_2L)	250
	4-picoline	2.79(M_2L)	Spec	-31.4	-50	25	CCl_4 (2M + L <-> M_2L)	250
	4-picoline	2.42(M_2L)	Spec	3.3	54	25	C_6H_6 (2M + L <-> M_2L)	249, 250
	pyridine	2.64(M_2L)	Spec	-59.4	-146	25	CCl_4 (2M + L <-> M_2L)	250
	pyridine	1.76(M_2L)	Spec	-14.6	-17	25	C_6H_6 (2M + L <-> M_2L)	250
	pyridine	2.57(M_2L)	Spec	-10.0	17	25	C_6H_6 (2M + L <-> M_2L)	249
	4-vinylpyridine	2.86(M_2L)	Spec	-6.7	33	25	C_6H_6 (2M + L <-> M_2L)	249
Porphyrin-40 (XXIX)	piperidine	-1.69(M_2L)	Spec	-23.0	-110	25	$CHCl_3$ (2M + L <-> M_2L)	251
Porphyrin-41 (XXIX)	4-carboxy-*n*-butyl-pyridine	3.67(M_2L)	Spec	29.3	176	25	C_6H_6 (2M + L <-> M_2L)	249
	4-cyanopyridine	1.25(M_2L)	Spec	31.4	134	25	C_6H_6 (2M + L <-> M_2L)	249
	4-picoline	1.10(M_2L)	Spec	-10.9	-17	25	C_6H_6 (2M + L <-> M_2L)	249
	pyridine	1.32(M_2L)	Spec	-31.4	134	25	C_6H_6 (2M + L <-> M_2L)	249
	4-vinylpyridine	2.64(M_2L)	Spec	-15.1	0	25	C_6H_6 (2M + L <-> M_2L)	249
Porphyrin-42 (XXIX)	piperidine	-0.25(M_2L)	Spec	-32.6	-114	25	$CHCl_3$ (2M + L <-> M_2L)	251
Porphyrin-43 (XXIX)	pyridine	-0.61(M_2L)	Spec	-17.8	-70.3	30	2,6-lutidine (M + ML <-> M_2L)	229
Porphyrin-44 (XXIX)	4-aminopyridine	5.65(M_2L)	Spec	-67.4	-117	25	C_6H_6 (2M + L <-> M_2L)	249
	4-carboxy-*n*-butyl-pyridine	2.93(M_2L)	Spec	-42.3	-84	25	C_6H_6 (2M + L <-> M_2L)	249
	4-cyanopyridine	3.45(M_2L)	Spec	-107	-293	25	CCl_4 (2M + L <-> M_2L)	250
	4-cyanopyridine	3.01(M_2L)	Spec	-37.7	-67	25	C_6H_6 (2M + L <-> M_2L)	249, 250
	4-cyanopyridine	2.71(M_2L)	Spec	-80.8	-218	25	$CHCl_3$ (2M + L <-> M_2L)	250
	4-picoline	2.79(M_2L)	Spec	-103	-293	25	CCl_4 (2M + L <-> M_2L)	250
	4-picoline	6.60(M_2L)	Spec	-58.6	-67	25	C_6H_6 (2M + L <-> M_2L)	249, 250
	4-picoline	1.10(M_2L)	Spec	-51.0	-151	25	$CHCl_3$ (2M + L <-> M_2L)	250
	pyridine	0.44(M_2L)	Spec	-66.9	-209	25	CCl_4 (2M + L <-> M_2L)	250
	pyridine	1.32(M_2L)	Spec	-13.8	-21	25	C_6H_6 (2M + L <-> M_2L)	249, 250
	pyridine	0.22(M_2L)	Spec	-45.2	-146	25	$CHCl_3$ (2M + L <-> M_2L)	250
	4-vinylpyridine	3.74(M_2L)	Spec	-31.0	-33	25	C_6H_6 (2M + L <-> M_2L)	249
Porphyrin-45 (XXIX)	piperidine	-1.39(M_2L)	Spec	-21.8	-99.6	25	$CHCl_3$ (2M + L <-> M_2L)	251
Porphyrin-46 (XXIX)	piperidine	0.15(M_2L)	Spec	-32.6	-107	25	$CHCl_3$ (2M + L <-> M_2L)	251
Porphyrin-47 (XXIX)	piperidine	-1.70(M_2L)	Spec	-18.0	-88.3	25	$CHCl_3$ (2M + L <-> M_2L)	251
Porphyrin-48 (XXIX)	pyridine	-0.55(M_2L)	Spec	-16.3	-64.4	30	2,6-lutidine (M + ML <-> M_2L)	229
Porphyrin-49 (XXIX)	pyridine	-0.49(M_2L)	Spec	-16.7	-64.4	30	2,6-lutidine (M + ML <-> M_2L)	229
Porphyrin-50 (XXX)	pyridine	0.34	Spec			25	$CDCl_3$	243

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
Porphyrin-51 (XXX)	pyridine	0.9	Spec			25	$CDCl_3$	243
Porphyrin-52 (XXX)	pyridine	3.9	Spec			25	$CDCl_3$	243
Porphyrin-53 (XXX)	pyridine	-1.0	Spec			25	$CDCl_3$	243
Porphyrin-54 (XXX)	pyridine	1.5	Spec			25	$CDCl_3$	243
Porphyrin-55 (XXX)	pyridine	-2.1	Spec			25	$CDCl_3$	243
Porphyrin-56 (XXX)	pyridine	2.97	Spec			25	$CDCl_3$	243
Porphyrin-57 (XXX)	pyridine	1.58(M_2L)	Spec			25?	H_2O (2M + L <-> M_2L)	252
Porphyrin-58 (XXX)	pyridine	-1.23	Spec			25?	H_2O (2M + L <-> ML)	252
	pyridine	0.27(M_2L)	Spec			25?	H_2O (M + ML <-> M_2L)	252
Porphyrin-59 (XXX)	pyridine	0.54	Spec			25	$CDCl_3$	243
Porphyrin-60 (XXX)	pyridine	2.47	Spec			25	$CDCl_3$	243
Porphyrin-61 (XXX)	pyridine	-1.15(M_2L)	Spec	-16.6	-77.0	30	2,6-lutidine (M + ML <-> M_2L)	229
Porphyrin-62 (XXX)	4-carboxy-*n*-butyl-pyridine	3.15(M_2L)	Spec	-37.2	-63	25	C_6H_6 (2M + L <-> M_2L)	249
	4-cyanopyridine	2.79(M_2L)	Spec	-49.0	-100	25	C_6H_6 (2M + L <-> M_2L)	249
	4-picoline	3.74(M_2L)	Spec	-36.4	-50	25	C_6H_6 (2M + L <-> M_2L)	249
	pyridine	2.42(M_2L)	Spec	-21.8	-25	25	C_6H_6 (2M + L <-> M_2L)	249
	4-vinylpyridine	3.67(M_2L)	Spec	-42.7	-67	25	C_6H_6 (2M + L <-> M_2L)	249
Porphyrin-63 (XXX)	piperidine	-2.04(M_2L)	Spec	-11.7	-78.7	25	$CHCl_3$ (2M + L <-> M_2L)	251
	piperidine	-2.08(M_2L)	Spec	-20.3	-105	34	THF (2M + L <-> M_2L)	253
Porphyrin-64 (XXX)	piperidine	-0.89	Spec	-9.62	-48.5	34	THF	253
Porphyrin-65 (XXX)	pyridine	-0.84(M_2L)	Spec	-15.8	-68.2	30	2,6-lutidine (M + ML <-> M_2L)	229
Porphyrin-66 (XXX)	pyridine	2.30	Spec			25	Diox	254
Porphyrin-67 (XXX)	piperidine	-1.02(M_2L)	Spec	-9.54	-50.2	30	2,6-lutidine (M + ML <-> M_2L)	229
	pyridine	-1.17(M_2L)	Spec	-12.2	-62.8	30	2,6-lutidine (M + ML <-> M_2L)	229
	pyrrolidine	-1.02(M_2L)	Spec	-10.3	-52.7	30	2,6-lutidine (M + ML <-> M_2L)	229
Porphyrin-68 (XXX)	pyridine	3.46	UV			25?	CH_2Cl_2	255, 256
	triethylene-diamine	5.38(1)	UV	-62	-103	25?	CH_2Cl_2	256
	triethylene-diamine	≥4(2)	UV			25?	CH_2Cl_2	256
Porphyrin-69 (XXX)	H_2O	4.47	Spec			25?	C_6H_6	252, 257
	aniline	1.66	Spec			25?	C_6H_6	252, 257
	benzyl alcohol	3.46	Spec			25?	C_6H_6	252, 257
	benzylamine	4.43	Spec			25?	C_6H_6	252, 257
	dimethylaniline	1.02	Spec			25?	C_6H_6	252, 257
	n-heptylamine	5.19	Spec			25?	C_6H_6	252, 257
	1-octanol	3.66	Spec			25?	C_6H_6	252, 257
	phenol	1.19	Spec			25?	C_6H_6	252, 257
	quinoline	4.12	Spec			25?	C_6H_6	252, 257
Porphyrin-70 (XXX)	pyridine	-1.13(M_2L)	Spec	-10.7	-57.3	30	2,6-lutidine (M + ML <-> M_2L)	229
Porphyrin-71 (XXX)	pyridine	3.60	Spec			29.9	C_6H_6 (estimated K)	228
	pyridine	-0.08(M_2L)	Spec	-10.9	-38	29.9	C_6H_6 (M + ML <-> M_2L)	228
Porphyrin-72 (XXX)	pyridine	3.72	Spec	-37.7	-54	29.9	C_6H_6	228
Porphyrin-73 (XXXI)	*N,N'*-diimidazolyl-methane	>6.6	Spec			18	C_6H_6 (4 coordination <-> 5 coordination)	230

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	N,N'-diimidazolyl-methane	4.90	Spec			18	C_6H_6 (K = averged value for two porphyrin moieties), (5 coordination <-> 6 coordination)	230
	N,N'-diimidazolyl-methane	5.1	Spec			18	DMF (5' coordination <-> 5# coordination)	230
	N,N'-diimidazolyl-methane	3.7	Spec			18	DMF (K = averged value for two porphyrin moieties), (5# coordination <-> 6 coordination)	230
	dimethylformamide	1.23	Spec			?	C_6H_6	230
	1-methylimidazole	3.5	Spec			18	C_6H_6 (K = averged value for two porphyrin moieties), (4 coordination <-> 5 coordination)	230
	1-methylimidazole	4.90	Spec			18	C_6H_6 (K = averged value for two porphyrin moieties), (5 coordination <-> 6 coordination)	230
Porphyrin-74 (XXXI)	*N,N'*-diimidazolyl-methane	6.6	Spec			-20	DMF	230
	4,4'-dipyridyl-methane	6.7	Spec			-20	DMF	230
	1-methylimidazole	3.3	Spec			-20	DMF (K = averged value for two porphyrin moieties)	230
Porphyrin-75 (XXXI)	4,4'-dipyridyl-methane	2.09	Spec			24	DMF	230
Porphyrin-76 (XXXI)	*N,N'*-diimidazolyl-methane	7.5	Spec			24	C_6H_6	230
	4,4'-dipyridyl-methane	6.6	Spec			24	C_6H_6	230
	1-methylimidazole	4.7	Spec			24	C_6H_6	230
	1-methylimidazole	4.93(M_2L)	Spec			24	C_6H_6	230
	4-picoline	4.13	Spec			24	C_6H_6	230
	4-picoline	4.20(M_2L)	Spec			24	C_6H_6	230
Porphyrin-77 (XXXI)	4,4'-bipyridine	3.26	Spec			25?	CH_2Cl_2	258
	1,2-bis(4-piperidyl)ethane	4.52	Spec	-60	-120	25?	CH_2Cl_2	258
	1,2-bis(4-pyridyl)-ethane	3.63	Spec			25?	CH_2Cl_2	258
	piperidine	4.08	Spec			25?	CH_2Cl_2	258
	pyrazine	2.26	Spec			25?	CH_2Cl_2	258
	pyridine	3.11	Spec			25?	CH_2Cl_2	258
	triethylamine	4.69	Spec	-60	-120	25?	CH_2Cl_2	258
Porphyrin-78 (XXXI)	4,4'-bipyridine	2.88	Spec			25?	CH_2Cl_2	258
	1,2-bis(4-piperidyl)ethane	4.15	Spec	-50	-100	25?	CH_2Cl_2	258
	1,2-bis(4-pyridyl)-ethane	3.11	Spec			25?	CH_2Cl_2	258
	piperidine	3.61	Spec			25?	CH_2Cl_2	258
	pyrazine	1.64	Spec			25?	CH_2Cl_2	258
	pyridine	2.56	Spec			25?	CH_2Cl_2	258
	triethylamine	4.36	Spec	-55	-100	25?	CH_2Cl_2	258
	guest-29[e]	3.11	Spec			25?	CH_2Cl_2	258
Porphyrin-79 (XXXII)	pyridine	2.01	UV			25?	CH_2Cl_2	256
	pyridine	1.34(M_2L)	UV			25?	CH_2Cl_2	256
	triethylene-diamine	~6	UV			25?	CH_2Cl_2	256
Porphyrin-80 (XXXII)	pyridine	2.01	UV			25?	CH_2Cl_2	256
	pyridine	1.34(M_2L)	UV			25?	CH_2Cl_2	256
	triethylene-diamine	~7	UV			25?	CH_2Cl_2	256
Porphyrin-81 (XXXII)	4-*t*-butylpyridine	2.63	UV			25?	CH_2Cl_2	255

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	4-*t*-butylpyridine	2.06(M_2L)	UV			25?	CH_2Cl_2	255
	pyridine	2.02	UV			25?	CH_2Cl_2	255, 256
	pyridine	2.31(M_2L)	UV			25?	CH_2Cl_2	255, 256
	triethylene-diamine	7.87	UV	-77	-121	25?	CH_2Cl_2 (guest bound inside cavity)	256
	triethylene-diamine	5.38	UV			25?	CH_2Cl_2 (guest bound outside cavity)	256
Porphyrin-82 (XXXII)	4,4'-bipyridine	3.58	Spec			25?	CH_2Cl_2 (guest bound outside cavity)	258
	4,4'-bipyridine	2.98(M_2L)	Spec			25?	CH_2Cl_2 (guest bound outside cavity)	258
	4,4'-bipyridine	3.11	Spec			25?	CH_2Cl_2 (guest bound inside cavity)	258
	1,2-bis(4-piperidyl)ethane	6.71	Spec	-70	-120	25?	CH_2Cl_2	258
	1,2-bis(4-piperidyl)ethane	nm(M_2L)	Spec			25?	CH_2Cl_2	258
	1,2-bis(4-pyridyl)-ethane	5.71	Spec			25?	CH_2Cl_2	258
	1,2-bis(4-pyridyl)-ethane	nm(M_2L)	Spec			25?	CH_2Cl_2	258
	piperidine	4.56	Spec			25?	CH_2Cl_2	258
	piperidine	3.95(M_2L)	Spec			25?	CH_2Cl_2	258
	pyrazine	2.78	Spec			25?	CH_2Cl_2	258
	pyrazine	2.18(M_2L)	Spec			25?	CH_2Cl_2	258
	pyridine	3.61	Spec			25?	CH_2Cl_2	258
	pyridine	3.04(M_2L)	Spec			25?	CH_2Cl_2	258
	triethylene-diamine	6.11	Spec	-100	-230	25?	CH_2Cl_2	258
	triethylene-diamine	3.11(M_2L)	Spec			25?	CH_2Cl_2	258
Porphyrin-83 (XXXII)	1,2-bis(4-pyridyl)-ethane	4.53	Spec			25?	CH_2Cl_2	258
	1,2-bis(4-pyridyl)-ethane	nm(M_2L)	Spec			25?	CH_2Cl_2	258
	pyridine	2.54	Spec			25?	CH_2Cl_2	258
	pyridine	2.26(M_2L)	Spec			25?	CH_2Cl_2	258
Porphyrin-84 (XXXII)	4,4'-bipyridine	3.26	Spec			25?	CH_2Cl_2 (guest bound outside cavity)	258
	4,4'-bipyridine	2.66(M_2L)	Spec			25?	CH_2Cl_2 (guest bound outside cavity)	258
	4,4'-bipyridine	3.00	Spec			25?	CH_2Cl_2 (guest bound inside cavity)	258
	1,2-bis(4-piperidyl)ethane	5.59	Spec	-50	-65	25?	CH_2Cl_2	258
	1,2-bis(4-piperidyl)ethane	nm(M_2L)	Spec			25?	CH_2Cl_2	258
	1,2-bis(4-pyridyl)-ethane	3.59	Spec			25?	CH_2Cl_2	258
	1,2-bis(4-pyridyl)-ethane	nm(M_2L)	Spec			25?	CH_2Cl_2	258
	piperidine	3.95	Spec			25?	CH_2Cl_2	258
	piperidine	3.32(M_2L)	Spec			25?	CH_2Cl_2	258
	pyrazine	1.84	Spec			25?	CH_2Cl_2	258
	pyrazine	1.23(M_2L)	Spec			25?	CH_2Cl_2	258
	pyridine	2.98	Spec			25?	CH_2Cl_2	258
	pyridine	2.52(M_2L)	Spec			25?	CH_2Cl_2	258
	triethylene-diamine	5.38	Spec	-95	-210	25?	CH_2Cl_2	258
	triethylene-diamine	4.00(M_2L)	Spec			25?	CH_2Cl_2	258
	guest-26[e]	5.41	Spec			25?	CH_2Cl_2	258, 259
	guest-26[e]	nm(M_2L)	Spec			25?	CH_2Cl_2	258, 259
Porphyrin-85 (XXXII)	*n*-butylamine	3.70	Spec			25	CH_2Cl_2	260, 261
	1,4-diaminobutane	5.78	Spec			25	CH_2Cl_2	260, 261
	1,2-diaminoethane	5.78	Spec			25	CH_2Cl_2	260, 261
	1,7-diaminoheptane	6.08	Spec			25	CH_2Cl_2	261
	1,7-diaminoheptane	6.30	Spec			25	CH_2Cl_2	260
	1,6-diaminohexane	6.48	Spec			25	CH_2Cl_2	260, 261

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	1,8-diaminooctane	5.48	Spec			25	CH_2Cl_2	260, 261
	1,5-diaminopentane	6.00	Spec			25	CH_2Cl_2	260, 261
	4,4'-dipyridine	7.48	Spec			25	CH_2Cl_2	260, 261
	pyridine	3.15	Spec			25	CH_2Cl_2	260, 261
Porphyrin-86 (XXXII)	4,4'-bipyridine	8.8	Spec			25?	CH_2Cl_2	245
	1,2-bis(4-pyridyl)-ethane	6.1	Spec			25?	CH_2Cl_2	245
	1,3-bis(4-pyridyl)-propane	5.1	Spec			25?	CH_2Cl_2	245
	pyridine	3.7	Spec			25?	CH_2Cl_2	245
	2,4,6-tri(4-pyridyl)-1,3,5-triazine	3.8	Spec			25?	CH_2Cl_2	245
Porphyrin-87 (XXXIII)	4,4'-bipyridine	4.20	Spec			25?	CH_2Cl_2 (microscopic K)	244
	1,2-bis(4-pyridyl)-ethane	6.65	Spec			25?	CH_2Cl_2 (microscopic K)	244
	pyridine	3.41	Spec			25?	CH_2Cl_2 (microscopic K)	244
	pyridine	3.41(M_2L)	Spec			25?	CH_2Cl_2 (microscopic K)	244
	2,4,6-tri(4-pyridyl)-1,3,5-triazine	7.64	Spec			25?	CH_2Cl_2 (microscopic K)	244
Porphyrin-88 (XXXIII)	4,4'-bipyridine	4.30	Spec			25?	CH_2Cl_2 (microscopic K)	244
	4,4'-bipyridine	3.43(M_2L)	Spec			25?	CH_2Cl_2 (microscopic K)	244
	1,2-bis(4-pyridyl)-ethane	6.63	Spec			25?	CH_2Cl_2 (microscopic K)	244
	1,2-bis(4-pyridyl)-ethane	3.45(M_2L)	Spec			25?	CH_2Cl_2 (microscopic K)	244
	pyridine	3.41	Spec			25?	CH_2Cl_2 (microscopic K)	244
	pyridine	3.41(M_2L)	Spec			25?	CH_2Cl_2 (microscopic K)	244
	pyridine	3.46(M_3L)	Spec			25?	CH_2Cl_2 (microscopic K)	244
	2,4,6-tri(4-pyridyl)-1,3,5-triazine	>9	Spec			25?	CH_2Cl_2 (microscopic K)	244
Porphyrin-89 (XXXIII)	4,4'-bipyridine	4.9	Spec			25?	CH_2Cl_2	245
	1,2-bis(4-pyridyl)-ethane	7.5	Spec			25?	CH_2Cl_2	245
	1,3-bis(4-pyridyl)-propane	8.8	Spec			25?	CH_2Cl_2	245
	pyridine	3.6	Spec			25?	CH_2Cl_2	245
	2,4,6-tri(4-pyridyl)-1,3,5-triazine	10.0	Spec			25?	CH_2Cl_2	245
Porphyrin-90 (XXXIII)	3,5-lutidine	<1	NMR			20	MeOD-d_3	262
	3,5-lutidine	<1	UV			20	MeOH	262
	pyridine	1.95	NMR			20	MeOD-d_3	262
	pyridine	1.85	UV			20	MeOH	262
Porphyrin-91 (XXXIV)	pyridine	3.67	NMR			20	$CDCl_3$	262
Porphyrin-92 (XXXIV)	pyridine	1.99	NMR			20	MeOD-d_3	262
Porphyrin-93 (XXXIV)	acenaphthylene	3.02	NMR			20	MeOD-d_3/D_2O/CD_3CO_2D (95:4.85:0.15 v/v)	263
	anthracene	2.66	NMR			20	MeOD-d_3/Me_2SO-d_6/D_2O/CD_3CO_2D (90:5:4.85:0.15 v/v)	263
	naphthalene	2.52	NMR			20	MeOD-d_3/D_2O/CD_3CO_2D (95:4.85:0.15 v/v)	263
	phenanthrene	3.12	NMR			20	MeOD-d_3/D_2O/CD_3CO_2D (95:4.85:0.15 v/v)	263
	pyrene	2.20	NMR			20	MeOD-d_3/D_2O/CD_3CO_2D (95:4.85:0.15 v/v)	263
Porphyrin-94 (XXXIV)	phenanthrene	4.60	UV			20	2,2,2-trifluoroethanol (high-spin complex)	263
Porphyrin-95 (XXXV)	4-ethylpyridine	2.73	NMR/UV			20	$CDCl_3$/$CHCl_3$	242
	imidazole	4.85	NMR/UV			20	$CDCl_3$/$CHCl_3$	242
	3,5-lutidine	4.67	NMR/UV			20	$CDCl_3$/$CHCl_3$	242
	purine	6.32	NMR/UV			20	$CDCl_3$/$CHCl_3$	242
	pyrazine N-oxide	4.04	NMR/UV			20	$CDCl_3$/$CHCl_3$	242
	pyridine	3.48	NMR/UV			20	$CDCl_3$/$CHCl_3$	242
	3-pyridinol	5.15	NMR/UV			20	$CDCl_3$/$CHCl_3$	242
	4-pyridinol	4.64	NMR/UV			20	$CDCl_3$/$CHCl_3$	242
	tropine	2.54	NMR/UV			20	$CDCl_3$/$CHCl_3$	242

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
			5. Miscellaneous (cont.)					
			c. Other					
Other-1 (XXXVI)	catechol	2.70	NMR			25	$CDCl_3$	264
	hydroquinone	2.74	NMR			25	$CDCl_3$	264
	resorcinol	3.51	NMR			25	$CDCl_3$	264
Other-2 (XXXVI)	catechol	<1.70	NMR			25	$CDCl_3$	264
	hydroquinone	<1.70	NMR			25	$CDCl_3$	264
	resorcinol	1.70	NMR			25	$CDCl_3$	264
Other-3 (XXXVI)	catechol	1.60	NMR			25	$CDCl_3$	264
	hydroquinone	3.73	NMR			25	$CDCl_3$	264
	resorcinol	3.30	NMR			25	$CDCl_3$	264
Other-4 (XXXVI)	2-bromohydroquinone	3.26	NMR			25	$CDCl_3$	264
	catechol	1.85	NMR	-22.0	-36	25	$CDCl_3$	264
	2-chlorohydroquinone	3.18	NMR			25	$CDCl_3$	264
	4,5-dibromocatechol	3.08	NMR			25	$CDCl_3$	264
	2,3-dibromohydroquinone	3.15	NMR			25	$CDCl_3$	264
	2,5-dibromohydroquinone	nm	NMR			25	$CDCl_3$	264
	2,3-dichlorohydroquinone	2.86	NMR			25	$CDCl_3$	264
	2,5-dichlorohydroquinone	nm	NMR			25	$CDCl_3$	264
	2,3-dicyanohydroquinone	3.62	NMR			25	$CDCl_3$/MeCN-d_3 (80:20 v/v)	264
	2,3-dicyanohydroquinone	5.36	NMR			25	$CDCl_3$ (calculated K)	264
	2,3-dicyanohydroquinone	5.48	Sol			25	$CDCl_3$	264
	hydroquinone	1.08	NMR			25	$CDCl_3$/MeCN-d_3 (80:20 v/v)	264
	hydroquinone	2.81	NMR			25	$CDCl_3$	264
	hydroquinone	3.08	Sol			25	$CDCl_3$	264
	resorcinol	3.46	NMR			25	$CDCl_3$	264
Other-5 (XXXVI)	1,3-dinitrobenzene	-0.52	UV			25?	$CHCl_3$/Me_2SO (75:25 v/v) without KSCN	265
	1,3-dinitrobenzene	-0.30	UV			25?	$CHCl_3$/Me_2SO (75:25 v/v) in presence of 4 equivalents of KSCN	265
	1,3-dinitrobenzene	0.08	UV			25?	$CHCl_3$/Me_2SO (90:10 v/v) without KSCN	265
	1,3-dinitrobenzene	0.86	UV			25?	$CHCl_3$/Me_2SO (90:10 v/v) in presence of 8 mM KSCN (L is converted into *anti-anti* conformer)	265
Other-6 (XXXVI)	4-aminopyridine	3.89	Polg			20	MeCN, 01 M Et_4NClO_4	266
	aniline	<1.87	Polg			20	MeCN, 01 M Et_4NClO_4	266
	benzamide	2.81	Polg			20	MeCN, 01 M Et_4NClO_4	266
	benzonitrile	2.16	Polg			20	MeCN, 01 M Et_4NClO_4	266
	benzylamine	3.43	Polg			20	MeCN, 01 M Et_4NClO_4	266
	4-*t*-butylpyridine	3.12	Polg			20	MeCN, 01 M Et_4NClO_4	266
	isoquinoline	2.70	Polg			20	MeCN, 01 M Et_4NClO_4	266
	2,6-lutidine	<1.87	Polg			20	MeCN, 01 M Et_4NClO_4	266
	methyl phenyl sulfoxide	2.75	Polg			20	MeCN, 01 M Et_4NClO_4	266
	N-phenylurea	<1.87	Polg			20	MeCN, 01 M Et_4NClO_4	266
	4-picoline	3.23	Polg			20	MeCN, 01 M Et_4NClO_4	266
	pyridine	2.73	Polg			20	MeCN, 01 M Et_4NClO_4	266
	pyridine *N*-Oxide	4.70	Polg			20	MeCN, 01 M Et_4NClO_4	266
Other-7 (XXXVI)	4-aminopyridine	>4.18	Polg			20	MeCN, 01 M Et_4NClO_4	266
	aniline	<1.87	Polg			20	MeCN, 01 M Et_4NClO_4	266
	benzamide	3.37	Polg			20	MeCN, 01 M Et_4NClO_4	266
	benzonitrile	2.63	Polg			20	MeCN, 01 M Et_4NClO_4	266
	benzylamine	3.55	Polg			20	MeCN, 01 M Et_4NClO_4	266
	4-*t*-butylpyridine	2.57	Polg			20	MeCN, 01 M Et_4NClO_4	266
	isoquinoline	2.69	Polg			20	MeCN, 01 M Et_4NClO_4	266

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	2,6-lutidine	2.13	Polg			20	MeCN, 01 M Et_4NClO_4	266
	methyl phenyl sulfoxide	2.51	Polg			20	MeCN, 01 M Et_4NClO_4	266
	N-phenylurea	2.55	Polg			20	MeCN, 01 M Et_4NClO_4	266
	4-picoline	2.99	Polg			20	MeCN, 01 M Et_4NClO_4	266
	pyridine	2.90	Polg			20	MeCN, 01 M Et_4NClO_4	266
	pyridine *N*-oxide	>4.70	Polg			20	MeCN, 01 M Et_4NClO_4	266
Other-8 (XXXVI)	4-aminopyridine	4.14	Polg			20	MeCN, 01 M Et_4NClO_4	266
	aniline	<1.87	Polg			20	MeCN, 01 M Et_4NClO_4	266
	benzamide	<1.87	Polg			20	MeCN, 01 M Et_4NClO_4	266
	benzonitrile	<1.87	Polg			20	MeCN, 01 M Et_4NClO_4	266
	benzylamine	3.48	Polg			20	MeCN, 01 M Et_4NClO_4	266
	4-*t*-butylpyridine	<1.87	Polg			20	MeCN, 01 M Et_4NClO_4	266
	isoquinoline	<1.87	Polg			20	MeCN, 01 M Et_4NClO_4	266
	2,6-lutidine	<1.87	Polg			20	MeCN, 01 M Et_4NClO_4	266
	methyl phenyl-sulfoxide	<1.87	Polg			20	MeCN, 01 M Et_4NClO_4	266
	4-picoline	2.80	Polg			20	MeCN, 01 M Et_4NClO_4	266
	N-phenylurea	<1.87	Polg			20	MeCN, 01 M Et_4NClO_4	266
	pyridine	<1.87	Polg			20	MeCN, 01 M Et_4NClO_4	266
	pyridine *N*-oxide	>4.70	Polg			20	MeCN, 01 M Et_4NClO_4	266
Other-9 (XXXVI)	urea	≤2	NMR			25	$CDCl_3$	267
	urea	≤2.70	Solv Extr			25?	$CHCl_3$	268
Other-10 (XXXVI)	urea	≥8	NMR			25	$CDCl_3$	267
	urea	≥5.78	Solv Extr			25?	$CHCl_3$	268
Other-11 (XXXVI)	urea	≥8.40	NMR			25	$CDCl_3$	267
	urea	≥6.60	Solv Extr			25?	$CHCl_3$	268
Other-12 (XXXVI)	urea	≥6	NMR			25	$CDCl_3$	267
	urea	≥4.30	Solv Extr			25?	$CHCl_3$	268
Other-13 (XXXVI)	1-butanol	0.90	NMR			~30	D_2O	269
Other-14 (XXXVI)	1-butanol	0.57	NMR			~30	D_2O	269
Other-15 (XXXVI)	benzyl alcohol	0.72	NMR			~30	D_2O	269
	1-butanol	0.62	NMR			~30	D_2O	269
	1-butanol	1.23	NMR			~30	D_2O (estimated K)	270
	2-methyl-2-propanol	-0.11	NMR			~30	D_2O	269
	1-propanol	0.89	NMR			~30	D_2O	269
Other-16 (XXXVI)	1-butanol	0.49	NMR			~30	D_2O	269
Other-17 (XXXVII)	4-aminopyridine	2.60	Spec	-33.6	-63	25	methyl benzoate [M + Co(II)L <-> MCo(II)L]	271
	4-cyanopyridine	0.307	Spec	-26.8	-84	25	methyl benzoate [M + Co(II)L <-> MCo(II)L]	271
	4-dimethylamino-pyridine	2.87	Spec	-36.9	-68	25	methyl benzoate [M + Co(II)L <-> MCo(II)L]	271
	2,6-lutidine	-0.044	Spec	-25.8	-88	25	methyl benzoate [M + Co(II)L <-> MCo(II)L]	271
	morpholine	2.08	Spec			25	methyl benzoate [M + Co(II)L <-> MCo(II)L]	271
	2-picoline	0.225	Spec	-24.4	-84	25	methyl benzoate [M + Co(II)L <-> MCo(II)L]	271
	3-picoline	1.26	Spec	-37.2	-78	25	methyl benzoate [M + Co(II)L <-> MCo(II)L]	271
	4-picoline	1.65	Spec	-37.0	-93	25	methyl benzoate [M + Co(II)L <-> MCo(II)L]	271
	piperidine	2.39	Spec			25	methyl benzoate [M + Co(II)L <-> MCo(II)L]	271
	pyridine	1.26	Spec	-45.2	-126	25	methyl benzoate [M + Co(II)L <-> MCo(II)L]	271
Other-18 (XXXVII)	4-aminopyridine	2.23	Spec			30	DCE [M + Co(II)L <-> MCo(II)L]	272
	4-cyanopyridine	0.78	Spec			30	DCE [M + Co(II)L <-> MCo(II)L]	272
	4-dimethylamino-pyridine	2.74	Spec			30	DCE [M + Co(II)L <-> MCo(II)L]	272
	2,6-lutidine	0.025	Spec			30	DCE [M + Co(II)L <-> MCo(II)L]	272
	2-picoline	0.43	Spec			30	DCE [M + Co(II)L <-> MCo(II)L]	272
	3-picoline	2.12	Spec			30	DCE [M + Co(II)L <-> MCo(II)L]	272
	4-picoline	1.86	Spec			30	DCE [M + Co(II)L <-> MCo(II)L]	272

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	pyridine	1.46	Spec			30	DCE [M + Co(II)L <-> MCo(II)L]	272
Other-19 (XXXVII)	4-aminopyridine	2.32	Spec			25	DCE [M + Co(III)LCN <-> MCo(III)LCN]	273
	4-cyanopyridine	0.42	Spec			25	DCE [M + Co(III)LCN <-> MCo(III)LCN]	273
	2,6-lutidine	-0.73	Spec			25	DCE [M + Co(III)LCN <-> MCo(III)LCN]	273
	2-picoline	-0.58	Spec			25	DCE [M + Co(III)LCN <-> MCo(III)LCN]	273
	4-picoline	1.83	Spec			25	DCE [M + Co(III)LCN <-> MCo(III)LCN]	273
	pyridine	1.41	Spec			25	DCE [M + Co(III)LCN <-> MCo(III)LCN]	273
Other-20 (XXXVII)	4-aminopyridine	2.35	Spec			30	DCE [M + Co(II)L <-> MCo(II)L]	272
	4-cyanopyridine	0.30	Spec			30	DCE [M + Co(II)L <-> MCo(II)L]	272
	4-dimethylamino-pyridine	2.77	Spec			30	DCE [M + Co(II)L <-> MCo(II)L]	272
	2,6-lutidine	0.22	Spec			30	DCE [M + Co(II)L <-> MCo(II)L]	272
	2-picoline	0.33	Spec			30	DCE [M + Co(II)L <-> MCo(II)L]	272
	3-picoline	1.83	Spec			30	DCE [M + Co(II)L <-> MCo(II)L]	272
	4-picoline	1.85	Spec			30	DCE [M + Co(II)L <-> MCo(II)L]	272
	pyridine	1.48	Spec			30	DCE [M + Co(II)L <-> MCo(II)L]	272
Other-21 (XXXVII)	4-aminopyridine	2.45	Spec			25	DCE [M + Co(III)LCN <-> MCo(III)LCN]	273
	4-cyanopyridine	0.45	Spec			25	DCE [M + Co(III)LCN <-> MCo(III)LCN]	273
	2,6-lutidine	-0.95	Spec			25	DCE [M + Co(III)LCN <-> MCo(III)LCN]	273
	2-picoline	-0.70	Spec			25	DCE [M + Co(III)LCN <-> MCo(III)LCN]	273
	4-picoline	1.90	Spec			25	DCE [M + Co(III)LCN <-> MCo(III)LCN]	273
	pyridine	1.43	Spec			25	DCE [M + Co(III)LCN <-> MCo(III)LCN]	273
Other-22 (XXXVII)	acenaphthene	3.20	Sol-EAS			27-29	H_2O	274, 275
	anthracene	4.36	Sol-EAS			27-29	H_2O	274, 275
	azulene	4.18	Calc'd			20-22	H_2O, (K calculated from transport rates)	275
	biphenyl	2.90	Sol-EAS			27-29	H_2O	276
	chrysene	4.85	Sol-EAS			27-29	H_2O	274, 275
	durene	3.20	Calc'd			20-22	H_2O, (K calculated from transport rates)	275
	durene	2.08	Sol-EAS			27-29	H_2O	274, 275
	fluoranthene	6.28	Calc'd			20-22	H_2O, (K calculated from transport rates)	275
	fluorene	3.56	Sol-EAS			27-29	H_2O	274, 275
	naphthalene	4.20	Calc'd			20-22	H_2O, (K calculated from transport rates)	275
	naphthalene	2.65	Sol-EAS			27-29	H_2O	274, 275
	phenanthrene	4.15	Sol-EAS			27-29	H_2O	274, 275
	pyrene	6.32	Calc'd			20-22	H_2O, (K calculated from transport rates)	275
	pyrene	4.63	Sol-EAS			27-29	H_2O	274, 275
Other-23 (XXXVII)	phenol blue	4.00	Spec			?	H_2O, pH 9.5	277
Amphotericin B	cholesterol	6.88	Spec			30	MeCN/H_2O (5:95)	278
	cholesterol	6.23	Spec			30	MeCN/H_2O (25:75)	278
	cholesterol	4.72	Spec			30	PC/cholesterol (3:1) vesicles	278
	ergosterol	6.18	Spec			30	MeCN/H_2O (5:95)	278
	ergosterol	6.00	Spec			30	MeCN/H_2O (25:75)	278

Table I (Continued)

ligand (chart)	neutral molecule[a]	log K[b]	method[c]	ΔH kJ/mol	ΔS J/K·mol	T, °C	conditions[d]	ref
	ergosterol	5.84	Spec			30	PC/ergosterol (3:1) vesicles	278
	desmosterol	4.11	Spec			30	PC/desmosterol (3:1) vesicles	278
	lanosterol	3.73	Spec			30	PC/lanosterol (3:1) vesicles	278
	stigmasterol	4.38	Spec			30	PC/stigmasterol (3:1) vesicles	278
	β-sitosterol	4.66	Spec			30	PC/β-sitosterol (3:1) vesicles	278
Amphotericin B Borate	cholesterol	4.60	Spec			30	PC/cholesterol (3:1) vesicles	278
	desmosterol	4.28	Spec			30	PC/desmosterol (3:1) vesicles	278
	ergosterol	4.54	Spec			30	PC/ergosterol (3:1) vesicles	278
	stigmasterol	4.18	Spec			30	PC/stigmasterol (3:1) vesicles	278
	β-sitosterol	4.36	Spec			30	PC/β-sitosterol (3:1) vesicles	278
Amphotericin B Methyl Ester	cholesterol	5.81	Spec			30	PC/cholesterol (3:1) vesicles	278
	desmosterol	5.48	Spec			30	PC/desmosterol (3:1) vesicles	278
	ergosterol	5.99	Spec			30	PC/ergosterol (3:1) vesicles	278
	lanosterol	5.46	Spec			30	PC/lanosterol (3:1) vesicles	278
	stigmasterol	5.57	Spec			30	PC/stigmasterol (3:1) vesicles	278
	β-sitosterol	5.64	Spec			30	PC/β-sitosterol (3:1) vesicles	278

[a] Neutral Molecules: The names of neutral molecules are in alphabetical order except for H_2O, HBr, KCl, Cl_2, Br_2,I_2, ICl, and Xe which are listed in this order. Ac = acetyl, Ala = alanine, Bn = benzyl, Boc = butoxycarbonyl, *t*-Bu = *tert*-butyl, Et = ethyl, Leu = leucine, Me = methyl, Ph = phenyl, Ser = Serine, Thr = Threonine, Val = valine. [b] Reactions: The log K values are for 1:1 interactions unless consecutive reactions occur. Interactions of the1:1 type are either of neutral molecule (M)-ligand (L) type (ML, no further designation) or of less common neutral molecule-protonated-ligand type (indicated by MHL, etc., placed in parentheses following the log K value). Two kinds of consecutive reactions have been reported. The more numerous is that in which a neutral molecule interacts consecutively with the macrocycle to form M_2L species. Where this occurs, the second reaction is indicated by placing the reaction product (M_2L, etc.,) in parentheses after the log K value. The second,represented here by only one case (Porphyrin-68), is that in which the macrocycle interacts consecutively with neutral molecule. This interaction is indicated by (1) and (2) placed after the log K value. When no complexation between neutral molecule and macrocycle occurs, this fact is denoted by "none"; "nm" means the measured values were too small to determine log K; "ppt" or "decomp" means the value of log K was not determined because of precipitation or decomposition, respectively. [c] Methods: Cal = calorimetry, Calc'd = calculated value, CD = induced circular dichroism, EAS = electronic absorption spectra, Fluor = fluorescent spectroscopy, IR = infrared spectroscopy, Kin = kinetic (calculated from kinetic data), NMR = nuclear magnetic resonance spectroscopy, PhotoTit = phototitration, Polg = polarography, Pot= potentiometry, Sol = solid-liquid extraction, Solv Extr = liquid-liquid extraction, Spec = spectrophotometry,Tit-EAS = electronic absorption titration, UV = ultraviolet spectroscopy, Volt = voltammetry. [d] Conditions: M = neutral molecule, L = ligand, borate-*d* = deuterated borate buffer, Bu = *n*-butyl, *t*-BuOH = *tert*-butyl alcohol, CAPS = 3-cyclohexylamino-1-propanesulfonate, DCE = 1,2-dichloroethane, DMAC = *N*,*N*-dimethylacetamide, DMF = *N*,*N*-dimethylformamide, DMF-d_7 = deuterated *N*,*N*-dimethylformamide, Diox = 1,4-dioxane, Et= ethyl, EtOH = ethanol, EtOD-d_5 = deuterated ethanol, Form = formaldehyde, HEPES = 4-(2-hydroxyethyl)-1-piperazineethanesulfonate, Me = methyl, MeCN = acetonitrile, MeCN-d_3 = deuterated acetonitrile, Me_2CO = acetone,Me_2CO-d_6 = deuterated acetone, $MeNO_2$ = nitromethane, MeOH = methanol, MeOD-d_3 = deuterated methanol, MES = 2-(*N*-morpholino)ethanesulfonate, Me_2SO = dimethyl sulfoxide, MeSO-d_6 = deuterated dimethyl sulfoxide, 2-Me-THF = 2-methyltetrahydrofuran, 2,2-Me_2-THF = 2,2-dimethyltetrahydrofuran, 2,2,5,5-Me_4-THF = 2,2,5,5-tetramethyltetrahydrofuran, NMF = *N*-methylformamide, PC = propylene carbonate, *i*-PrOH = *iso*-propyl alcohol, THF-D_8= deuterated tetrahydrofuran, toluene-d_8 = deuterated toluene, TRIS = tris(hydroxymethyl)aminomethane. [e] For structure see Chart XXXVIII-XXXIX. [f] For structure see Chart XXV.

Table II. ΔC_p Values for Neutral Molecule–Macrocycle Interaction in Solution

ligand (chart)	neutral molecule	ΔC_p,[a] J/mol·K	method[b]	T, °C	conditions[c]	ref
(1,4-B)$_4$30C4-3 (VII)	*p*-cresol	-460	Cal	20	H_2O	79
	1,4-dicyanobenzene	~0	NMR	2.8-42.8	D_2O	66
	1,4-dicyanobenzene	-126	Cal	20	H_2O	79
	1,4-dimethoxybenzene	-84	Cal	20	H_2O	79
	dimethyl 1,4-benzene-dicarboxylate	-251	Cal	20	H_2O	79
	1,4-dinitrobenzene	-167	Cal	20	H_2O	79
	hydroquinone	-251	Cal	20	H_2O	79
	4-nitrophenol	-209	Cal	20	H_2O	79
	4-nitrotoluene	-544	Cal	20	H_2O	79
	p-tolunitrile	-293	Cal	20	H_2O	79
	p-xylene	-84	Cal	20	H_2O	79
(1,4-B)$_2$32C4-2 (VIII)	isoquinoline	-105	NMR	21-61	D_2O, pD ~9 (borate-*d*)	89
	lepidine	-544	NMR	21-61	D_2O, pD ~9 (borate-*d*)	89
	1-methylindole	-502	NMR	21-61	D_2O, pD ~9 (borate-*d*)	89
	quinoline	-50	NMR	21-61	D_2O, pD ~9 (borate-*d*)	89
(1,4-Cy)$_2$32C4-1 (VIII)	isoquinoline	-255	NMR	21-61	D_2O, pD ~9 (borate-*d*)	89
	lepidine	-795	NMR	21-61	D_2O, pD ~9 (borate-*d*)	89
	1-methylindole	-502	NMR	21-61	D_2O, pD ~9 (borate-*d*)	89
	quinoline	-163	NMR	21-61	D_2O, pD ~9 (borate-*d*)	89
Cyclophane-3 (XVI)	pyrene	-502	Cal	15-35	MeOH	79

[a] Reactions: C_p values are for 1:1 interactions. [b] Methods: NMR = nuclear magnetic resonance spectroscopy, Cal = calorimetry. [c] Conditions: MeOH = methanol, borate-*d* = deuterated borate buffer.

Table III. Kinetic Parameters for Neutral Molecule–Macrocycle Interaction in Solution

ligand (chart)	neutral molecule	k_f, M^{-1} s^{-1}	k_d, s^{-1}	$\Delta H^{\ddagger}$,[a] kJ/mol	$\Delta S^{\ddagger}$,[a] J/K·mol	method[b]	T, °C	conditions[c]	ref
$N_4$14C4-2 (I)	ammonia	141	1.59			Spec	25	H_2O, I = 0.2 ($NaClO_4$) [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	aniline	10.7	1.98			Spec	25	H_2O, I = 0.2 ($NaClO_4$) [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	dimethylamine	846	1.73			Spec	25	H_2O, I = 0.2 ($NaClO_4$) [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	ethylamine	687	1.64			Spec	25	H_2O, I = 0.2 ($NaClO_4$) [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	methylamine	648	1.62			Spec	25	H_2O, I = 0.2 ($NaClO_4$) [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	piperidine	2325	2.86			Spec	25	H_2O, I = 0.2 ($NaClO_4$) [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	pyridine	1.55	2.08			Spec	25	H_2O, I = 0.2 ($NaClO_4$) [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
	trimethylamine	98.0	1.51			Spec	25	H_2O, I = 0.2 ($NaClO_4$) [M + $CuL(H_2O)^{2+}$blue <-> $MCuL^{2+}$ + H_2O]	23
15C5-1 (I)	KI	0.09×10^{-2}		60.7		Spec	25	$CHCl_3$, [L] = 0.60×10^{-2} M	300
	KI	0.11×10^{-2}				Spec	25	$CHCl_3$, [L] = 0.92×10^{-2} M	300
	KI	0.50×10^{-2}				Spec	16	$CHCl_3$, [L] = 1.82×10^{-2} M	300
	KI	7.05×10^{-2}				Spec	40	$CHCl_3$, [L] = 1.82×10^{-2} M	300
	KI	1.01×10^{-2}				Spec	25	$CHCl_3$, [L] = 10.83×10^{-2} M	300
	KI	1.10×10^{-2}				Spec	25	$CHCl_3$, [L] = 12.40×10^{-2} M	300
	KI	2.04×10^{-2}				Spec	32	$CHCl_3$, [L] = 12.40×10^{-2} M	300
	KI	1.27×10^{-2}				Spec	25	$CHCl_3$, [L] = 14.53×10^{-2} M	300
	I_2	1.42×10^{-3}				Spec	16	$CHCl_3$, [L] = 0.83×10^{-2} M	301
	I_2	0.88×10^{-3}				Spec	25	$CHCl_3$, [L] = 0.83×10^{-2} M	301
	I_2	0.64×10^{-3}				Spec	32	$CHCl_3$, [L] = 0.83×10^{-2} M	301
	I_2	1.25×10^{-3}				Spec	25	$CHCl_3$, [L] = 1.90×10^{-2} M	301
	I_2	1.59×10^{-3}				Spec	25	$CHCl_3$, [L] = 5.02×10^{-2} M	301
	I_2	4.73×10^{-3}				Spec	16	$CHCl_3$, [L] = 7.14×10^{-2} M	301
	I_2	3.17×10^{-3}				Spec	25	$CHCl_3$, [L] = 7.14×10^{-2} M	301
	I_2	1.22×10^{-3}				Spec	40	$CHCl_3$, [L] = 7.14×10^{-2} M	301
18C6-1 (II)	I_2	1.04×10^{-3}				Spec	25	$CHCl_3$, [L] = 0.83×10^{-2} M	301
	I_2	3.57×10^{-3}				Spec	25	$CHCl_3$, [L] = 7.14×10^{-2} M	301
	I_2	2.53×10^{-3}				Spec	32	$CHCl_3$, [L] = 7.14×10^{-2} M	301
	I_2	1.56×10^{-3}				Spec	40	$CHCl_3$, [L] = 7.14×10^{-2} M	301
$B_2$18C6-1 (II)	I_2	0.57×10^{-3}				Spec	16	$CHCl_3$, [L] = 0.83×10^{-2} M	301
	I_2	0.38×10^{-3}				Spec	25	$CHCl_3$, [L] = 0.83×10^{-2} M	301
	I_2	0.16×10^{-3}				Spec	40	$CHCl_3$, [L] = 0.83×10^{-2} M	301
[2.2.2]-1 (V)	H_2O	$\leq10^3$	$\leq10^8$			TJ	25	H_2O, I = 0.1 (Me_4NCl) (L + H_2O <-> HL)	302

Table III (Continued)

ligand (chart)	neutral molecule	k_f, M^{-1} s^{-1}	k_d, s^{-1}	$\Delta H^{\ddagger}$,[a] kJ/mol	$\Delta S^{\ddagger}$,[a] J/K·mol	method[b]	T, °C	conditions[c]	ref
(1,4-B)$_4$32C4-2 (VIII)	pyrene	~9×10^8	495			NMR	20	D_2O	303
Cryptophane-9 (XXIV)	ethanol		$t_{1/2}$=40min			NMR	22	$CDCl_3$	213
Cavitand-9 (XXV)	Cavitand-9[d]	1.4×10^5	106			NMR	12	$CDCl_3$	217
Carcerand-1 (XXVI)	Xe		2.5×10^{-4} min^{-1}			NMR	22	CD_2Cl_2 or $CDCl_3$ ($t_{1/2}$ = 47 h)	219
	acetonitrile		$t_{1/2}$=~13h			NMR	22	CD_2Cl_2	219
	carbon disulfide		$t_{1/2}$=>400h			NMR	22	CD_2Cl_2	219
	dibromo-methane		$t_{1/2}$=>400h			NMR	22	CD_2Cl_2	219
	N,N-dimethyl-acetamide		3.4×10^{-4} min^{-1}			NMR	140	1,2,4-$Cl_3C_6H_3$ ($t_{1/2}$ = 34 h)	219
	N,N-dimethyl-formamide		8.5×10^{-4} min^{-1}			NMR	140	1,2,4-$Cl_3C_6H_3$ ($t_{1/2}$ = 14 h)	219
	dimethyl sulfoxide		nm			NMR	140	1,2,4-$Cl_3C_6H_3$ (immeasurably slow)	219
	dimethyl sulfoxide		4.8×10^{-4} min^{-1}			NMR	195	1,2,4-$Cl_3C_6H_3$ ($t_{1/2}$ = 24 h)	219
Carcerand-2 (XXVII)	acetonitrile		0.02min^{-1}			NMR	80	$(CDCl_2)_2$ (M_2L -> M + ML)	304
	acetonitrile		0.05min^{-1}			NMR	90	$(CDCl_2)_2$ (M_2L -> M + ML)	304?
	acetonitrile		0.13min^{-1}			NMR	100	$(CDCl_2)_2$ (M_2L -> M + ML)	304
	acetonitrile		1.8 min^{-1}			NMR	110	$(CDCl_2)_2$ (M_2L -> M + ML)	304
Carcerand-3 (XXVII)	ferrocene		$t_{1/2}$=19.6h			NMR	25	$CDCl_3$	305
	hexachloro-butadiene		$t_{1/2}$=3.2h			NMR	25	$CDCl_3$	305
Porphyrin-13 (XXVIII)	imidazole	3.2×10^9		31.4	41.4	TJ	25	1-chlorobutane	237
	2-picoline	6.9×10^8	2.5×10^4			TJ	-32.2	1-chlorobutane	237
	2-picoline	1.6×10^9		7.5	43.9	TJ	25	1-chlorobutane	237
	pyridine	8.3×10^8	5.1×10^4	43.9(d)		TJ	9.8	chlorobenzene	237
	pyridine	1×10^9		9.83	-41.0	TJ	25	chlorobenzene	237
	pyridine	3.5×10^9		16.3	-8.8	TJ	25	1-chlorobutane	237
	pyridine	3.2×10^9		28.0	34.3	TJ	25	toluene	237
Porphyrin-7 (XXXII)	triethylene-diamine	5×10^4				Spec	27	$(CHCl_2)_2$ (bimolecular binding mechanism)	256
Porphyrin-80 (XXXII)	triethylene-diamine	1×10^5				Spec	27	$(CHCl_2)_2$ (bimolecular binding mechanism)	256
Porphyrin-81 (XXXII)	triethylene-diamine			94(d)	77(d)	NMR	27	$(CDCl_2)_2$ (unimolecular exchange mechanism)	256

[a] Generally, the $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$ values are calculated from k_f data. In those cases where these values are based on k_d values, a d is placed in parentheses following the value. [b] Methods: NMR = nuclear magnetic resonance spectroscopy, Spec = spectrophotometry, TJ = temperature jump. [c] Conditions: M = neutral molecule, L = ligand, Me = methyl, $t_{1/2}$ = half-life. [d] For structure see Chart XXV.

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